# 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

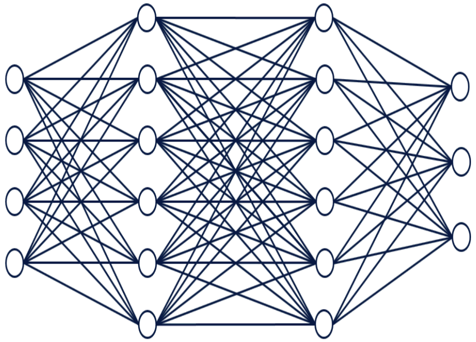
Peter Frazier

Ziv Scully

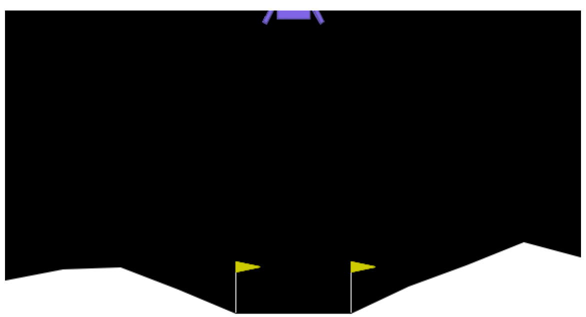
Alexander Terenin

# World of Parameter Optimization

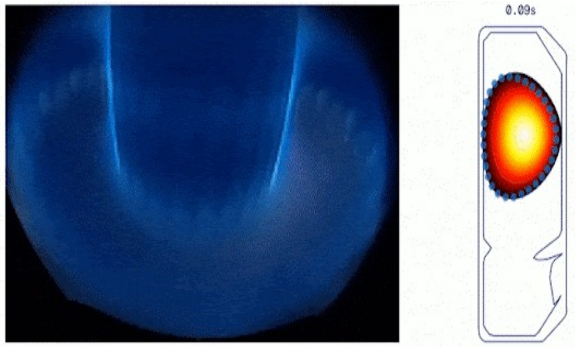
Hyperparameter tuning:

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:

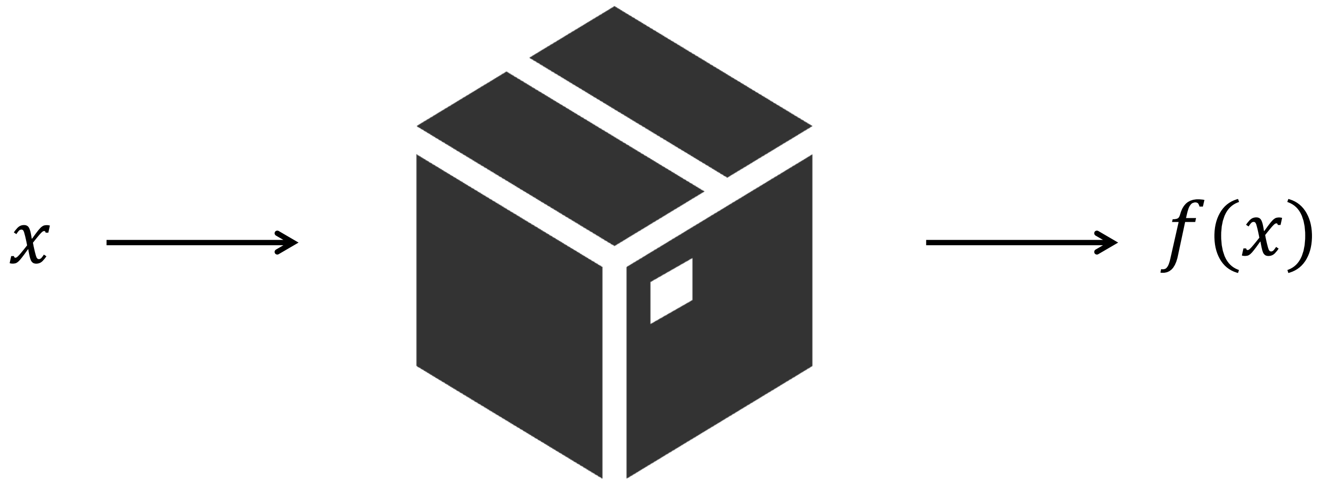
$x$  $f(x)$

# Optimizing Black-box Functions

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

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

# Optimizing Black-box Functions




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

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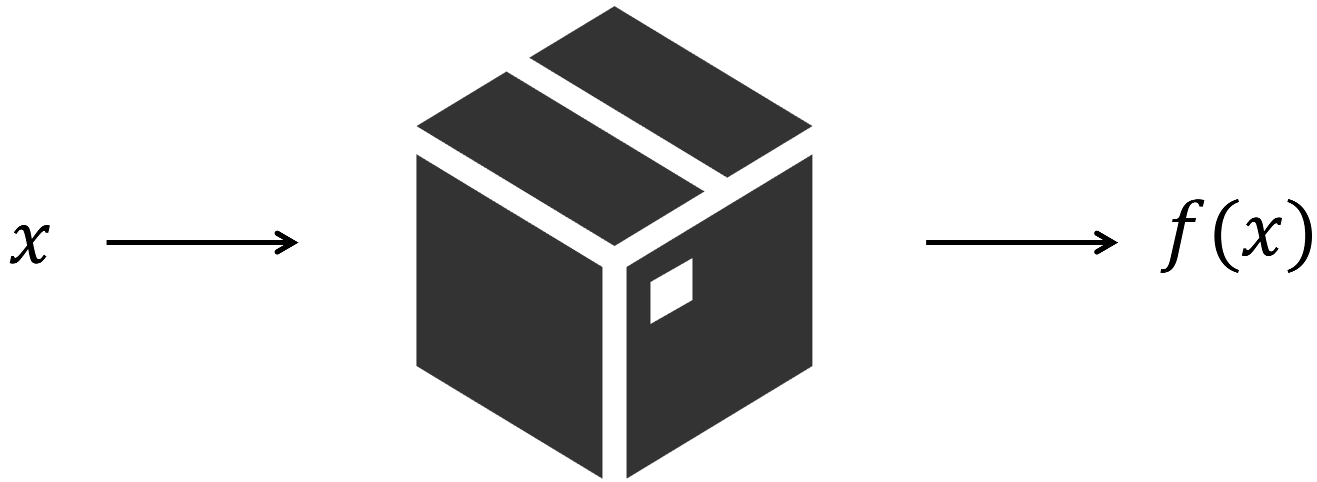
# Optimizing Black-box Functions




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

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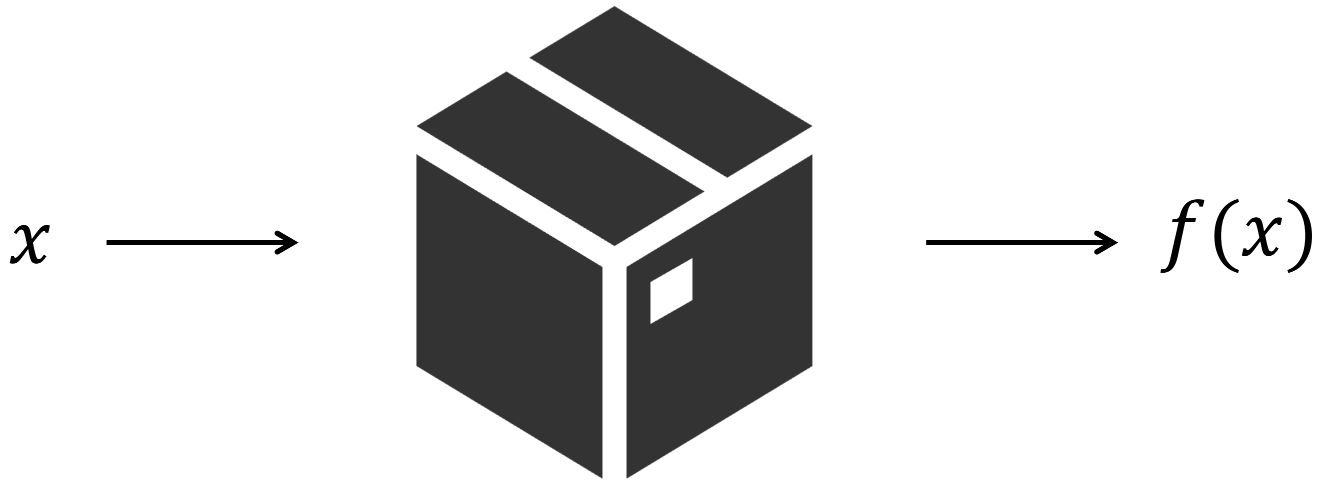


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# Bayesian Optimization

$x \longrightarrow$

$\longrightarrow f(x)$

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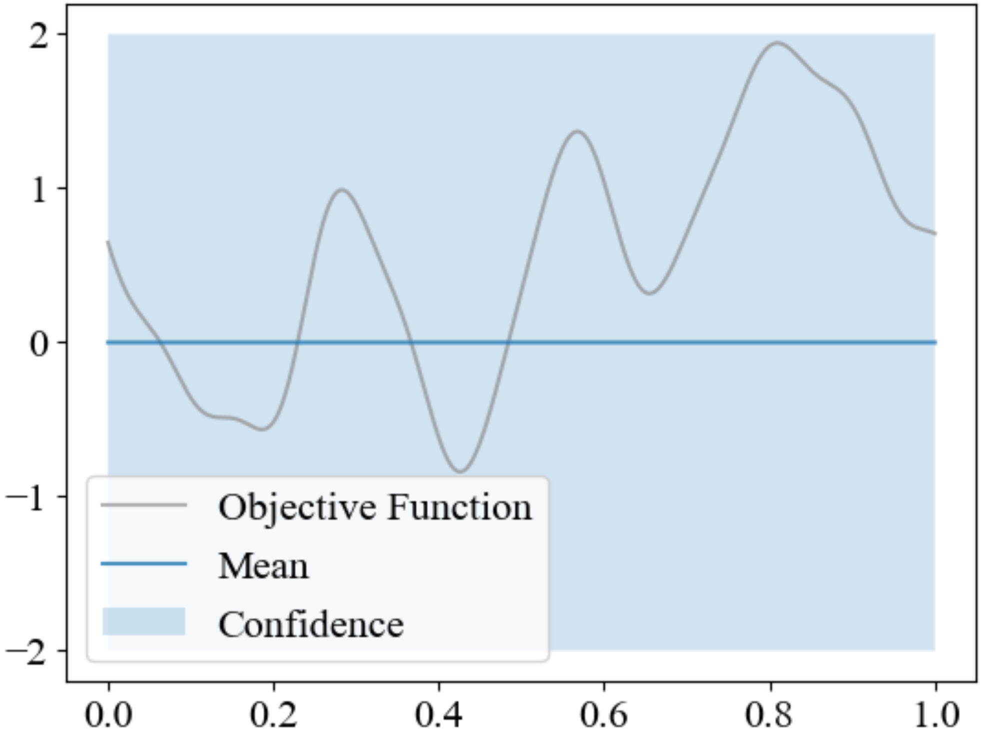
# Bayesian Optimization

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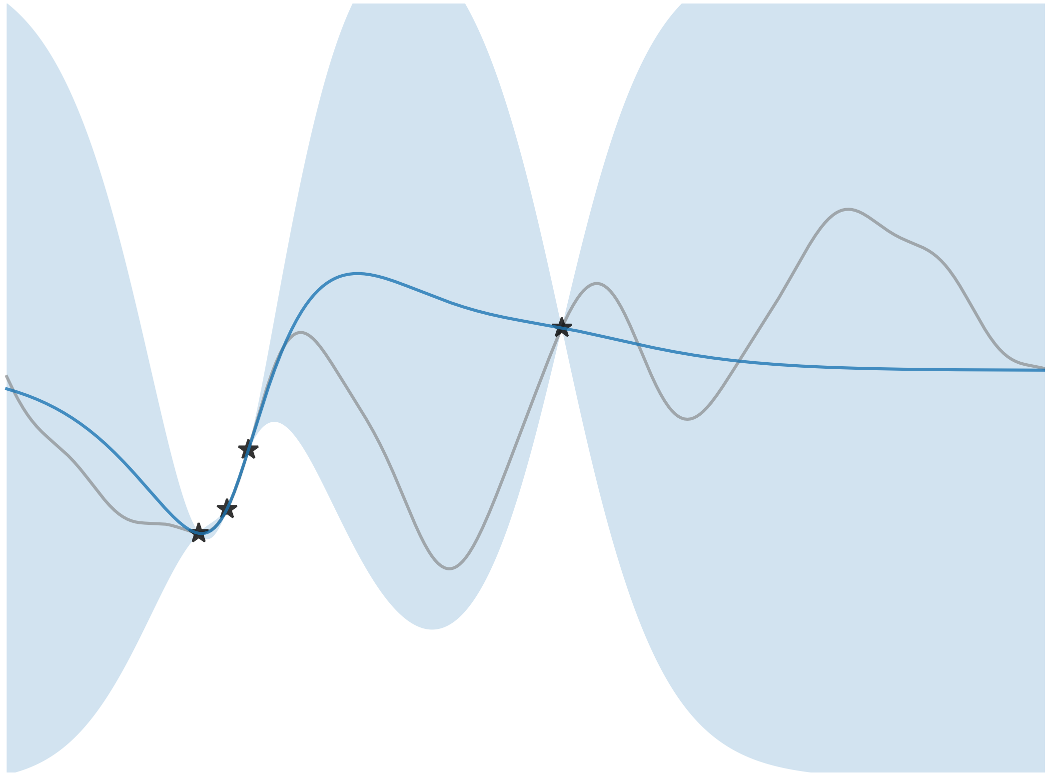
$f$ ~Gaussian Process

