

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

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Qian Xie (Cornell ORIE)

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

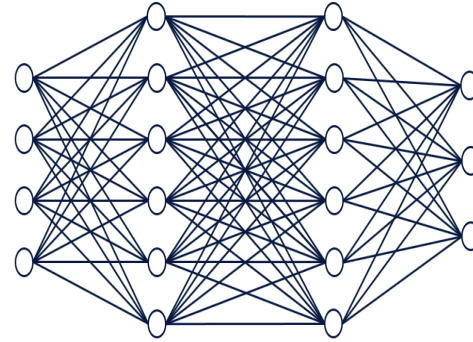


Alexander Terenin

# World of Parameter Optimization

Hyperparameter tuning:

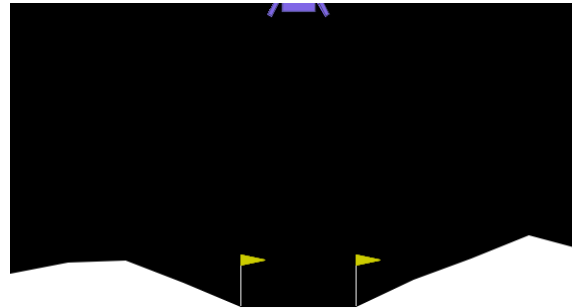
Training parameters →



→ Accuracy

Control optimization:

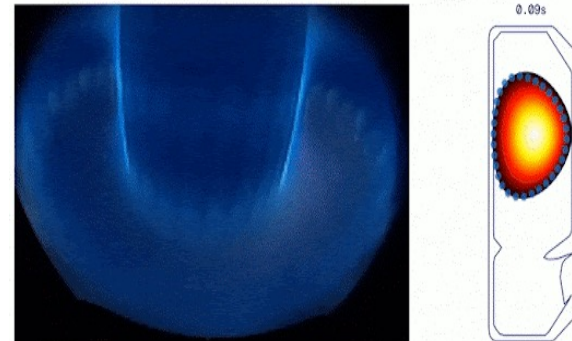
Control parameters →



→ Reward

Plasma physics:

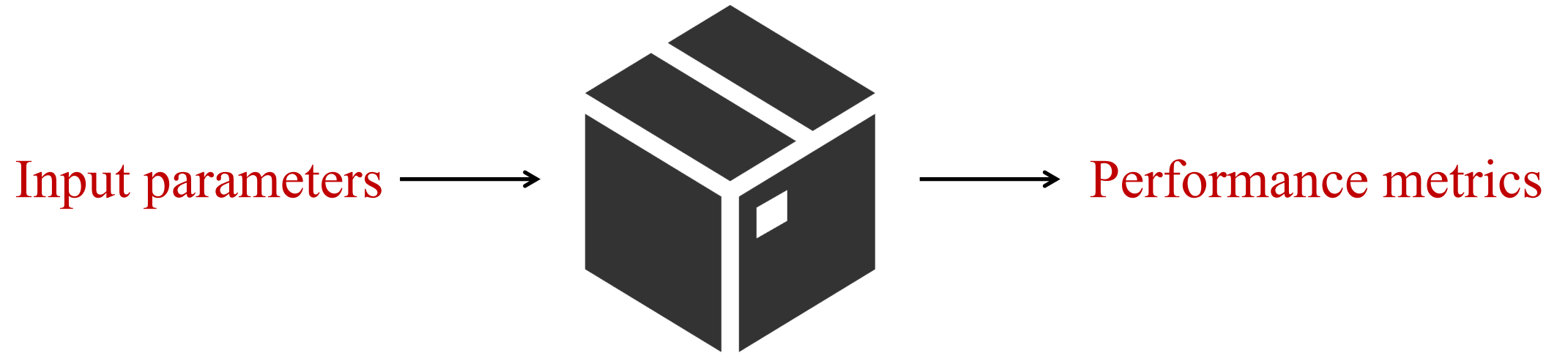
Reactor parameters →



→ Stability

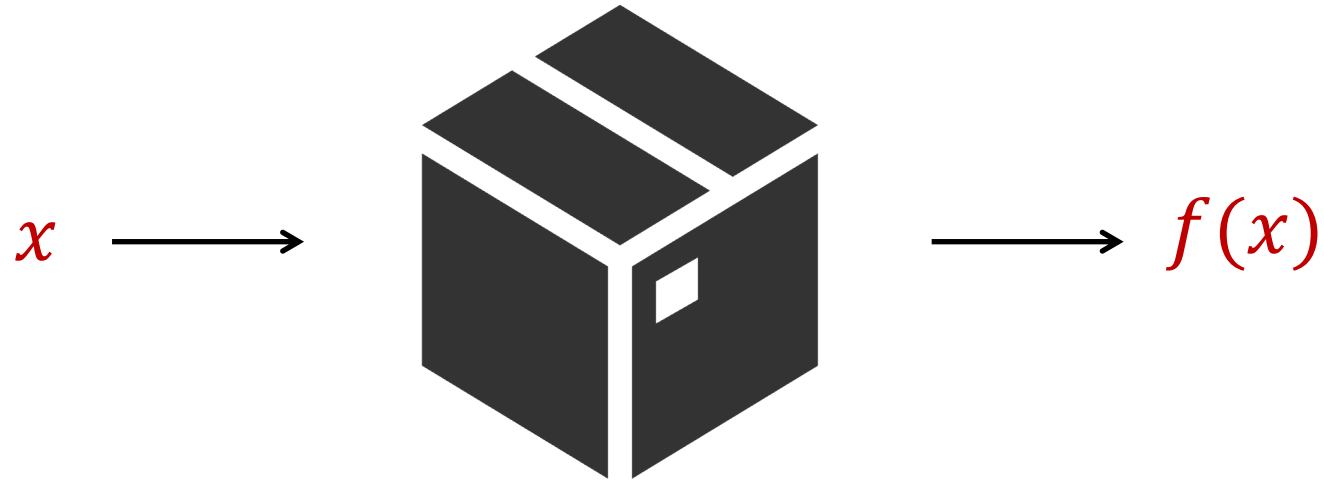
# World of Parameter Optimization

Black-box optimization:

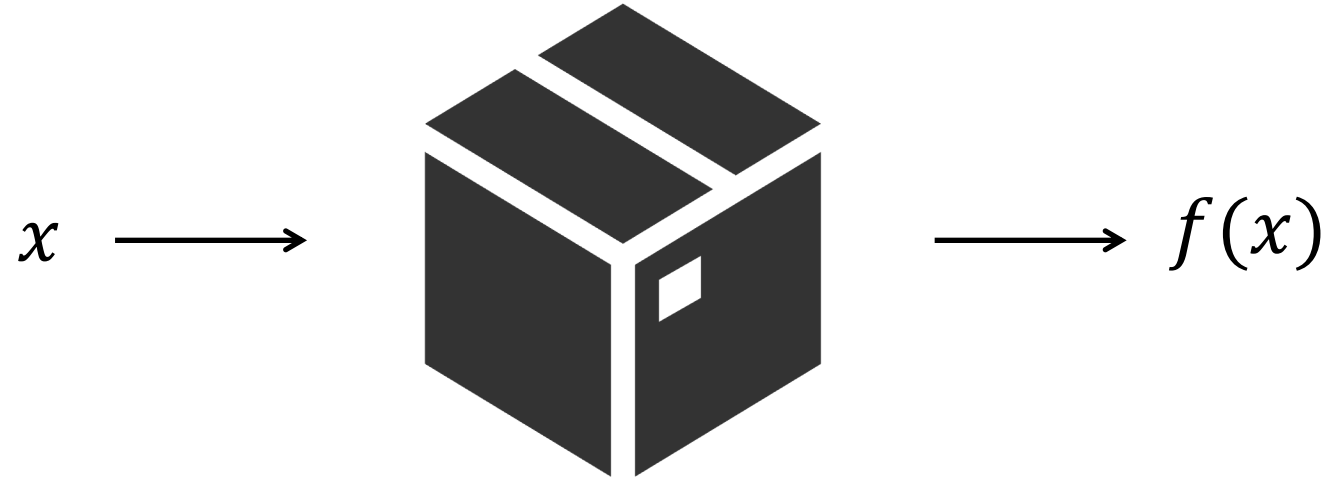


# World of Parameter Optimization

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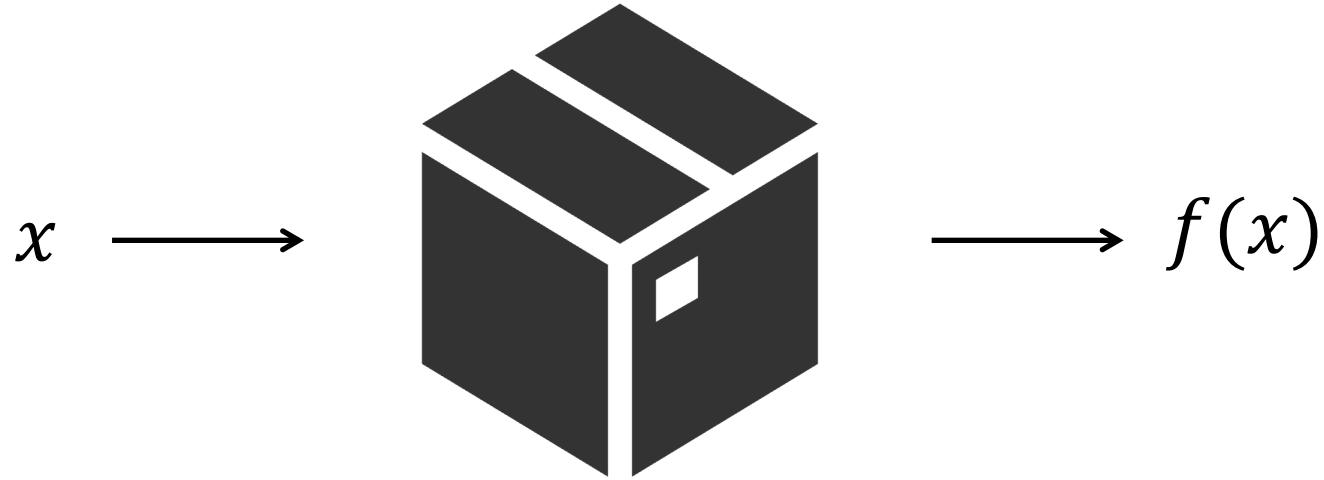


# Optimizing Black-box Functions



Goal:  **$\max_{x \in \mathcal{X}} f(x)$**

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$f \sim \text{Stochastic Process}$

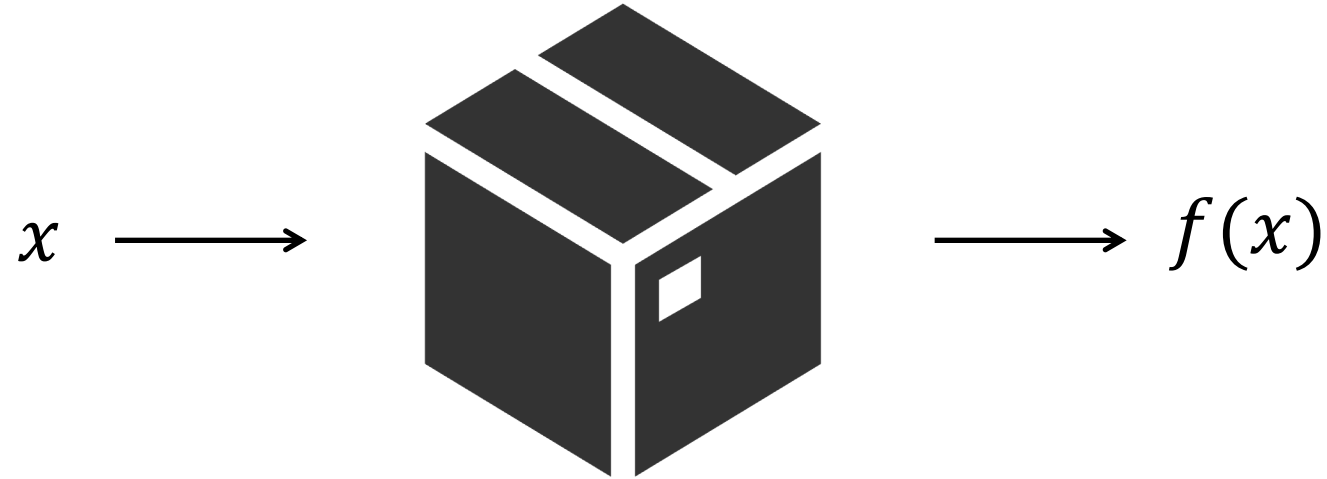
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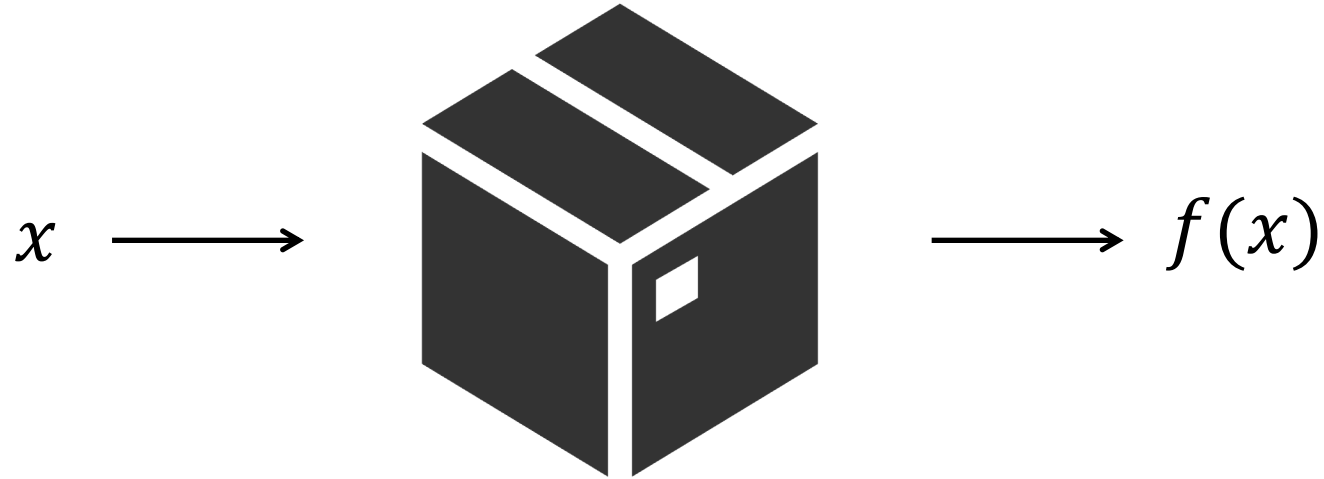