# Bayesian Optimization



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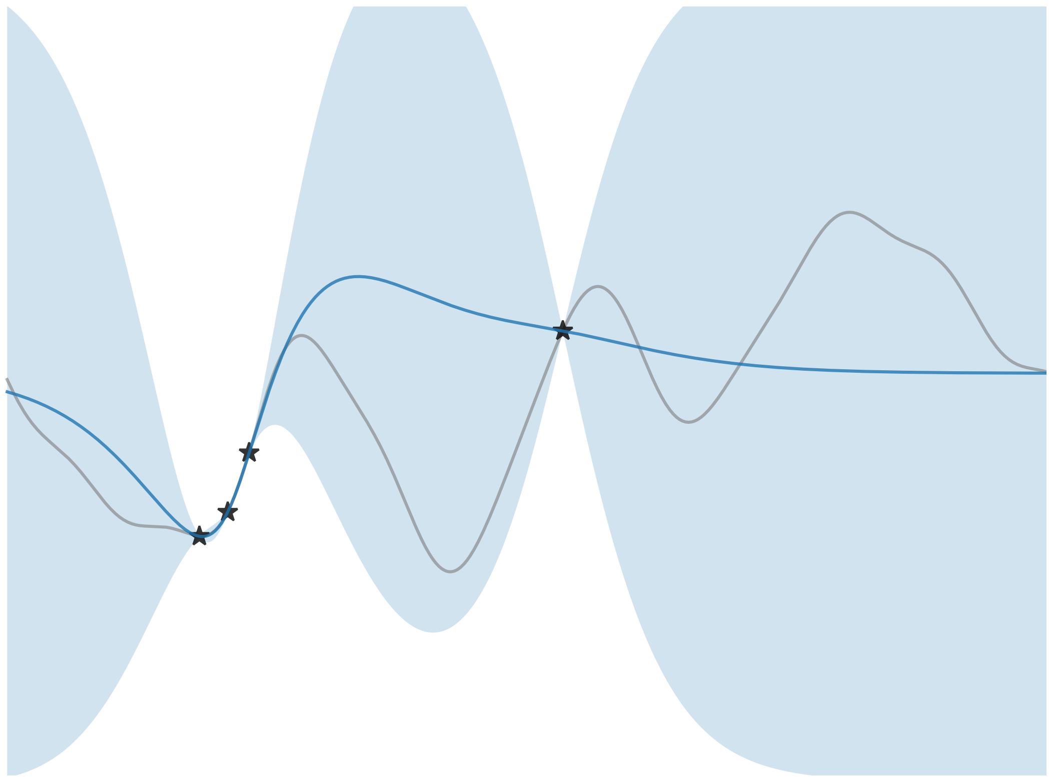
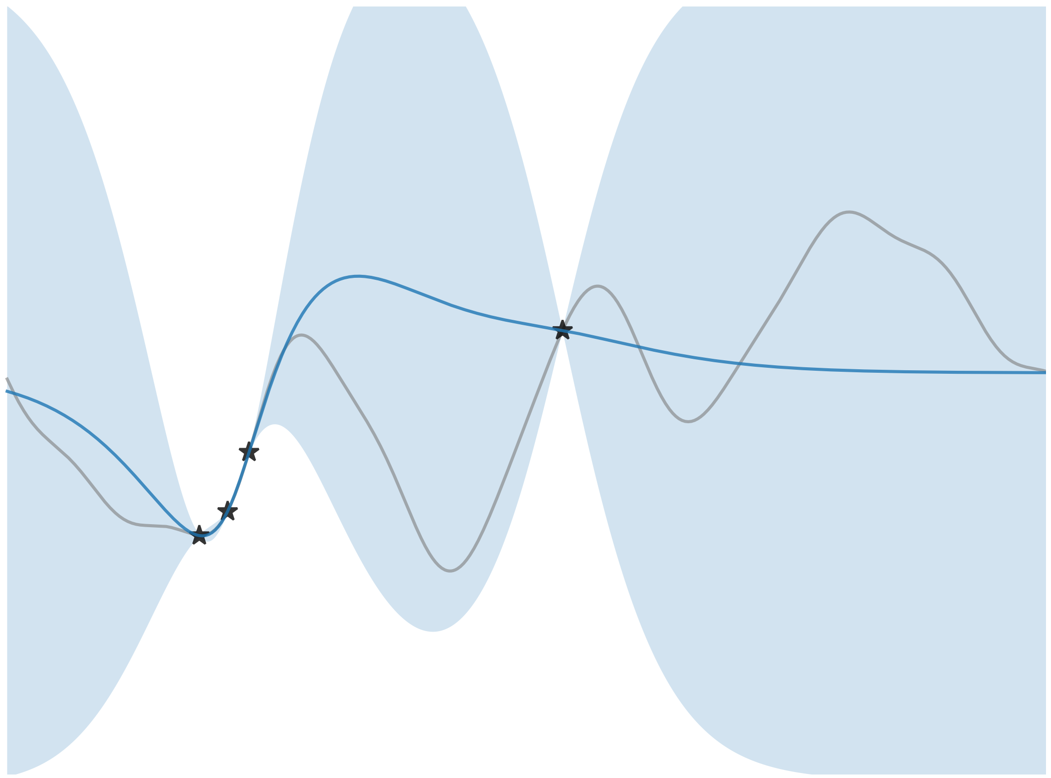


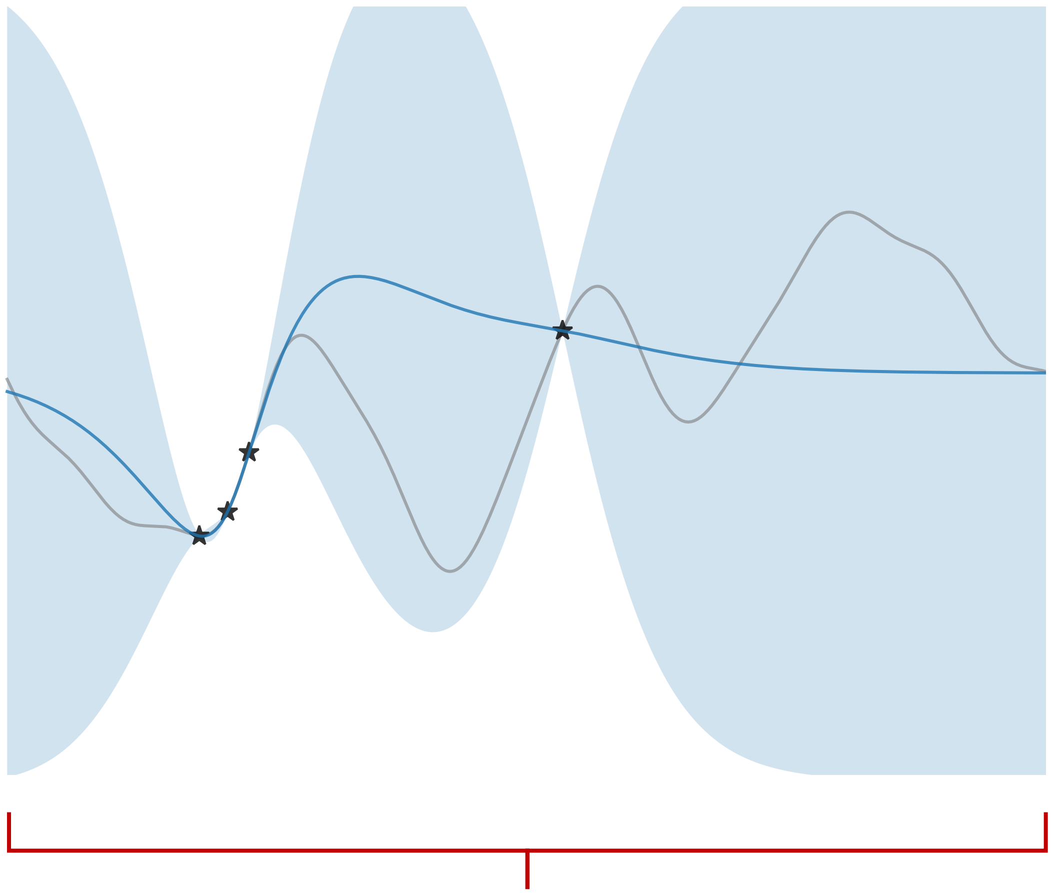
What to evaluate next?

# Bayesian Optimization



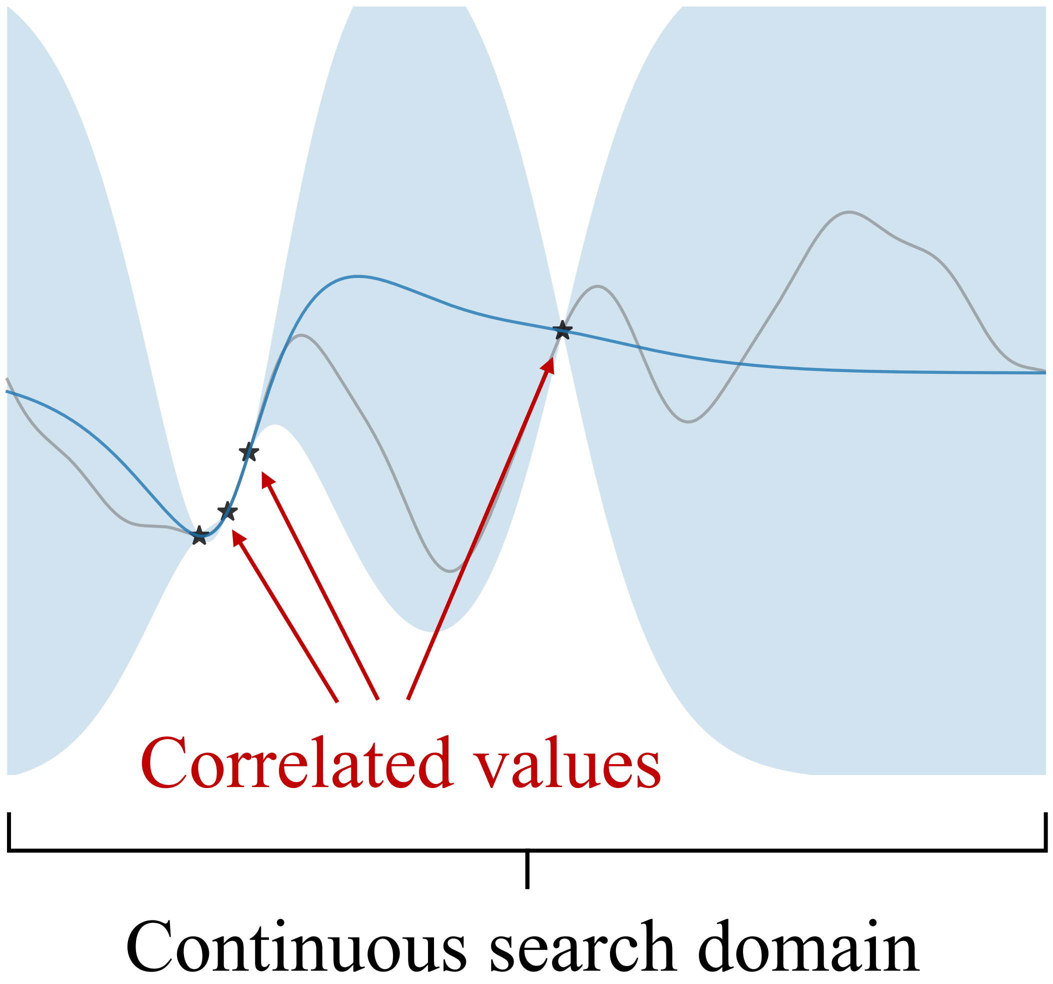
Optimal policy?

# Challenges of Bayesian Optimization

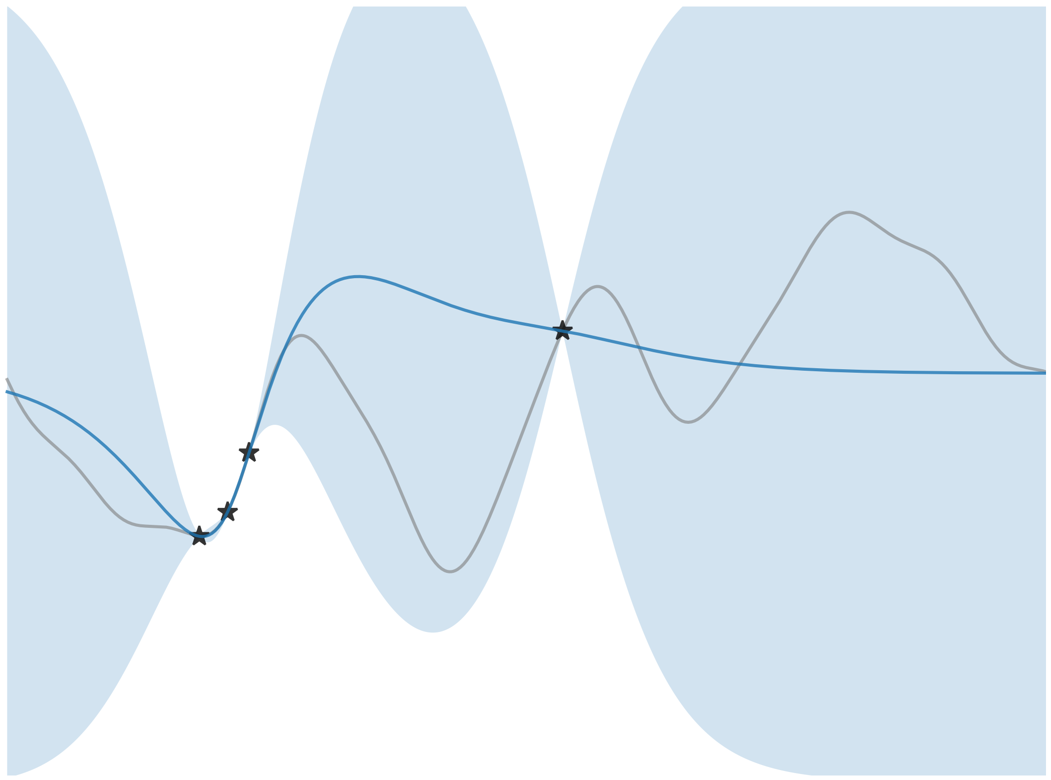


Continuous search domain

# Challenges of Bayesian Optimization

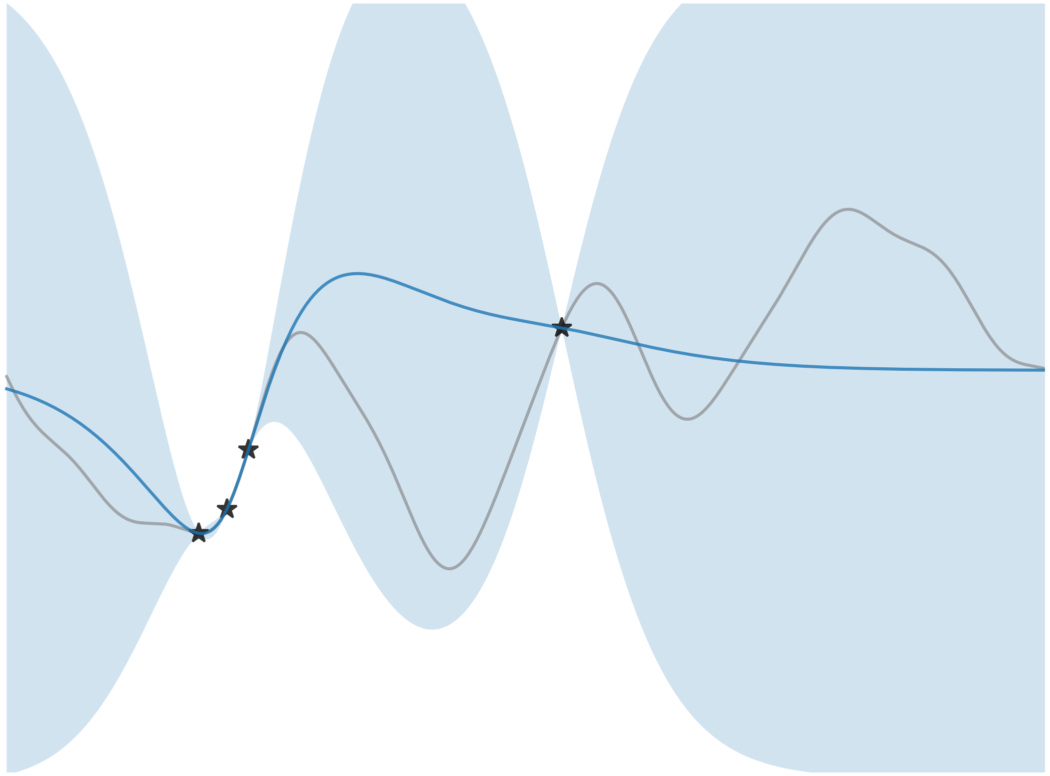


# Challenges of Bayesian Optimization



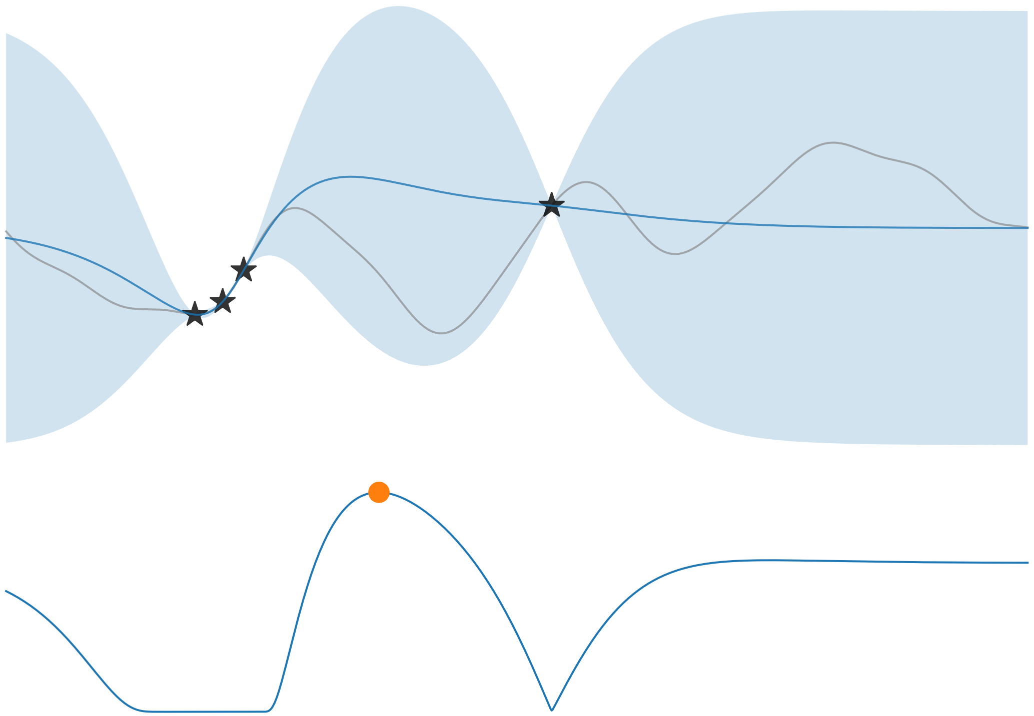
Correlation & continuity $\Longrightarrow$ Intractable MDP

# Challenges of Bayesian Optimization



Intractable MDP $\Longrightarrow$ Optimal policy unknown

# Popular Policy: Expected Improvement

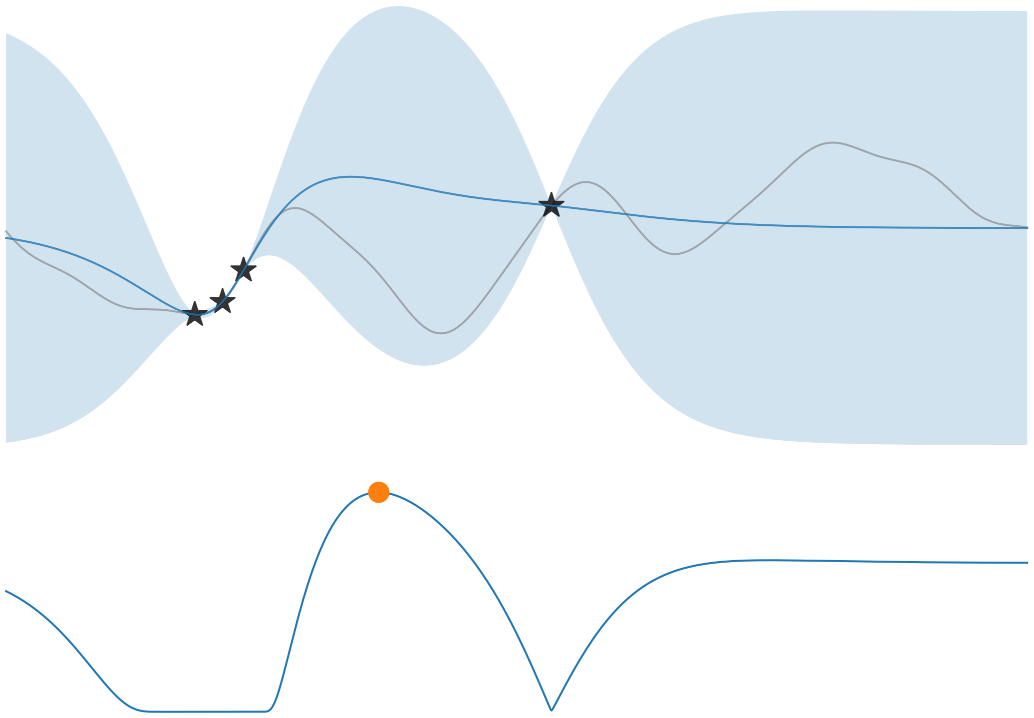


current best observed

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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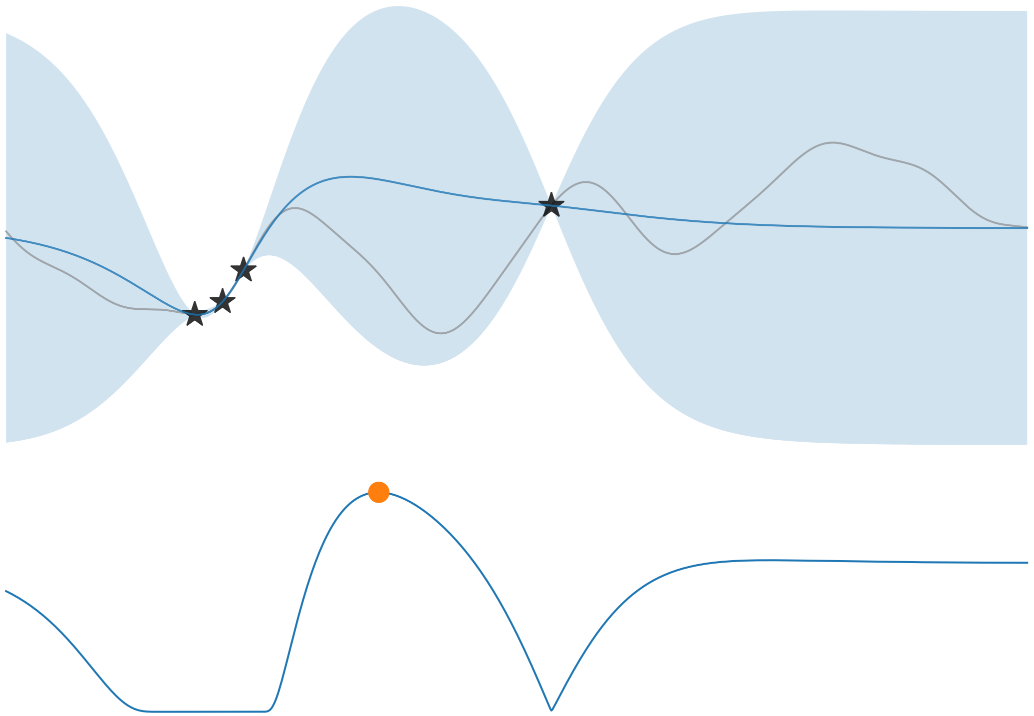

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One-step approximation to MDP

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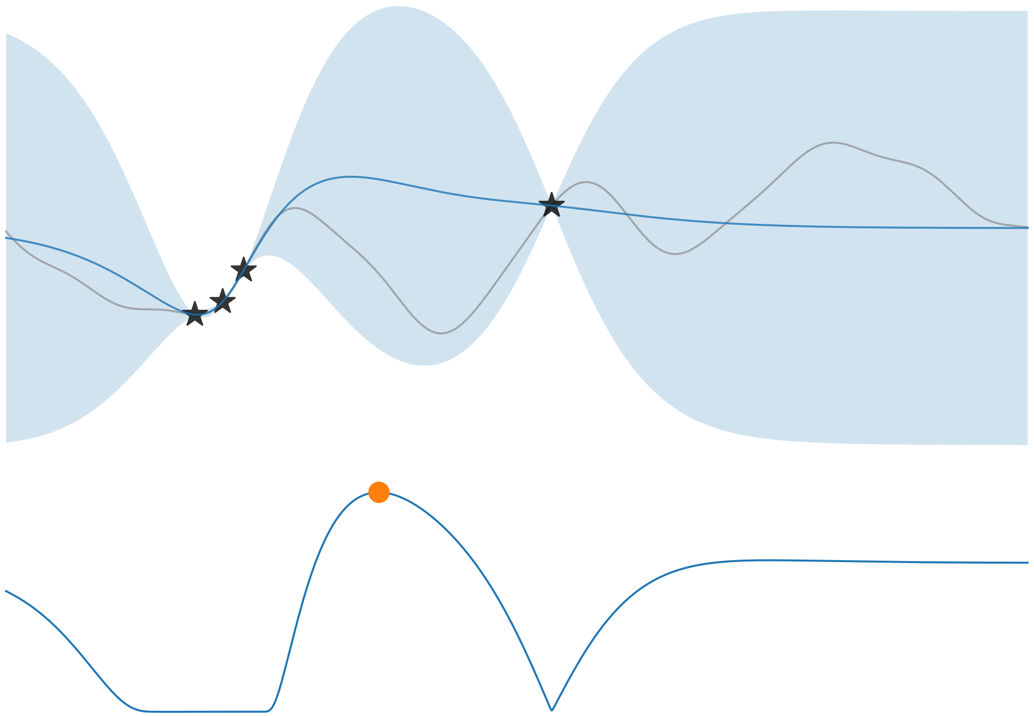

Other improvement-based policy:

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

# Approaches to Bayesian Optimization

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

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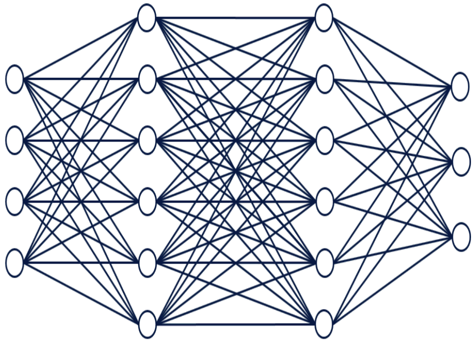
Why another approach?