# Optimizing Black-box Functions



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

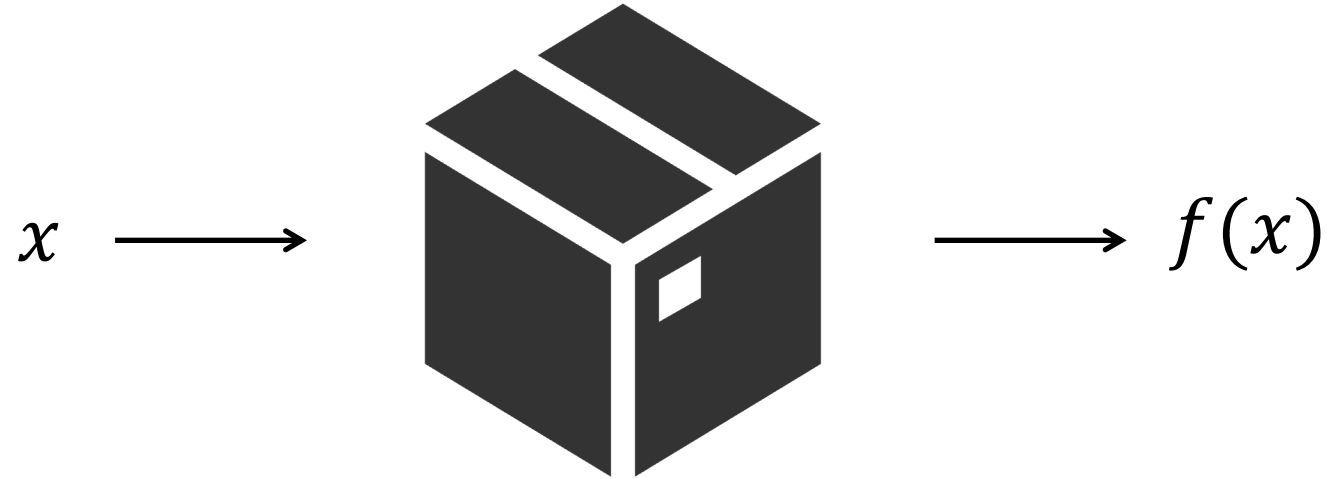
# Optimizing Black-box Functions



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

$f \sim \text{Gaussian Process}$

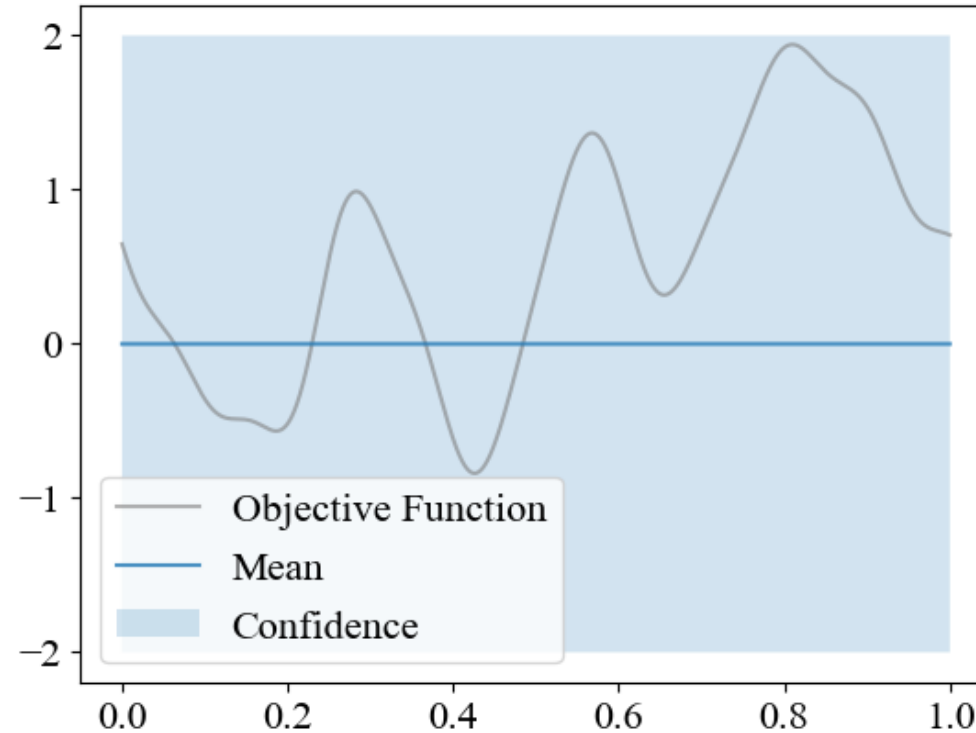
# Bayesian Optimization



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

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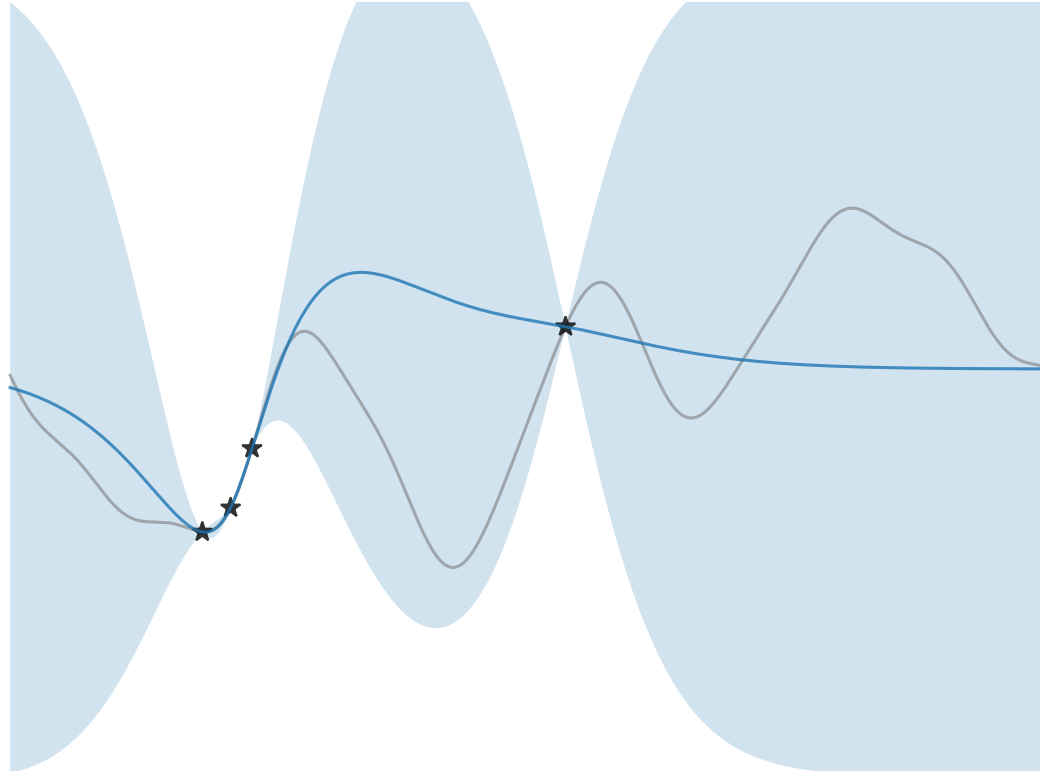
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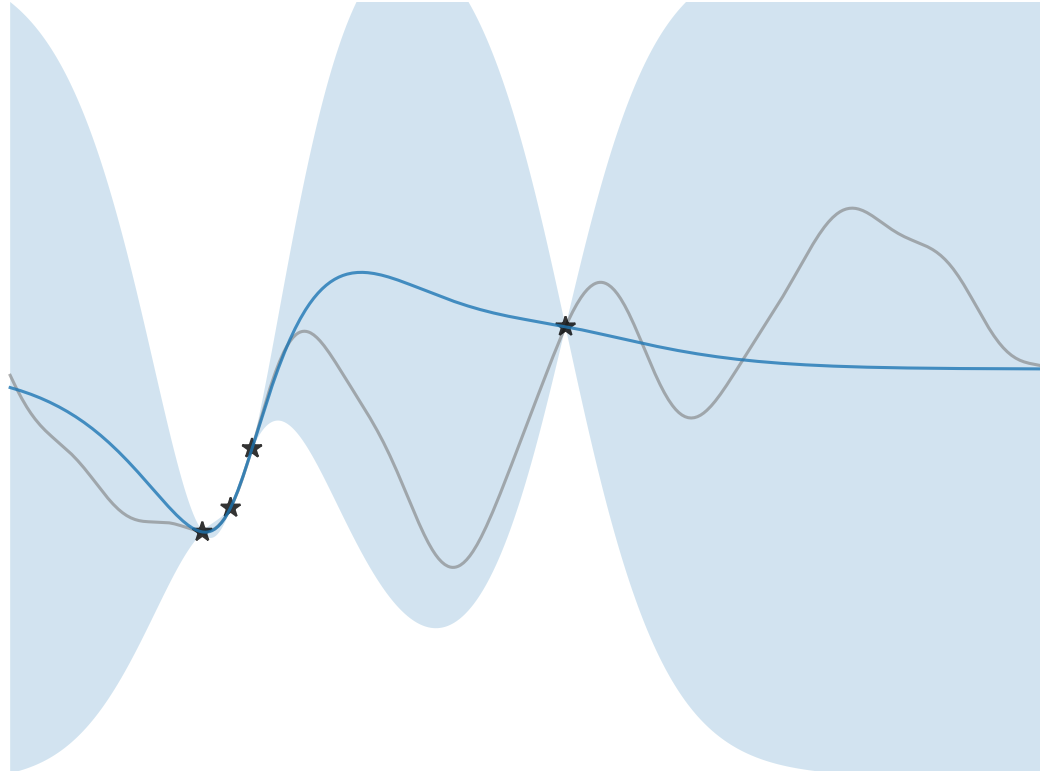
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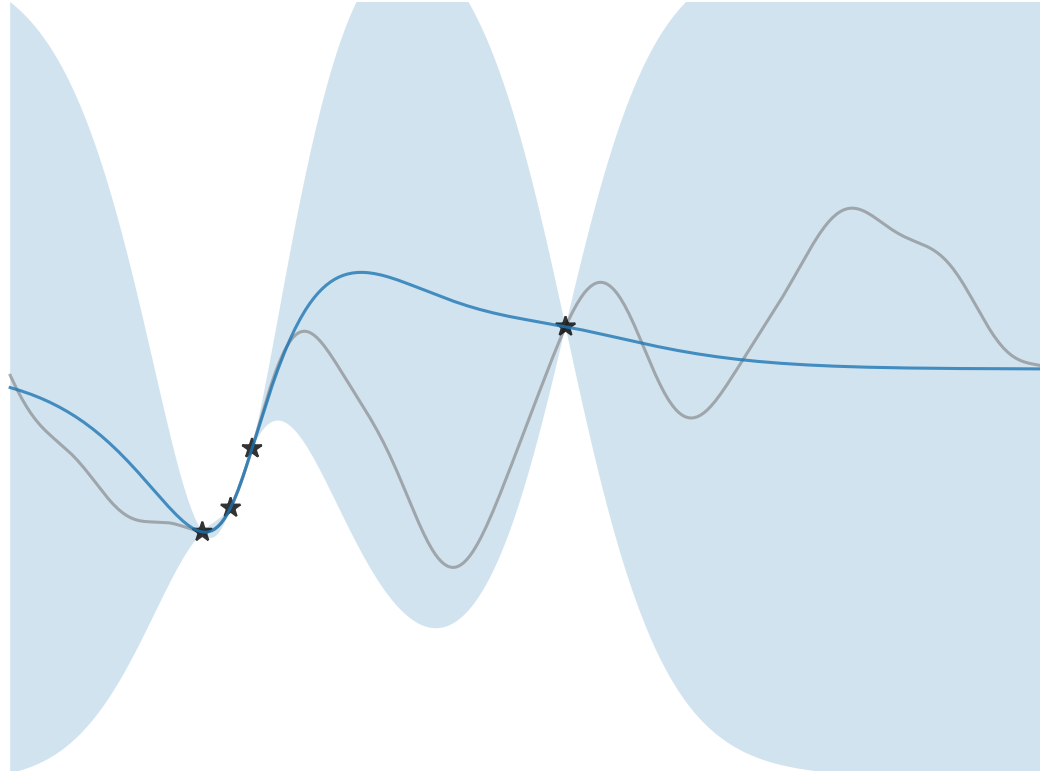
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# Bayesian Optimization