# Challenge: Varying Evaluation Costs

Hyperparameter tuning:

Training parameters →  → Accuracy

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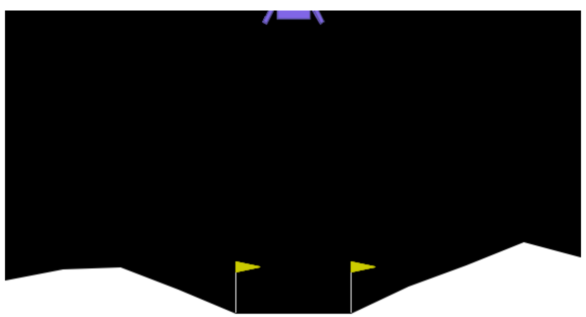
Control parameters →  → Reward

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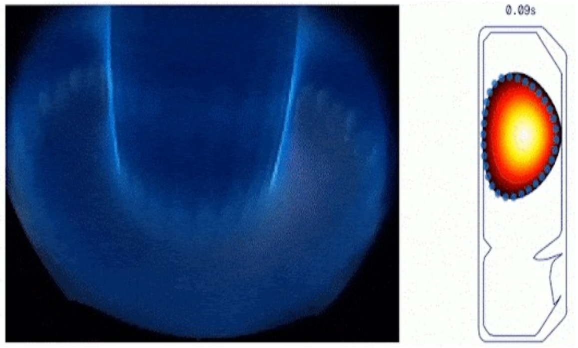
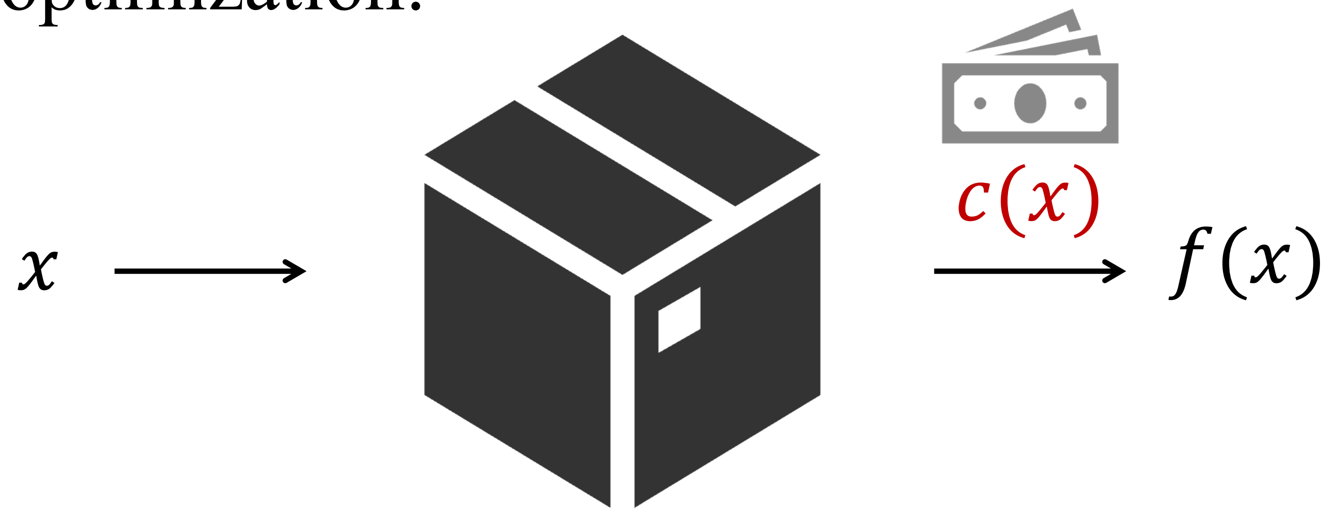
Reactor parameters → 

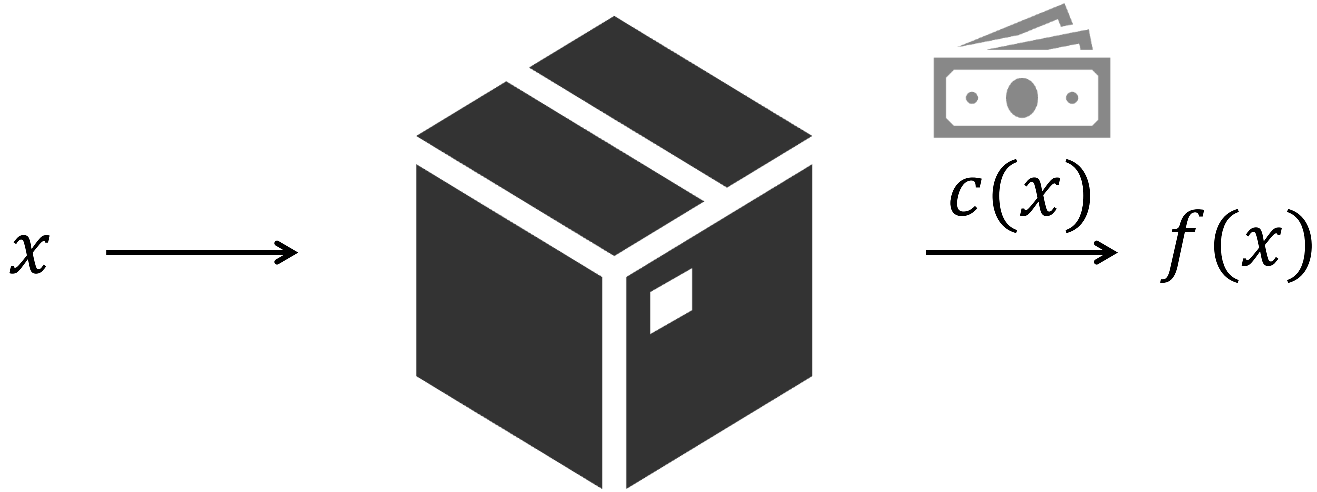
→ Stability

# Challenge: Varying Evaluation Costs

Black-box optimization:



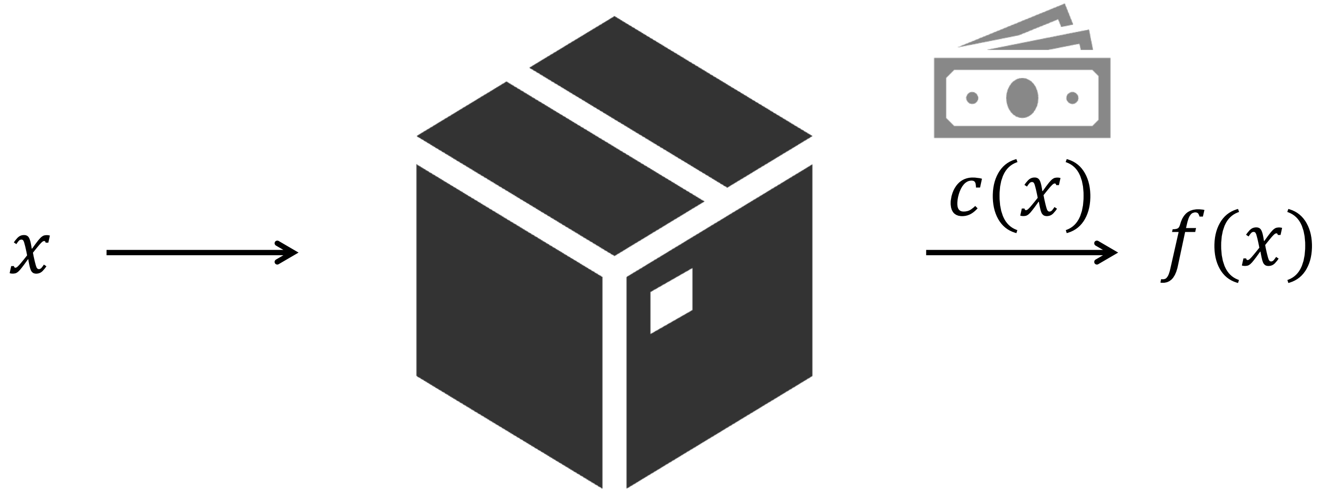
# Challenge: Varying Evaluation Costs




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

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

# Cost-aware Bayesian Optimization

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[Lee, Perrone, Archambeau, Seeger’21]

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

# Cost-aware Bayesian Optimization

Uniform costs

Expected improvement

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

Varying costs

# Cost-aware Bayesian Optimization

## Uniform costs

Expected improvement

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

## Varying costs

Expected improvement per cost

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

# Cost-aware Bayesian Optimization

## Uniform costs

Expected improvement

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

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Why divide?

# Cost-aware Bayesian Optimization

Uniform costs

Expected improvement

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

Varying costs

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Why divide?

Our view: lack of a guidance to incorporate costs

# Cost-aware Bayesian Optimization

**Uniform costs**

Expected improvement

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

**Varying costs**

Expected improvement per cost

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

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 | Varying costs |
|---|---|
| Expected improvement | Expected improvement per cost |
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| Upper Confidence Bound | ? |
| Thompson Sampling | ? |

# Cost-aware Bayesian Optimization

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| ⋮ | ⋮ |

New design principle: Gittins Index

# Cost-aware Bayesian Optimization

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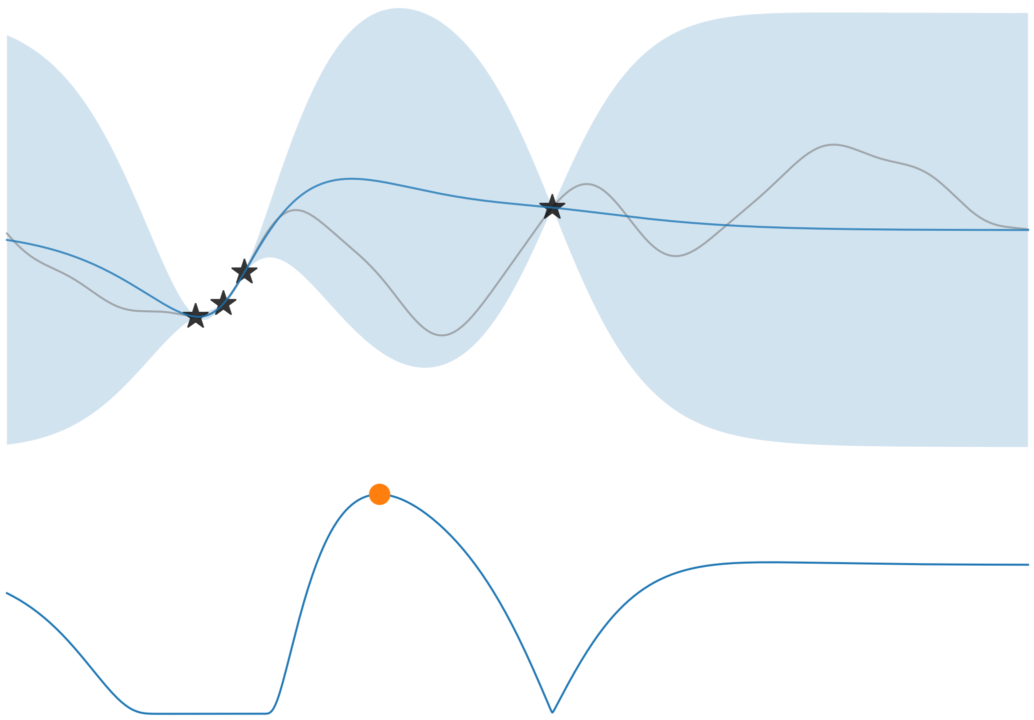
New design principle: Gittins Index