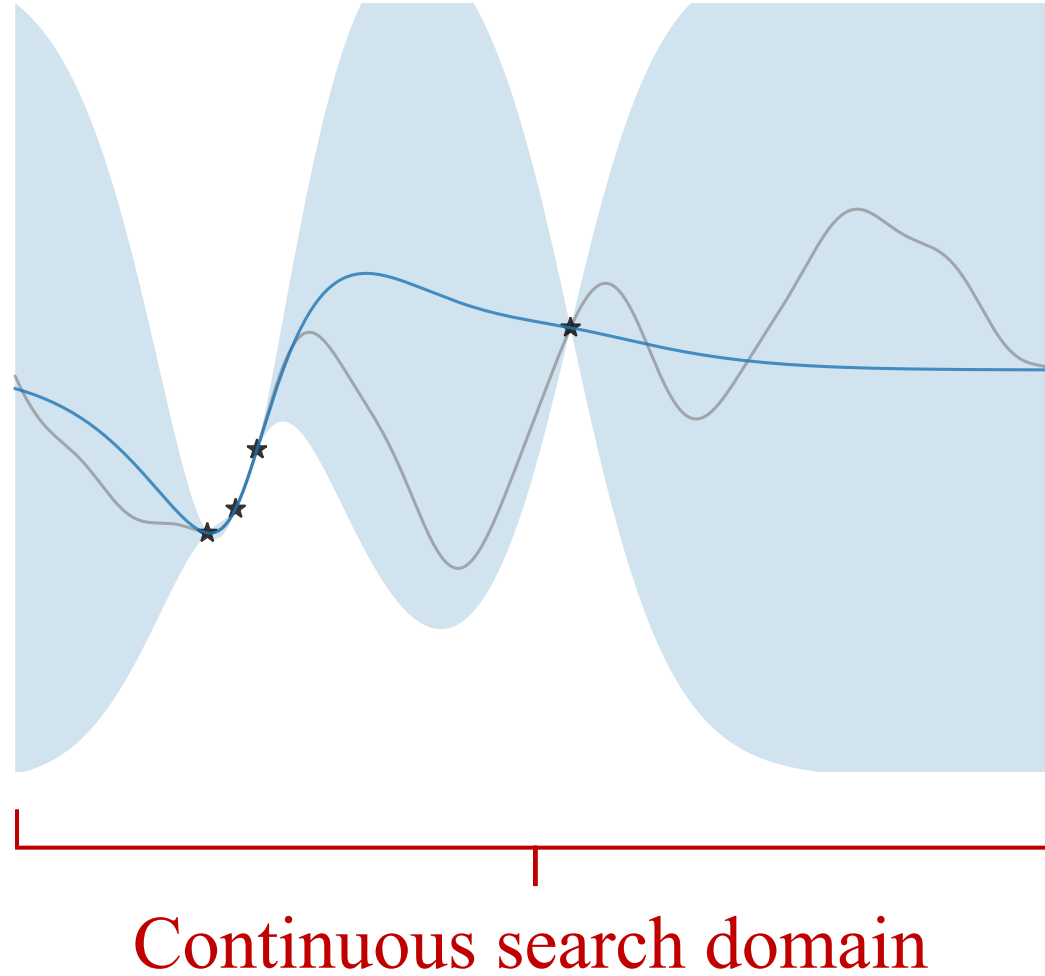
What to evaluate next?

# Bayesian Optimization



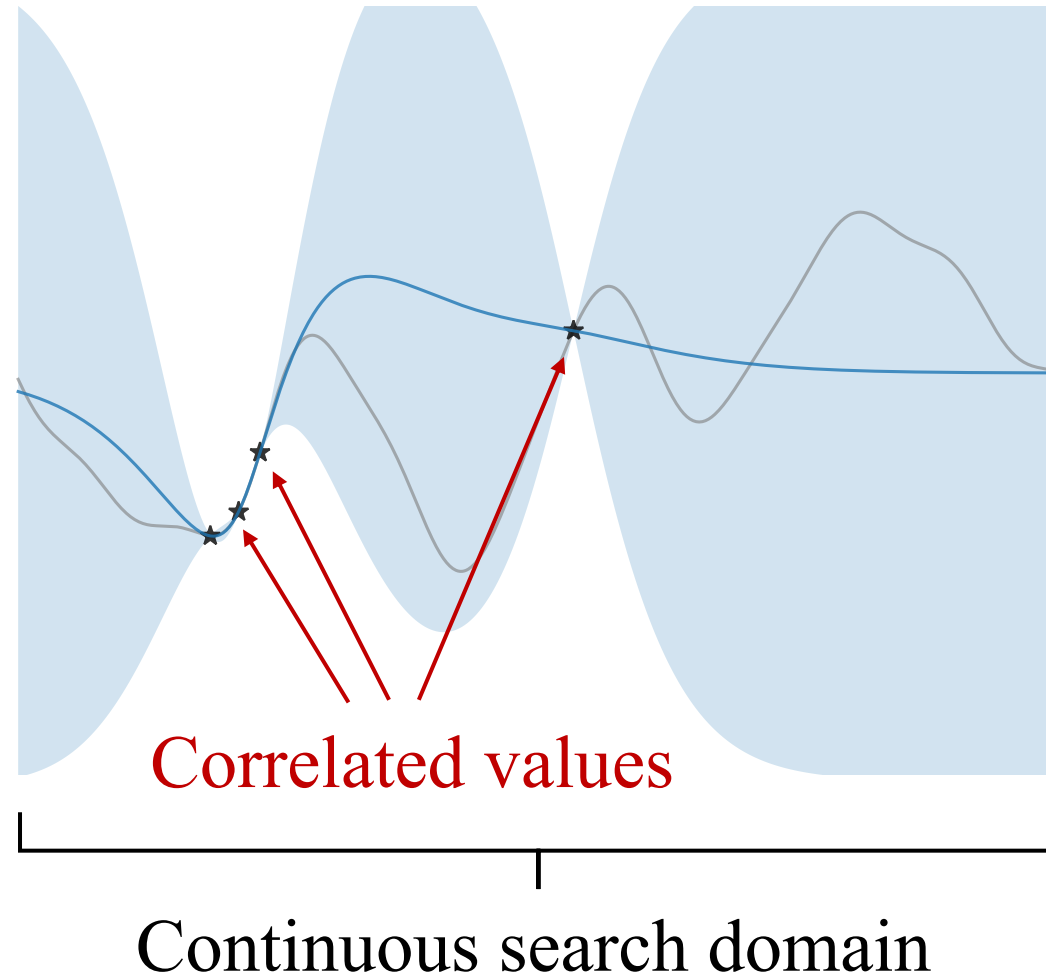
Optimal policy?