Cost-aware

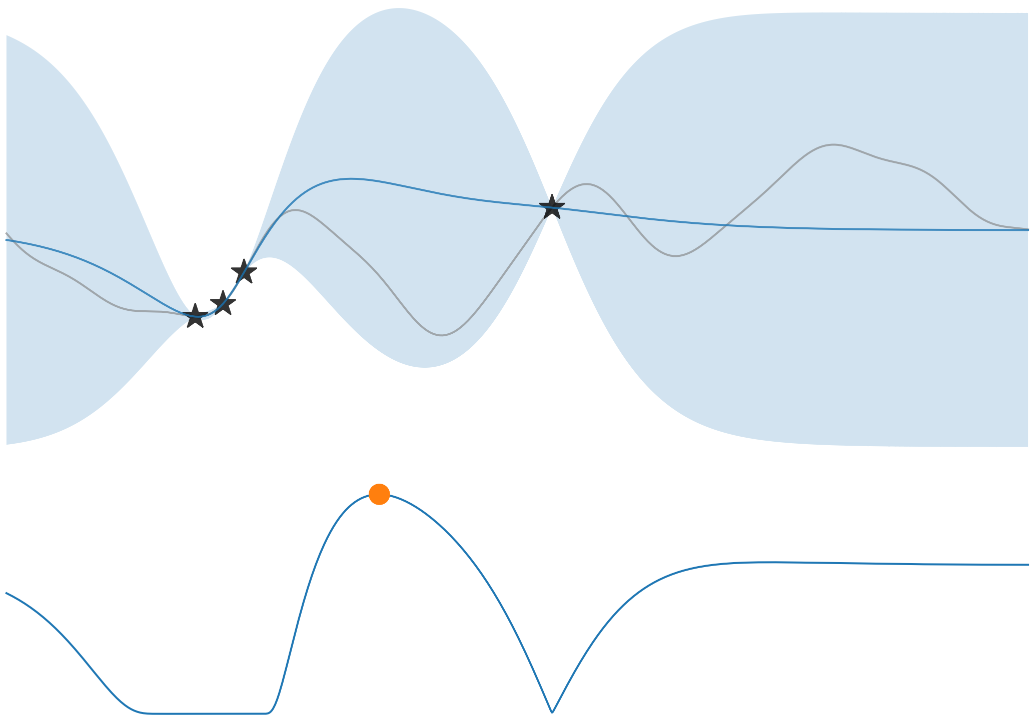
# Expected Improvement



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

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

## Expected Improvement



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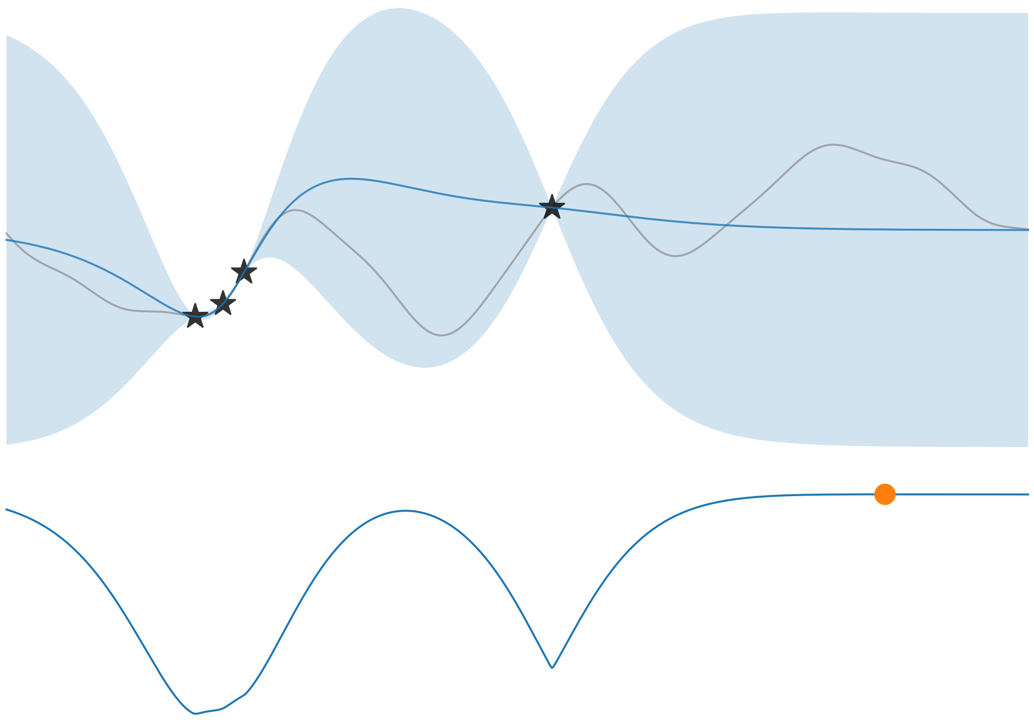
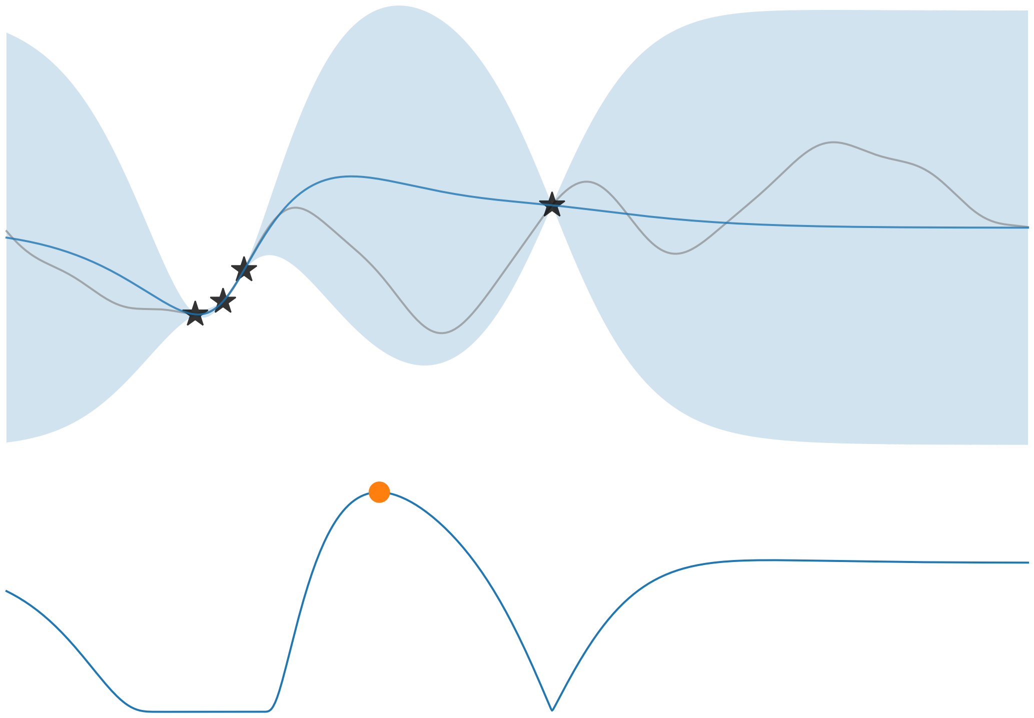
## Gittins Index



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

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

## Expected Improvement



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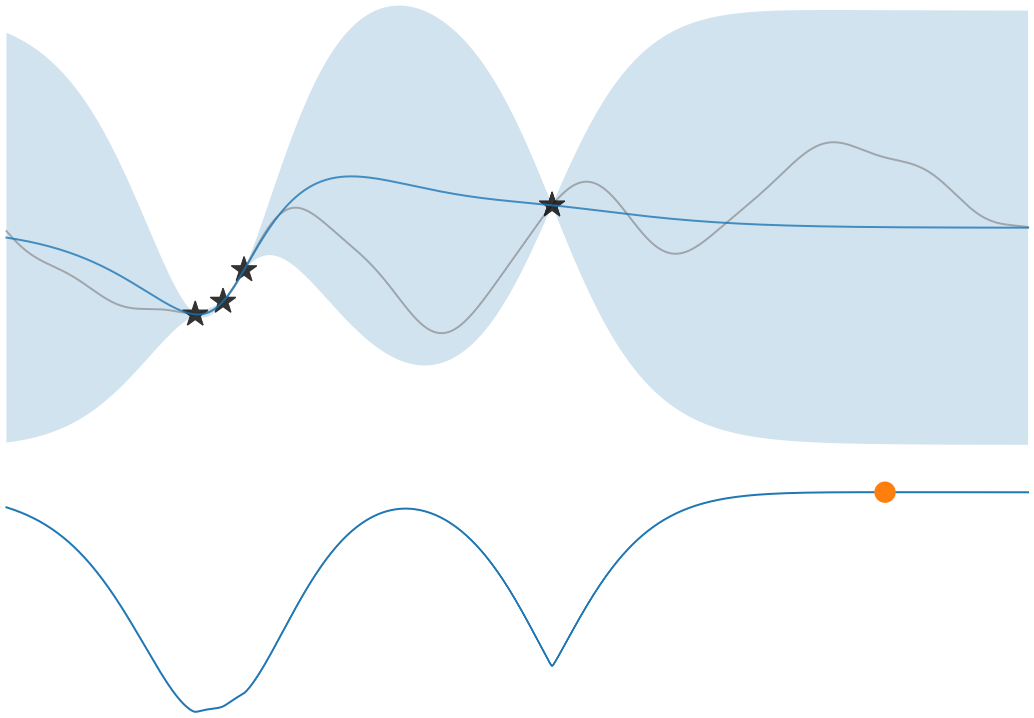
One-step approximation to MDP

## Gittins Index



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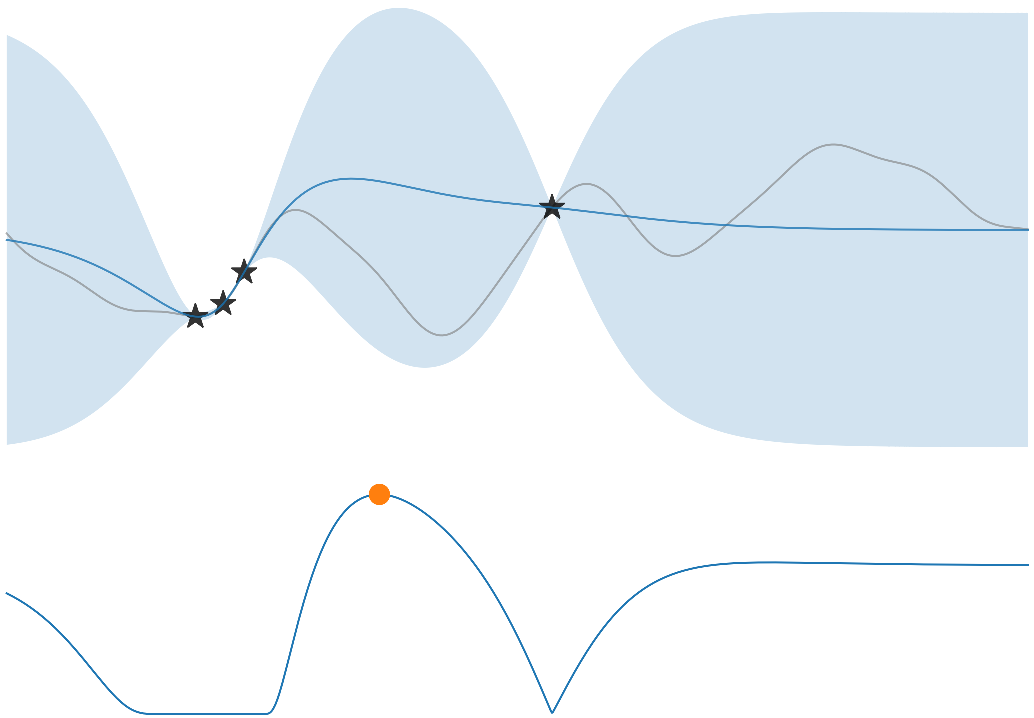

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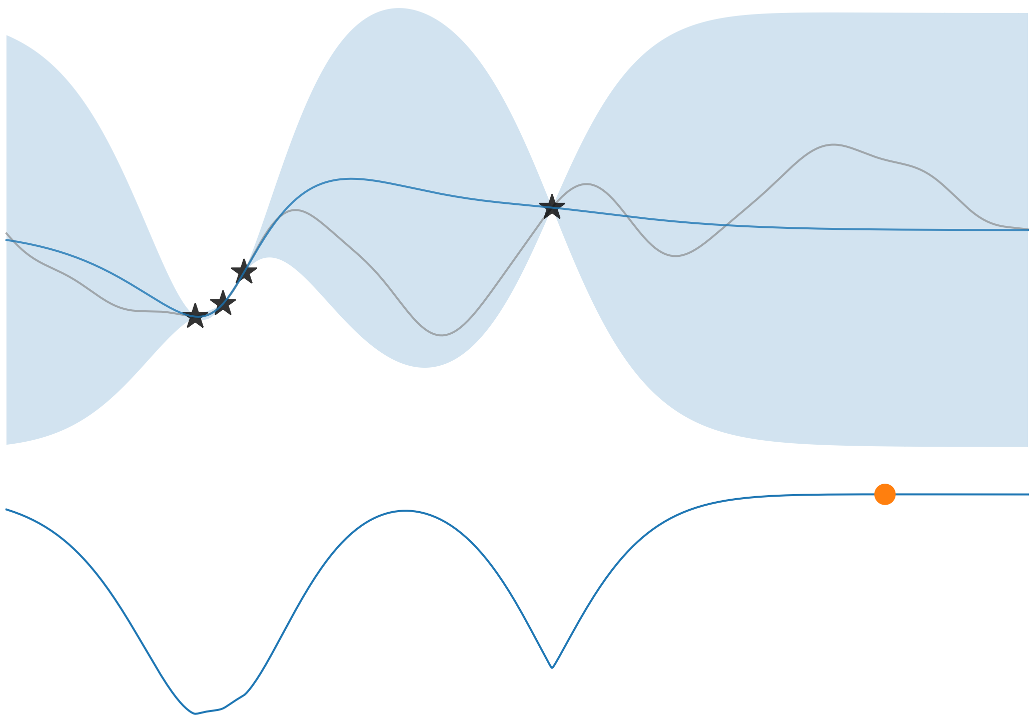
Temporal simplification to MDP