# Challenges of Bayesian Optimization

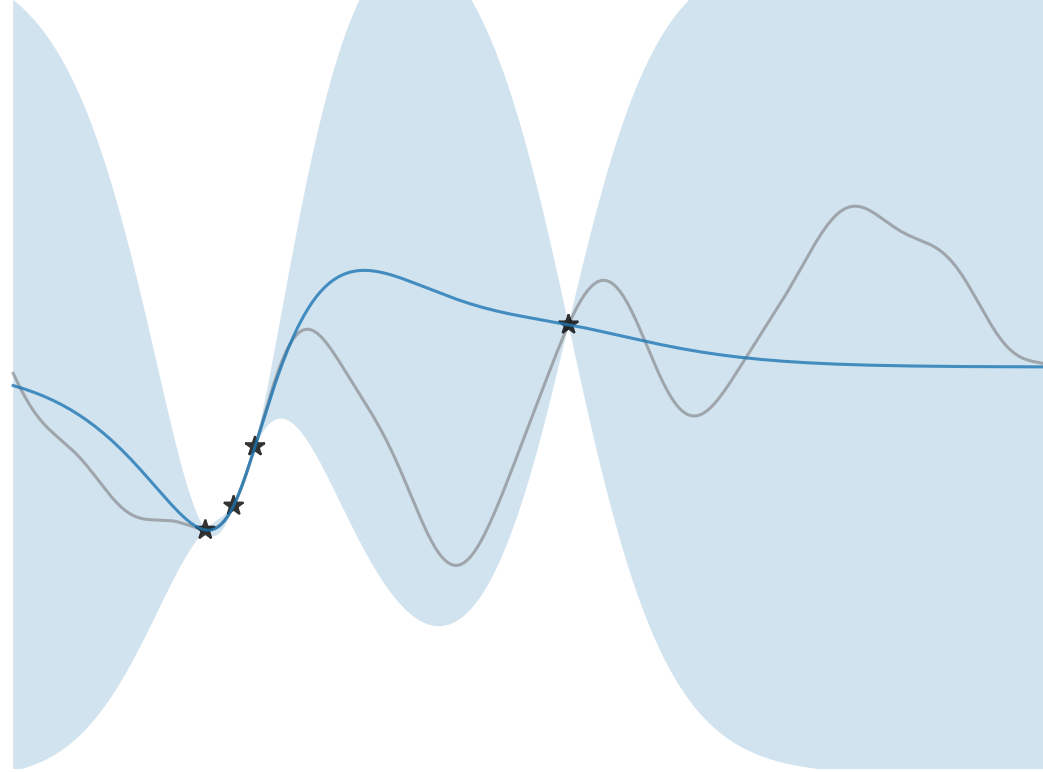




# Challenges of Bayesian Optimization

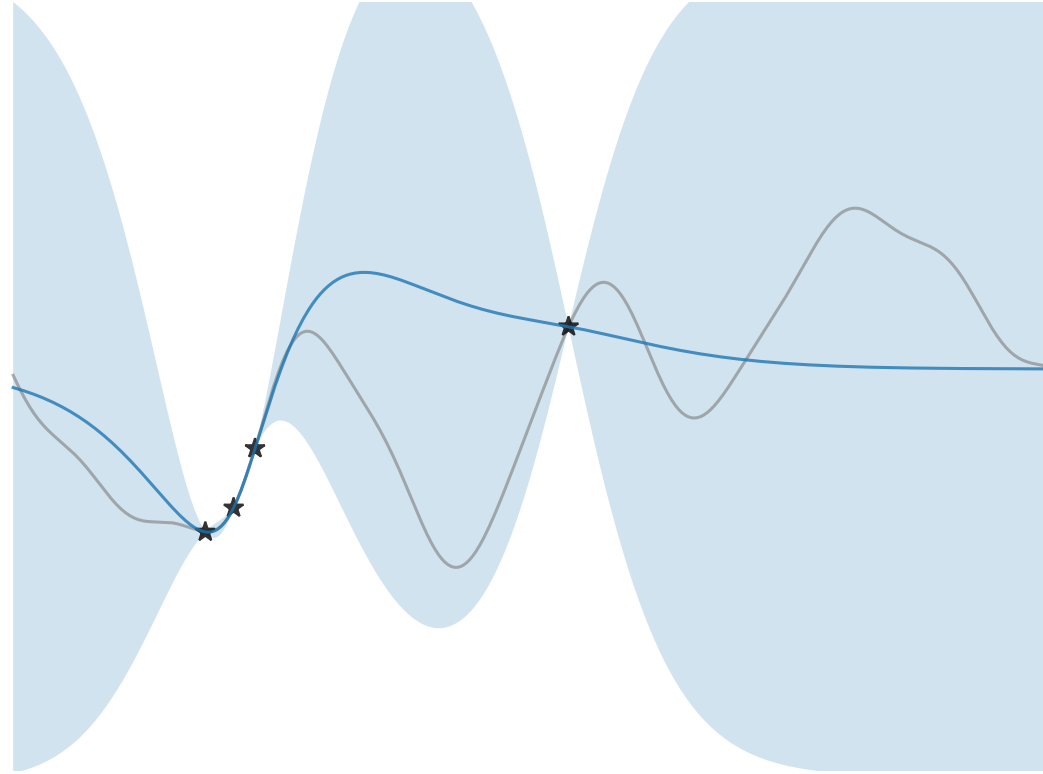


# Challenges of Bayesian Optimization



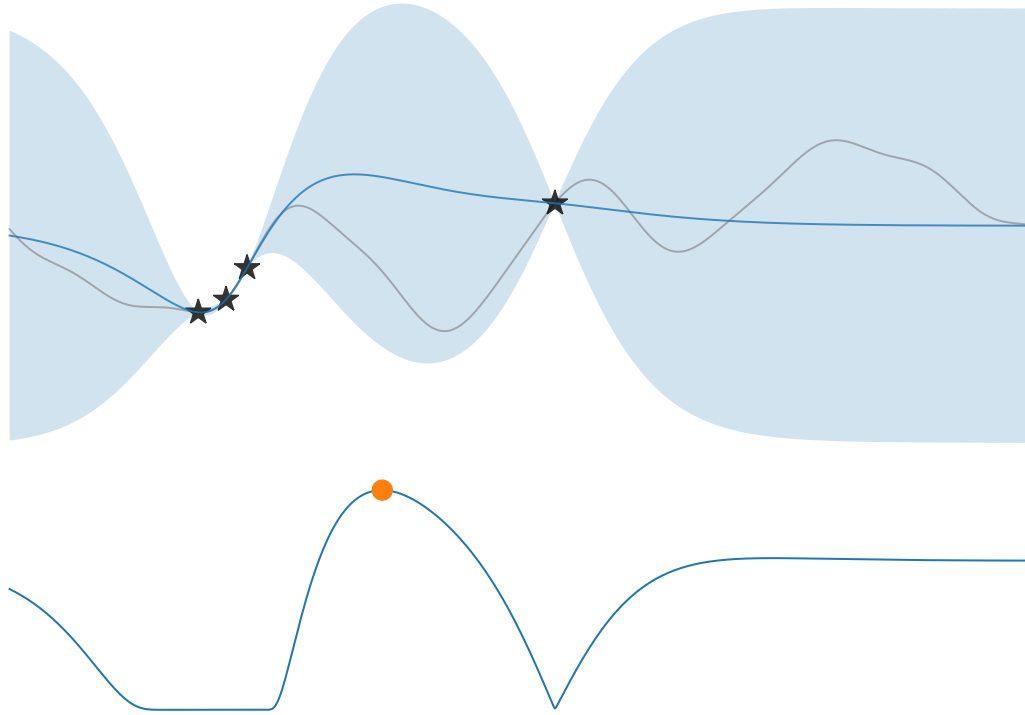
Correlation & continuity  $\Rightarrow$  **Intractable MDP**

# Challenges of Bayesian Optimization



Intractable MDP  $\Rightarrow$  Optimal policy unknown

# Popular Policy: Expected Improvement

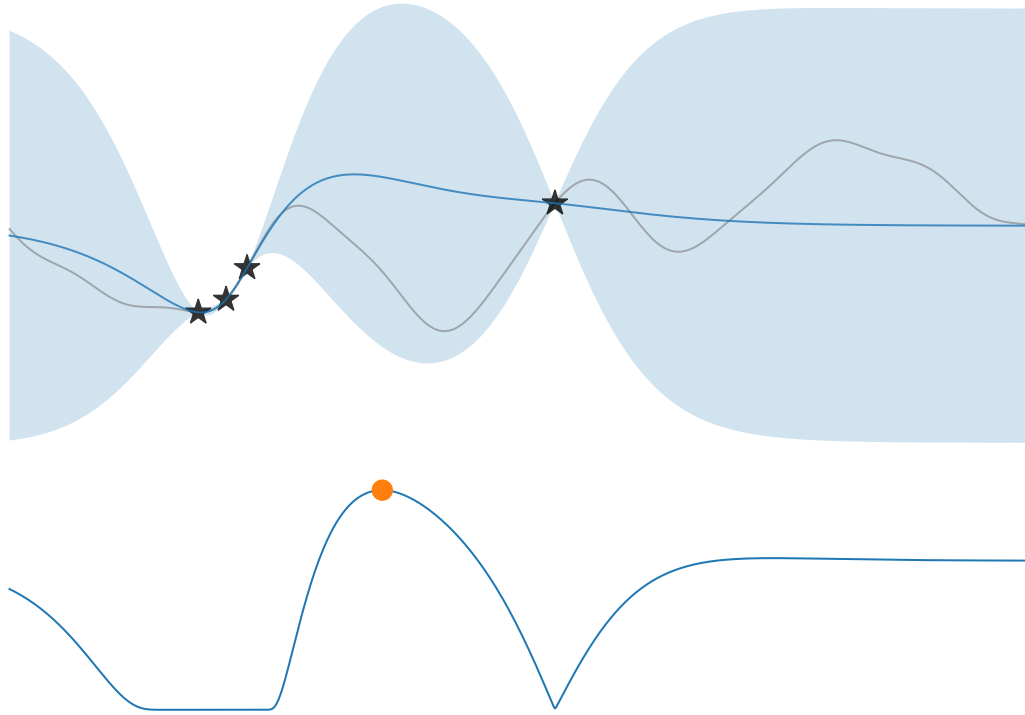


$$\text{EI}(x) = \mathbb{E}[\underbrace{\max(f(x) - y_{\text{best}}, 0)}_{\text{"improvement"}} \mid D]$$

current best observed

data

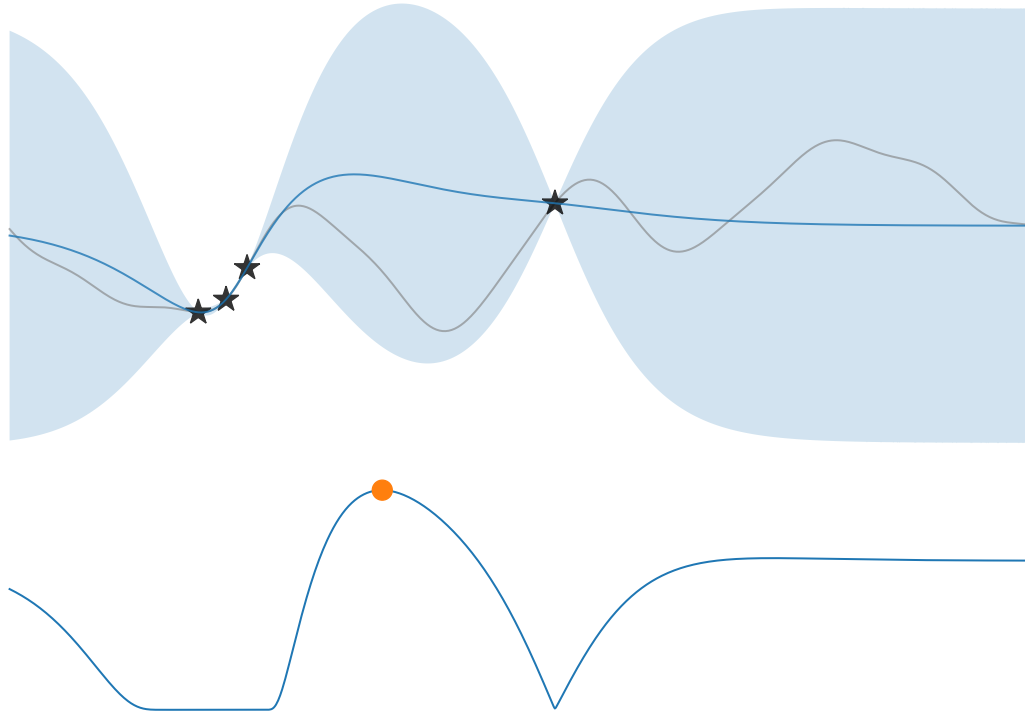
# Popular Policy: Expected Improvement



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

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

# Popular Policy: Expected Improvement

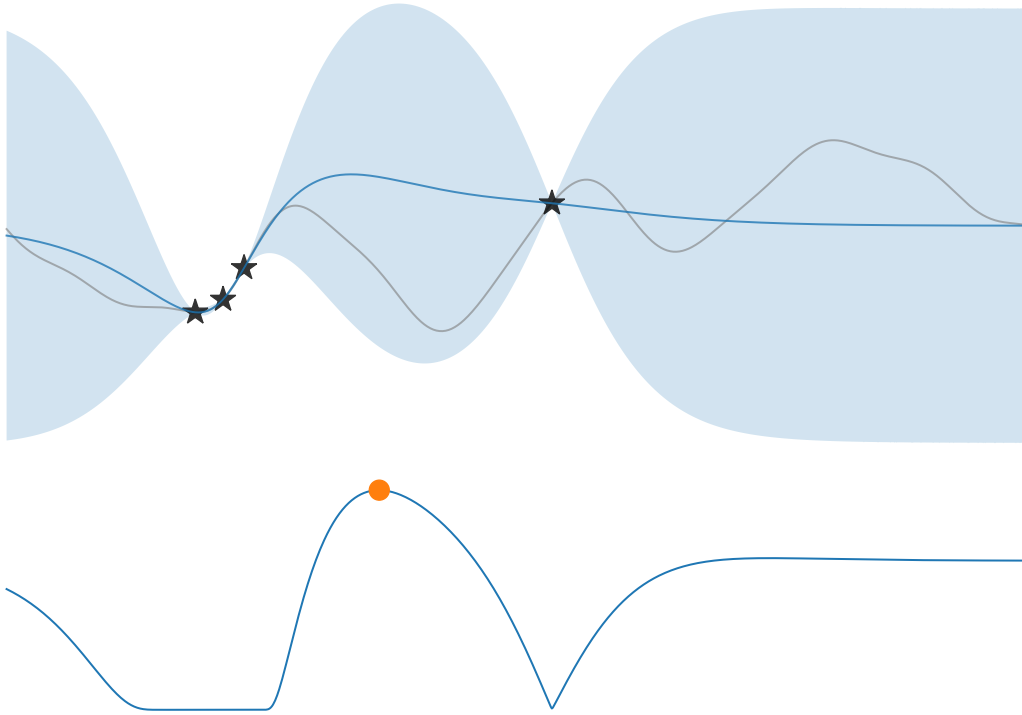


$$EI(x) = \mathbb{E}[\underbrace{\max(f(x) - y_{\text{best}}, 0)}_{\text{"improvement"}} \mid \underbrace{D}_{\text{data}}]$$

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

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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- Entropy-based:
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  - Predictive Entropy Search

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- Our work: Gittins Index

# Approaches to Bayesian Optimization

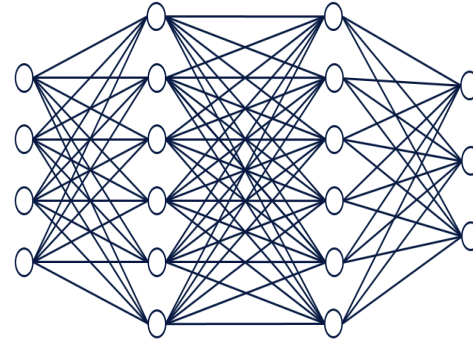
- Improvement-based
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- Our work: Gittins Index

Why another approach?