## Gittins Index



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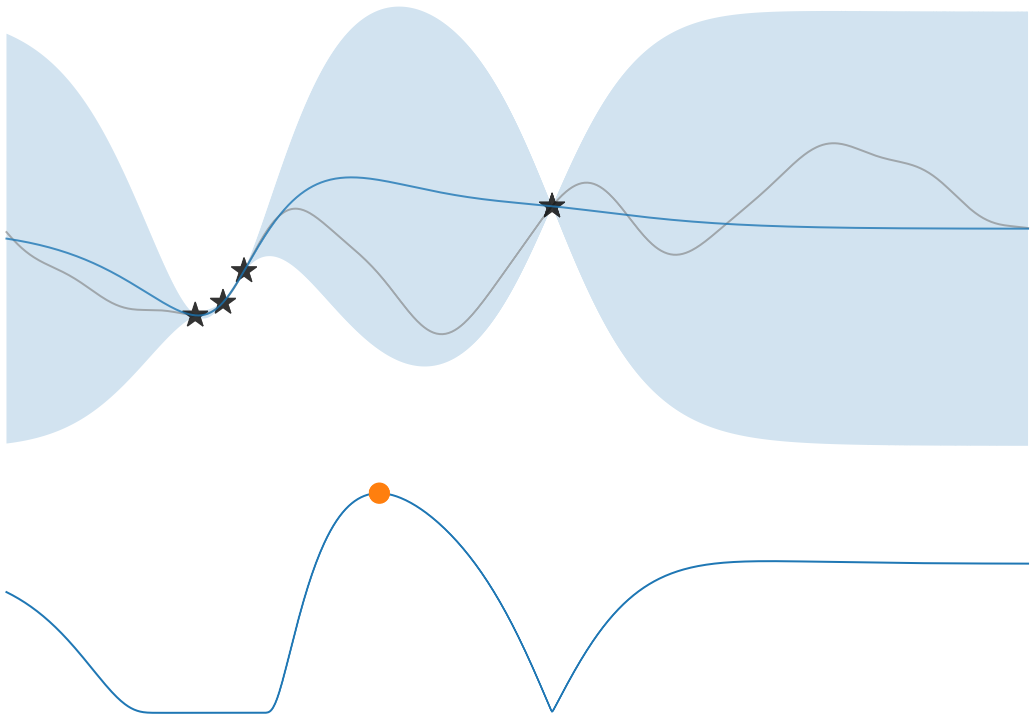

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Temporal simplification to MDP

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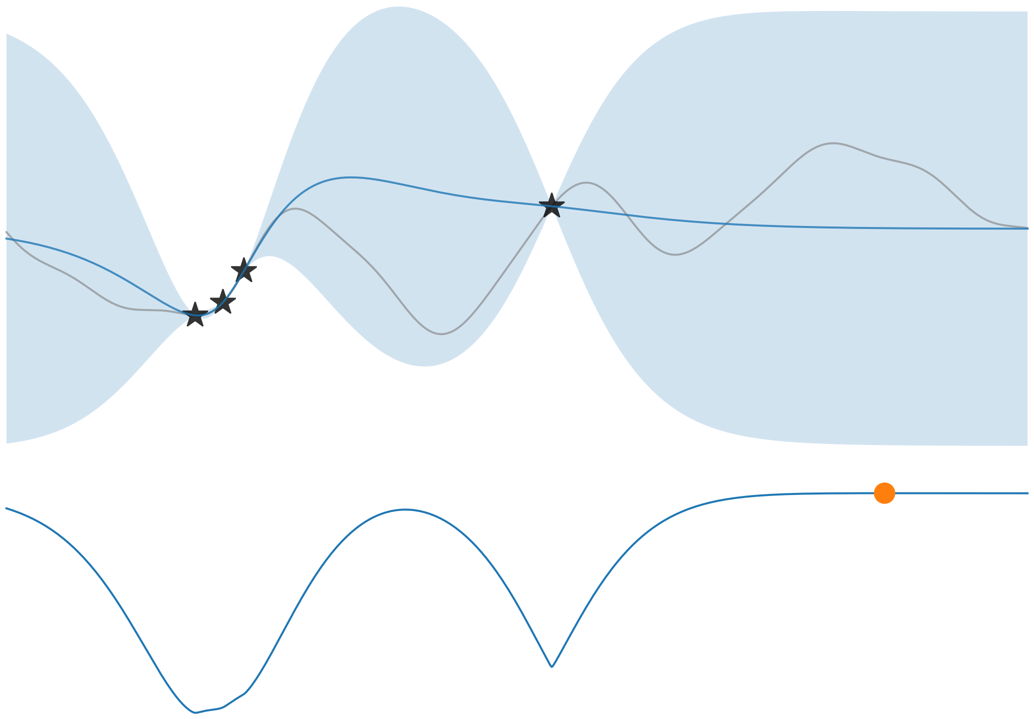
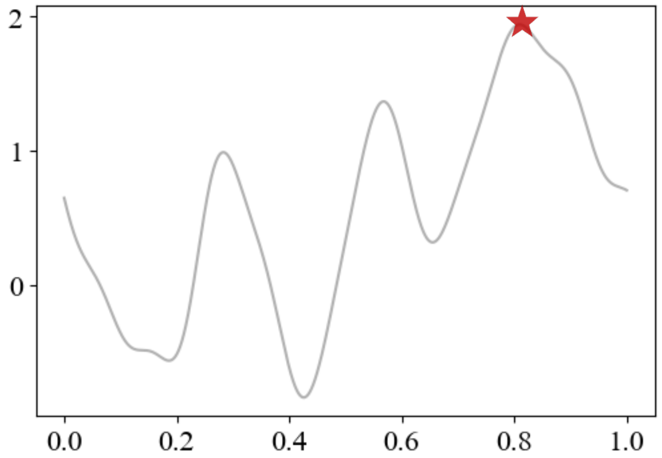


$$\mathrm{GI}_{f|D}(x) = g \text{ s.t. } \mathrm{EI}_{f|D}(x; g) = c(x)$$

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

Spatial simplification to MDP

# Our Approach: Spatial Simplification

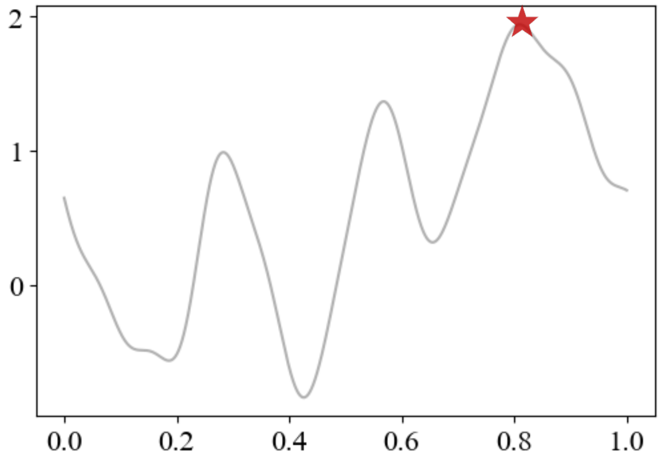



Bayesian Optimization

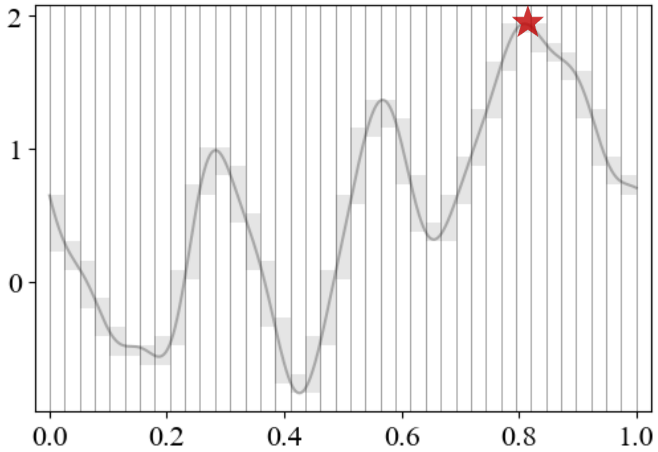
Continuous

Correlated

# Our Approach: Spatial Simplification




$\Longrightarrow$




Bayesian Optimization

Continuous $\Longrightarrow$ Discrete

Correlated

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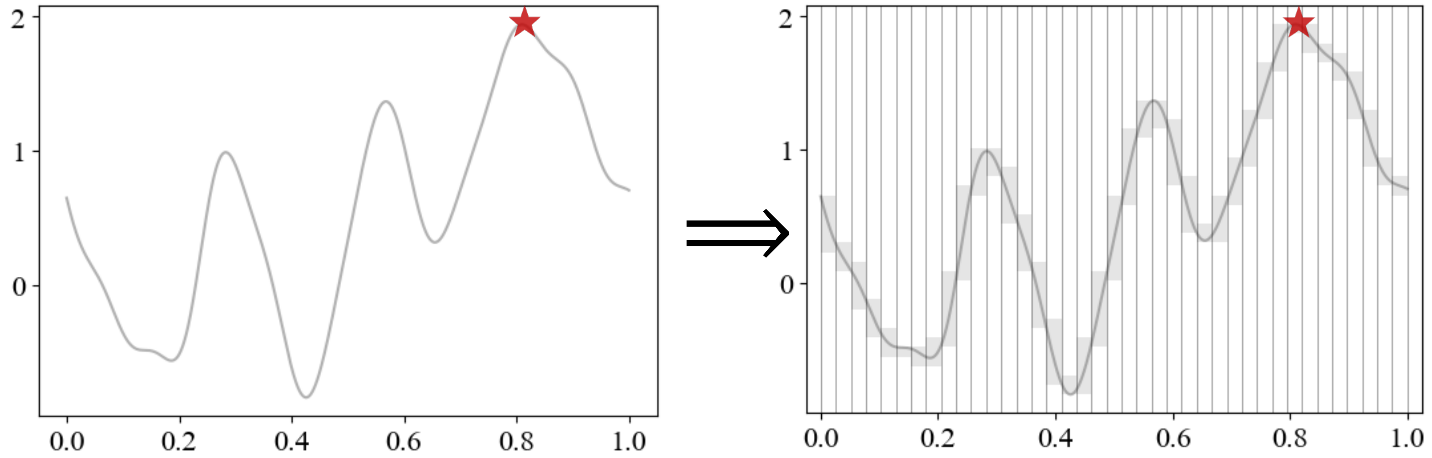


Bayesian Optimization

Continuous ⟹ Discrete

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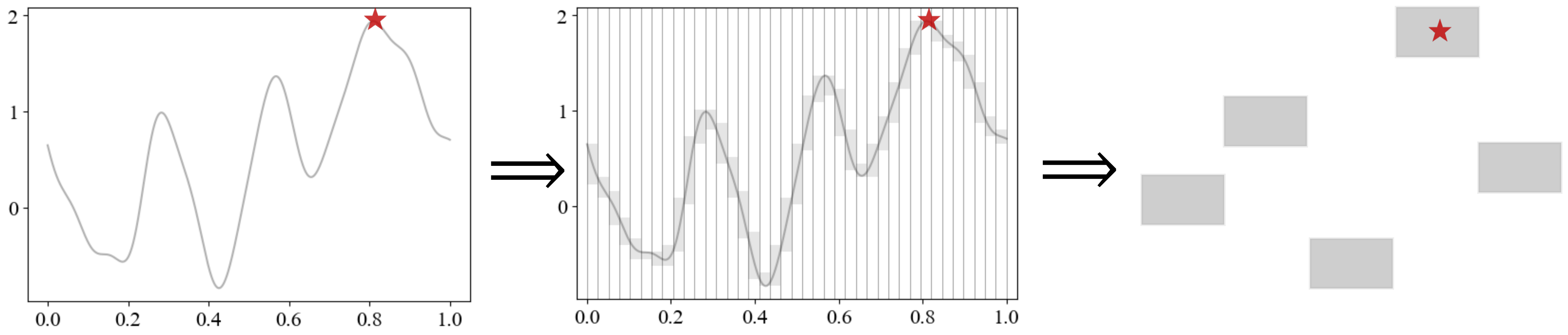


Bayesian Optimization

| | | |
|---|---|---|
| Continuous | ⟹ | Discrete |
| Correlated | ⟹ | Independent |

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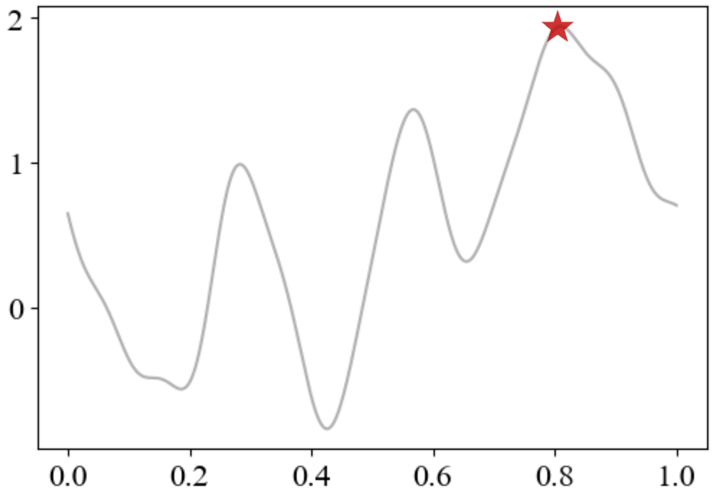
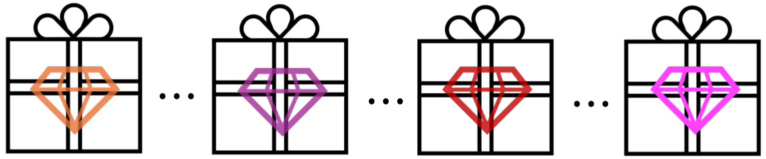



$\Longrightarrow$



Bayesian Optimization

Pandora's Box [Weitzman'79]

Continuous $\Longrightarrow$ Discrete

Correlated $\Longrightarrow$ Independent

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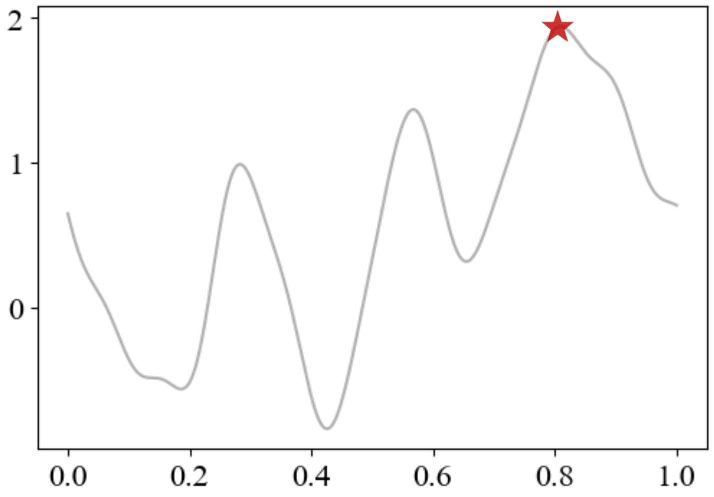