# Challenge: Varying Evaluation Costs

Hyperparameter tuning:

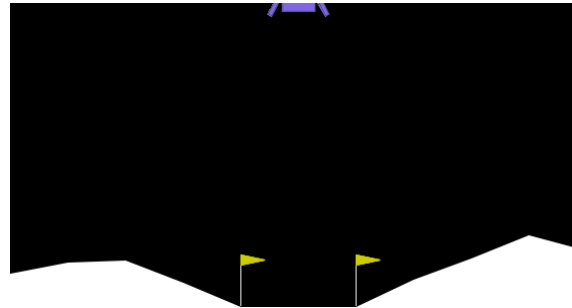
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→ Accuracy

Control optimization:

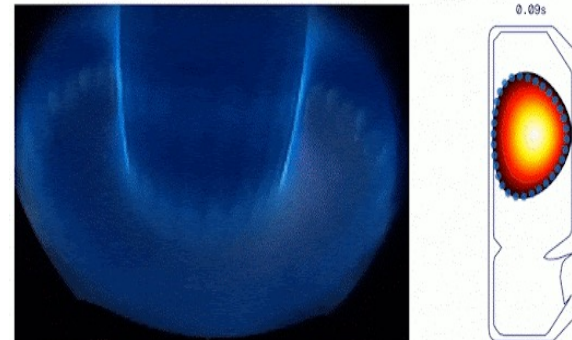
Control parameters →



→ Reward

Plasma physics:

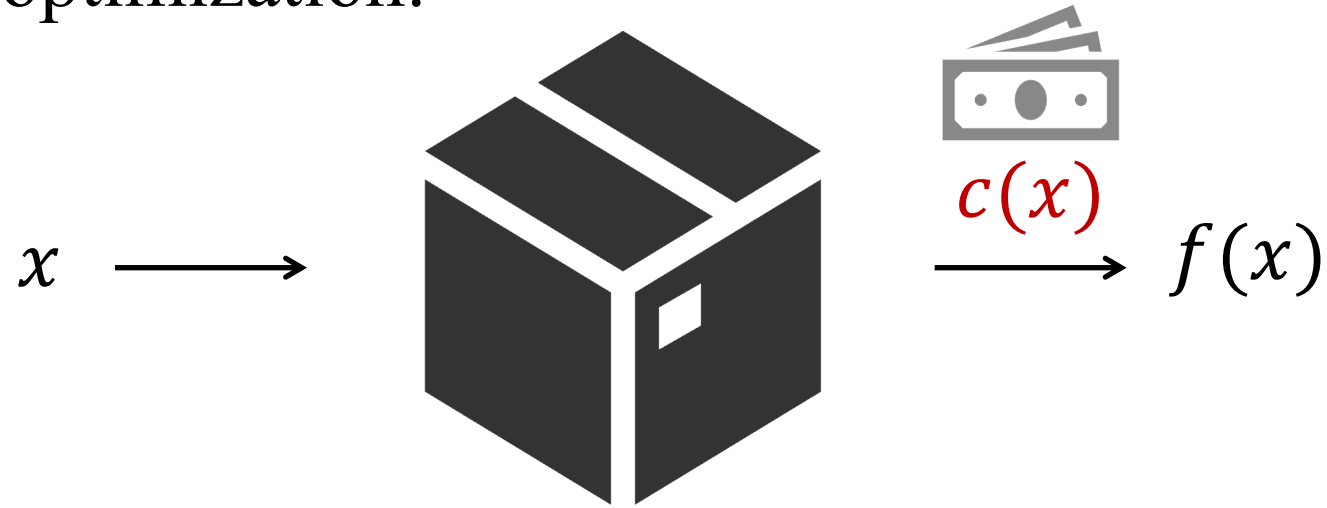
Reactor parameters →



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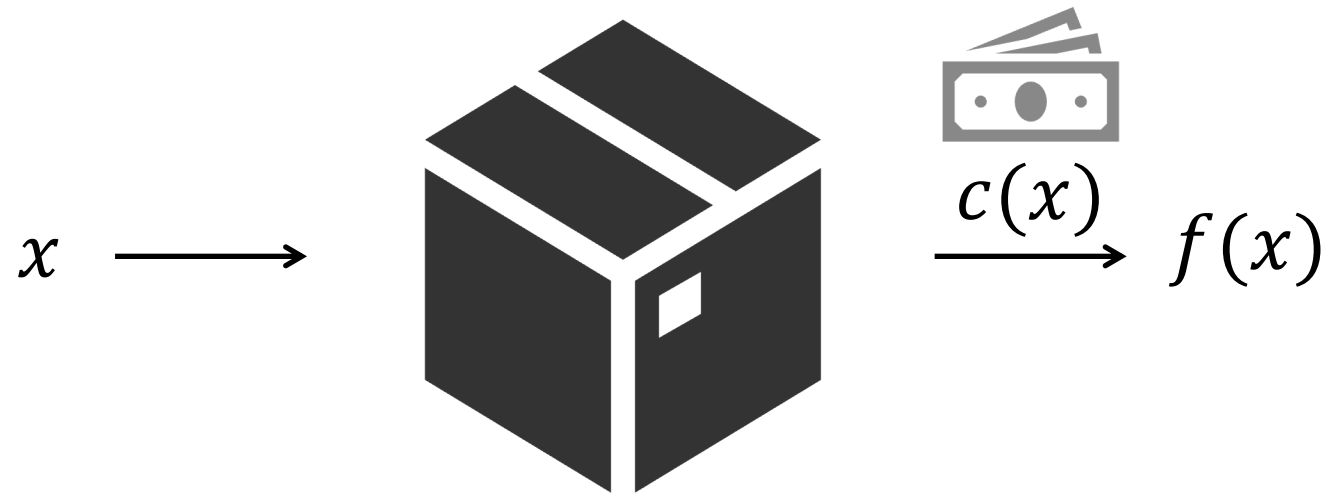
# Challenge: Varying Evaluation Costs

Black-box optimization:



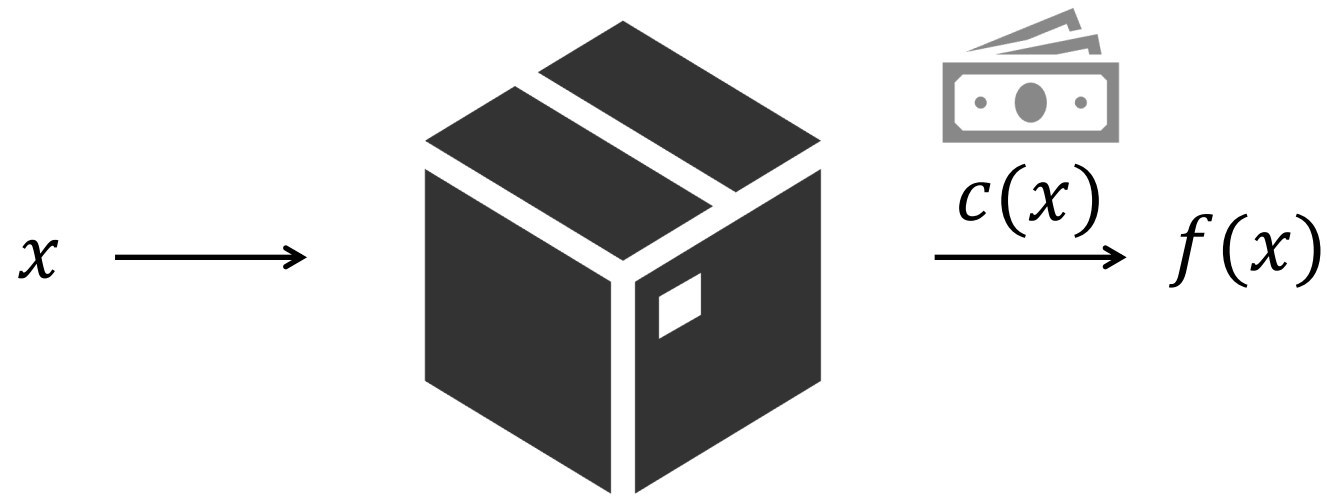


# Challenge: Varying Evaluation Costs



$$\begin{aligned} \text{Goal: } & \mathbf{\max} \mathbb{E} \max_{t=1,2,\dots,T} f(x_t) \\ \text{s.t. } & \mathbb{E} \sum_{t=1}^T c(x_t) \leq B \end{aligned}$$

# Cost-aware Bayesian Optimization



$$\text{Goal: } \mathbf{\max} \mathbb{E} \max_{t=1,2,\dots,T} f(x_t)$$
$$\text{s.t. } \mathbb{E} \sum_{t=1}^T c(x_t) \leq B$$

[Lee, Perrone, Archambeau, Seeger'21]

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

# Cost-aware Bayesian Optimization

Uniform costs

Varying costs

Expected improvement

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

# Cost-aware Bayesian Optimization

Uniform costs

Expected improvement

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

Varying costs

Expected improvement per cost

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

# Cost-aware Bayesian Optimization

Uniform costs

Expected improvement

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Varying costs

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

Why divide?