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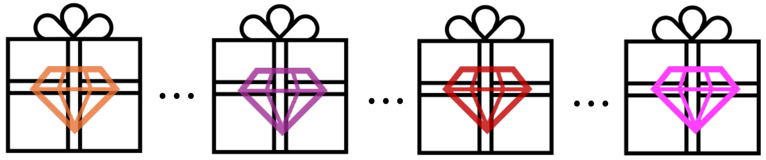


Bayesian Optimization

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Continuous $\Longrightarrow$ Discrete

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Optimal policy: Gittins index

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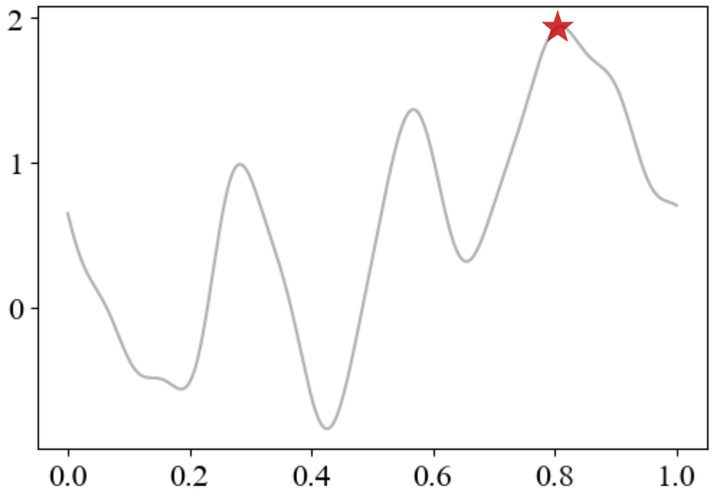


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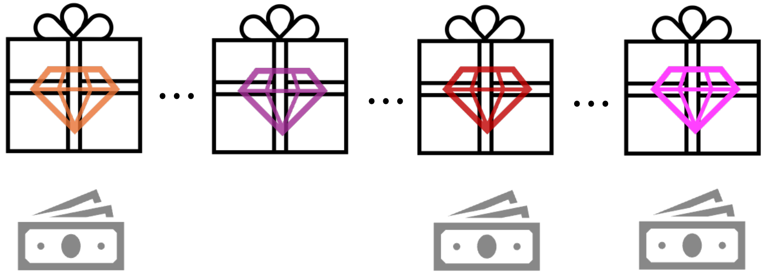


| Bayesian Optimization | | Pandora's Box |
|---|---|---|
| Continuous | $\Longrightarrow$ | Discrete |
| Correlated | $\Longrightarrow$ | Independent |

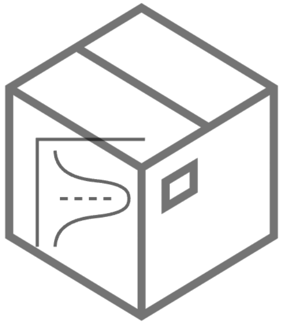
allow varying costs

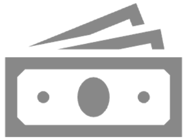
Optimal policy: Gittins index

# Intuition Behind Pandora's Box Gittins Index

1.5-box problem:

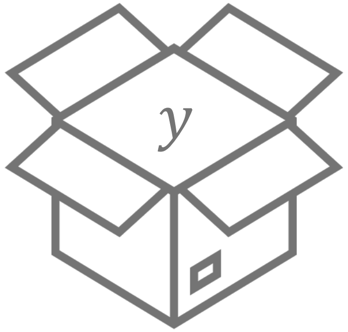
$f(x)$

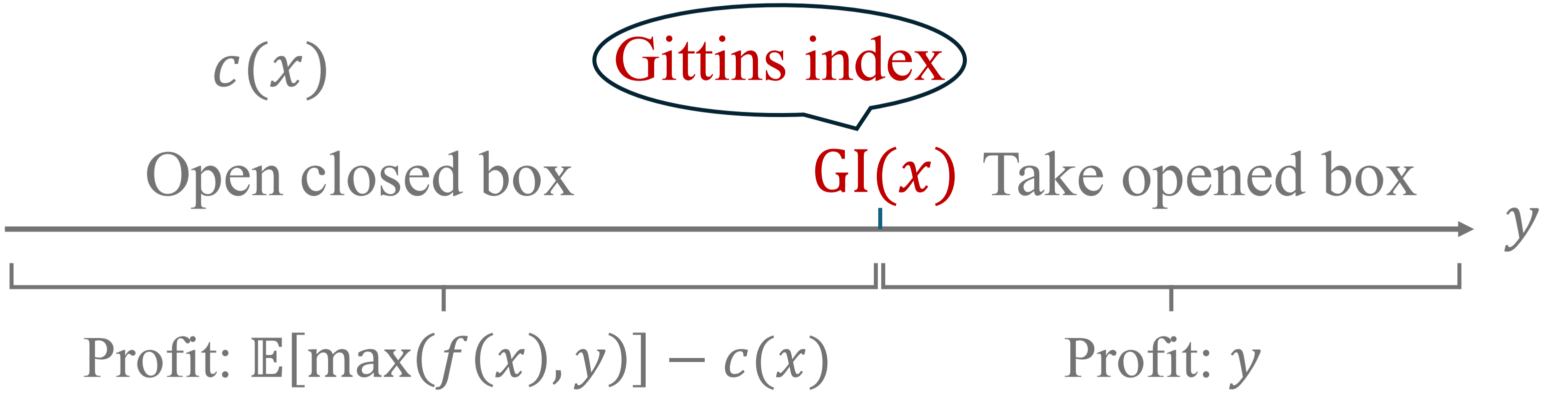




$c(x)$

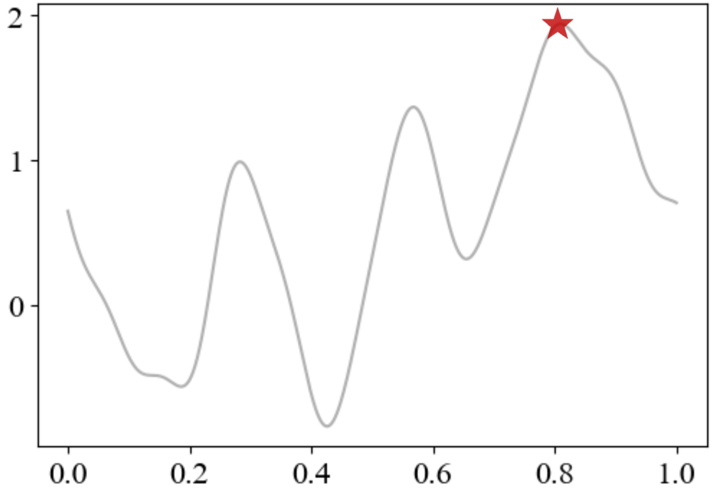
vs.



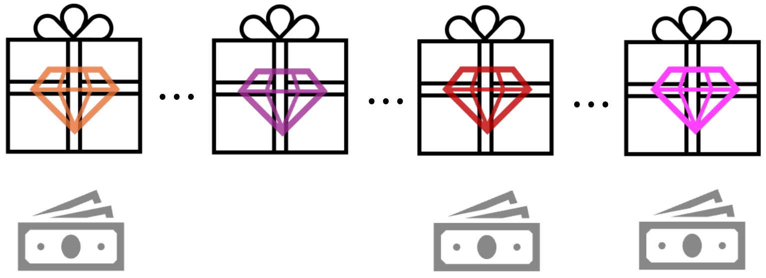

$\mathrm{GI}(x)$: solution $y$ to $\mathbb{E}[\max(f(x), y)] - c(x) = y$

# How to translate Gittins index?




Bayesian Optimization

$\Longrightarrow$




Pandora's Box

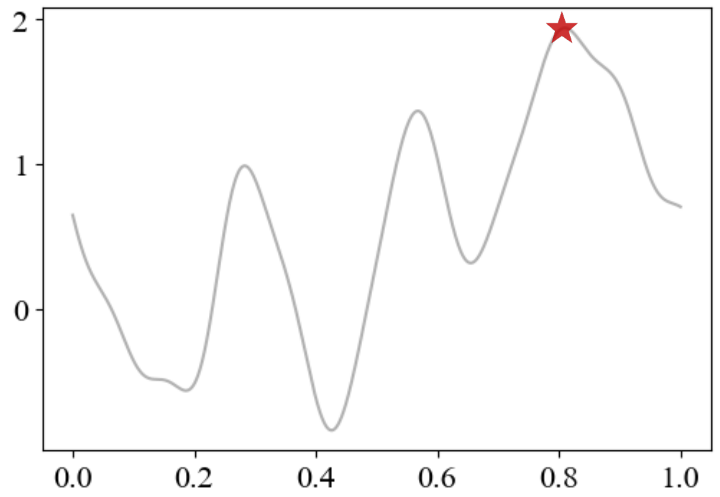
Continuous $\Longrightarrow$ Discrete

Correlated $\Longrightarrow$ Independent

How to translate?

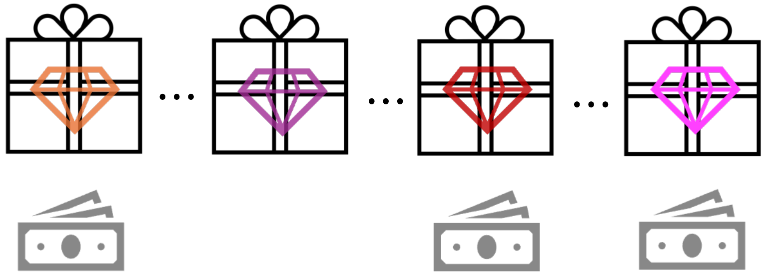
$\Longleftarrow$ Optimal policy: Gittins index

# How to translate Gittins index?




Bayesian Optimization

$\Longrightarrow$



Pandora's Box

Continuous $\Longrightarrow$ Discrete

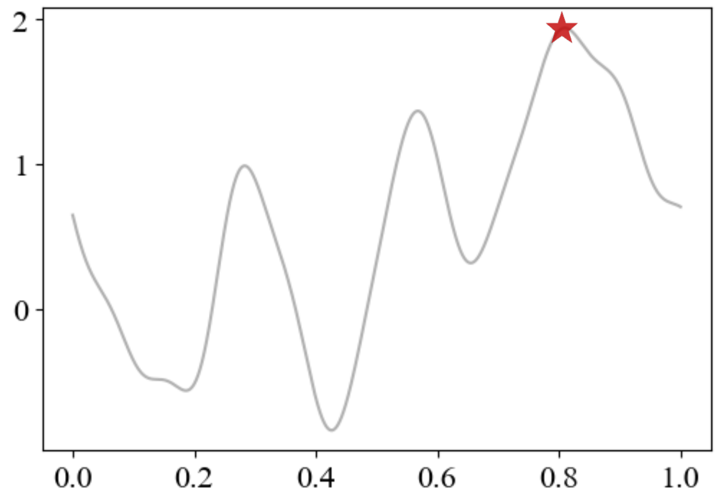
Correlated $\Longrightarrow$ Independent

incorporate posterior

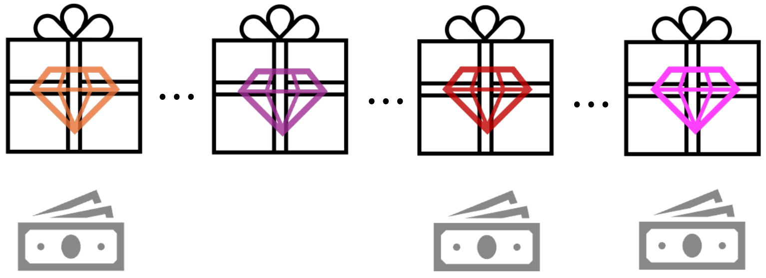
Our policy $\Longleftarrow$ Optimal policy: Gittins index

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

# Is Gittins good in Bayesian Optimization?




$\Longrightarrow$



Bayesian Optimization | Pandora's Box [Weitzman'79]

Continuous $\Longrightarrow$ Discrete

Correlated $\Longrightarrow$ Independent

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

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

# Experiment Setup: Objective Functions

Synthetic

## Samples from prior

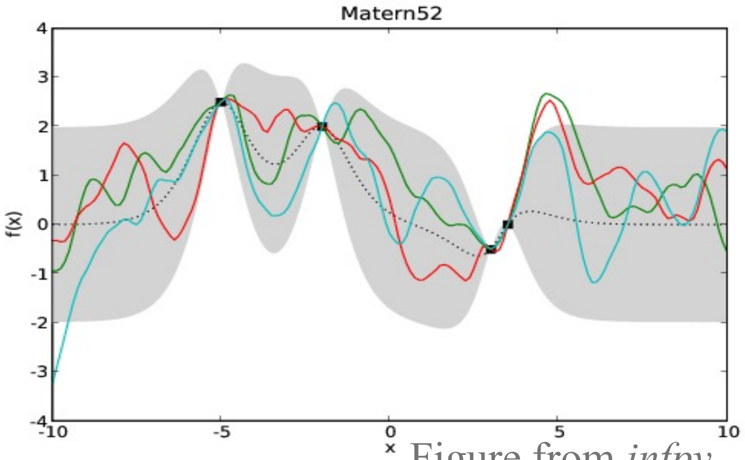



Figure from *infpy*

## Ackley function

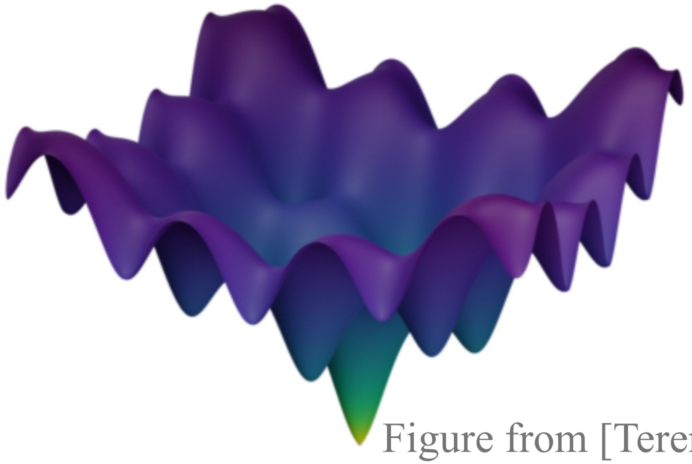


Figure from [Terenin’22]

Empirical

## Pest Control

Figure from ChatGPT

## Lunar Lander

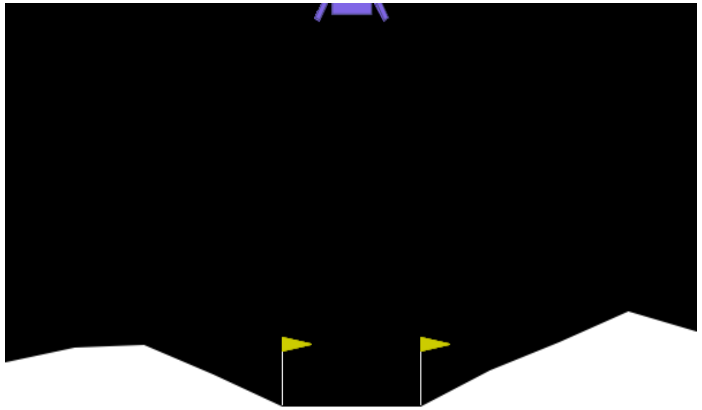
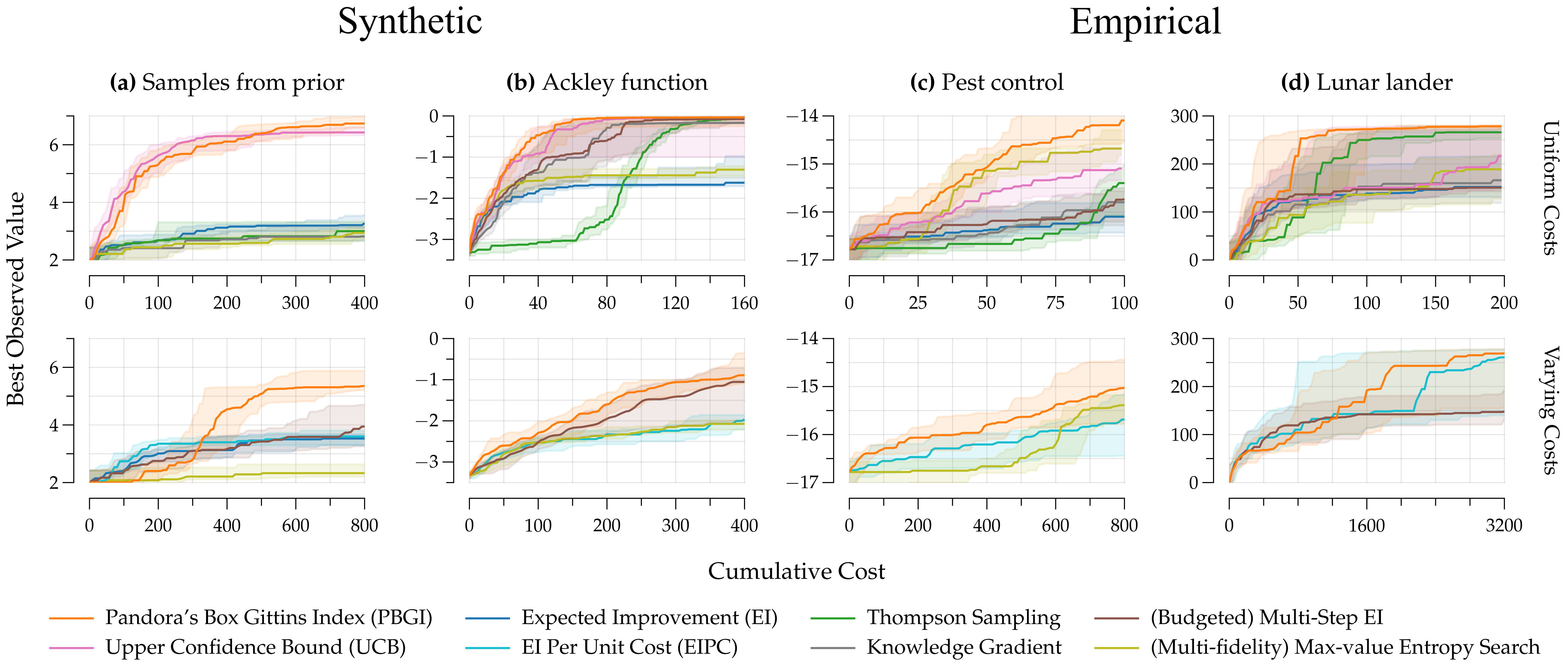


Figure from OpenAI Gym

# Experiment Results



# FAQ

- Easy-to-compute?

# FAQ

- Easy-to-compute?

  Yes, EI + bisection

# FAQ

- Easy-to-compute?

  Yes, EI + bisection
- Any theoretical results?

# FAQ

- Easy-to-compute?

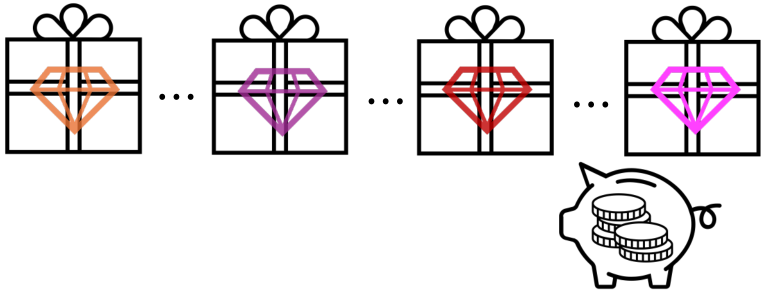
  Yes, EI + bisection

- Any theoretical results?

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

# Theoretical Result

**max** best observed under budget

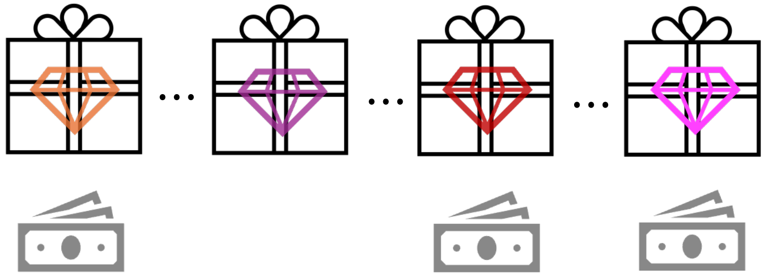


Budgeted Pandora's Box

Expected budget constraint

Optimal policy?

**max** (best observed – costs)



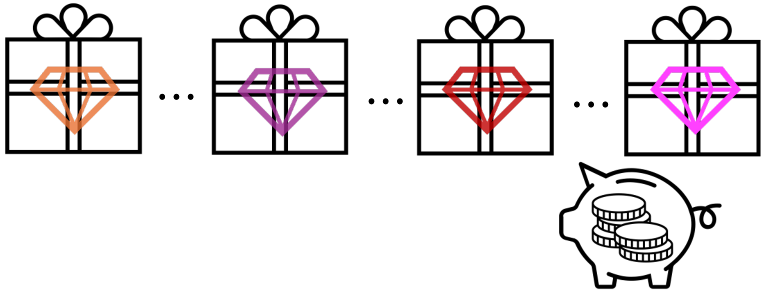
Pandora's Box

Cost per sample

Optimal policy: Gittins index

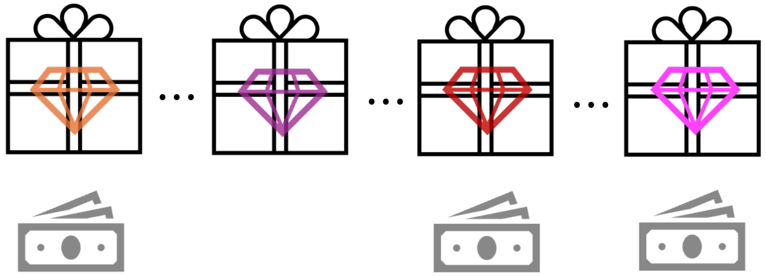
# Theoretical Result

**max** best observed under budget



$\Longleftarrow$

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



Budgeted Pandora's Box

Expected budget constraint

Optimal policy ✔

extension to [Aminian, Manshadi, Niazadeh'24]

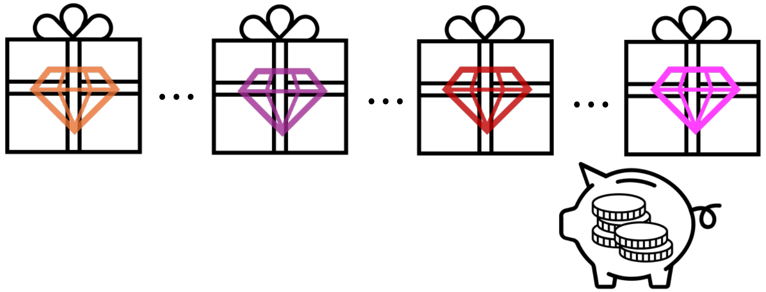
Pandora's Box

Cost per sample

Optimal policy: Gittins index

# Theoretical Result

**max** best observed under budget



Budgeted Pandora's Box

Expected budget constraint

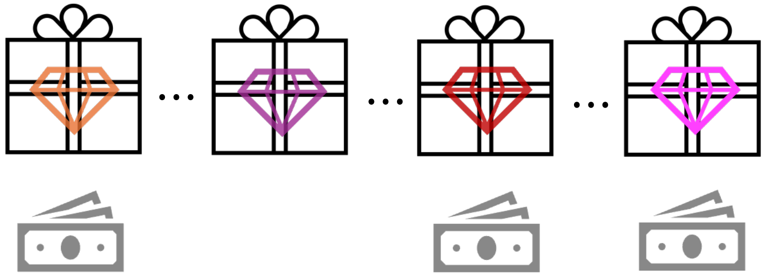
Optimal policy ✓

extension to [Aminian, Manshadi, Niazadeh'24]

$\Longleftarrow$

budget-dependent

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



Pandora's Box

Cost per sample

Optimal policy: Gittins index

# FAQ

- Easy-to-compute?

  Yes, EI + bisection
- Any theoretical results?

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

# FAQ

- Easy-to-compute?

  Yes, EI + bisection

- Any theoretical results?

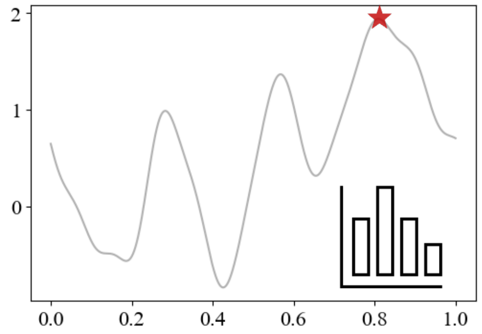
  Yes, expected-budget-constrained $\cong$ cost-per-sample

- Tuning parameters?

  Yes, control unit conversion

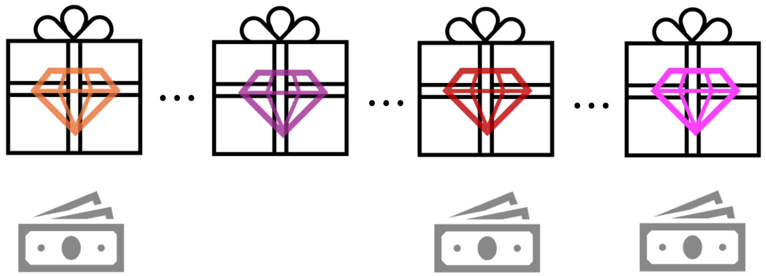
# New Design Principle: Gittins Index

## Problem



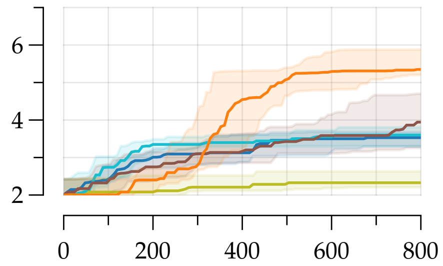

Bayesian optimization
with varying costs

## Key idea



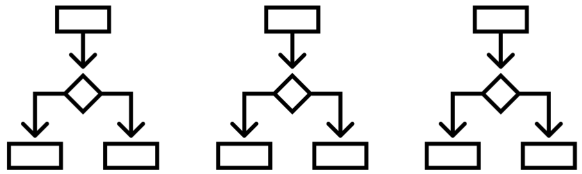

link to Pandora's box
and Gittins index theory

## Impact




competitive performance

## Future potential



black-box processes
with partial feedback