# Cost-aware Bayesian Optimization

Uniform costs

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

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

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

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

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

# Cost-aware Bayesian Optimization

Uniform costs

Expected improvement

Multi-step Lookahead EI

Varying costs

Expected improvement per cost

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

Expected improvement

Multi-step Lookahead EI

Upper Confidence Bound

Thompson Sampling

⋮

Varying costs

Expected improvement per cost

Budgeted Multi-step Lookahead EI

?

?

⋮

New design principle: Gittins Index

# Cost-aware Bayesian Optimization

Uniform costs

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Multi-step Lookahead EI

Upper Confidence Bound

Thompson Sampling

⋮

Varying costs

Expected improvement per cost

Budgeted Multi-step Lookahead EI

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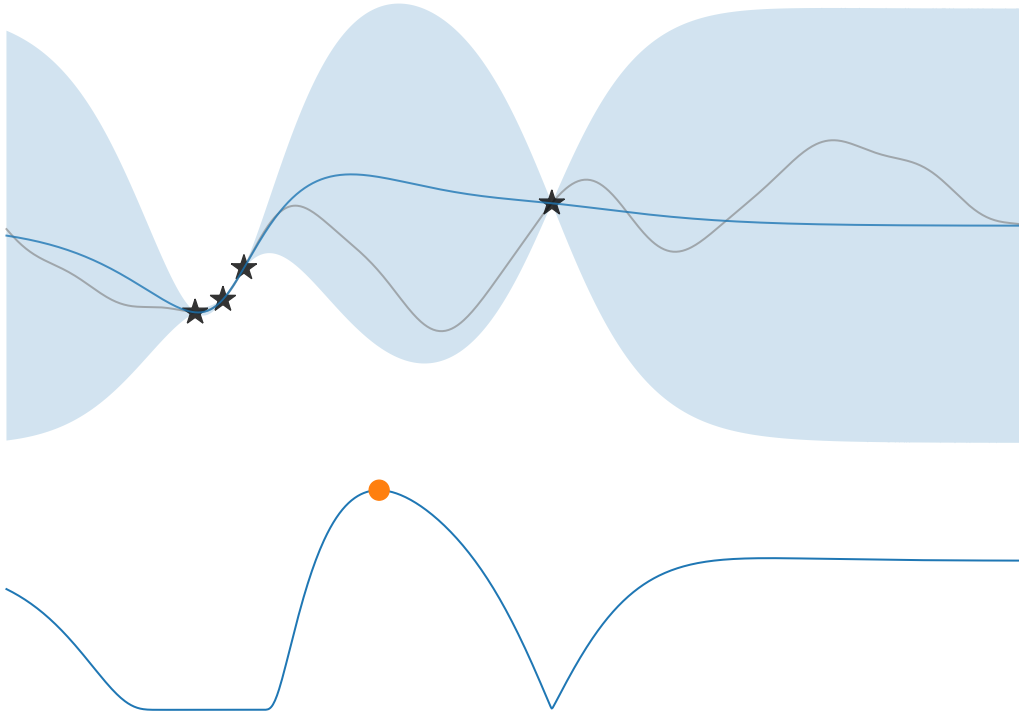
?

⋮

New design principle: Gittins Index

naturally cost-aware

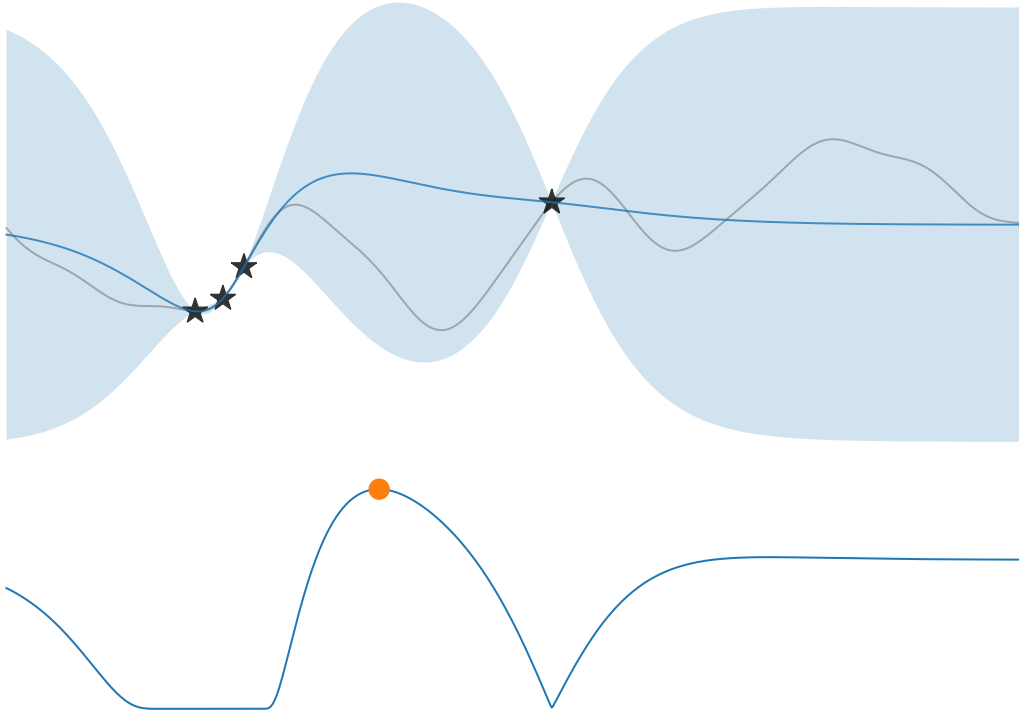
# Expected Improvement



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

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

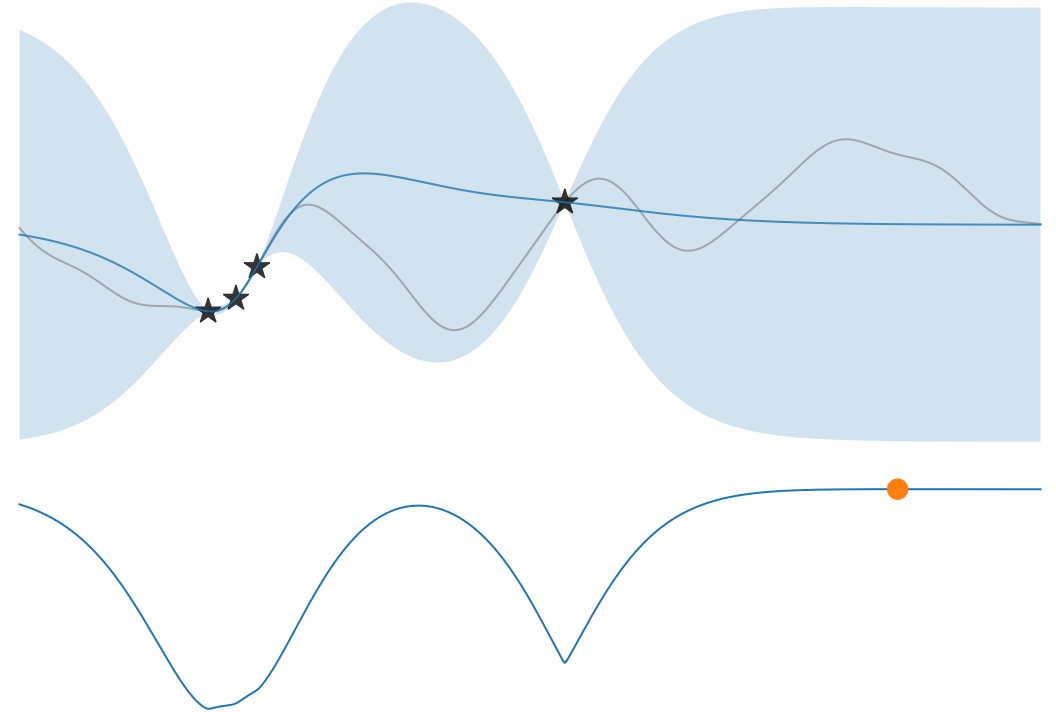
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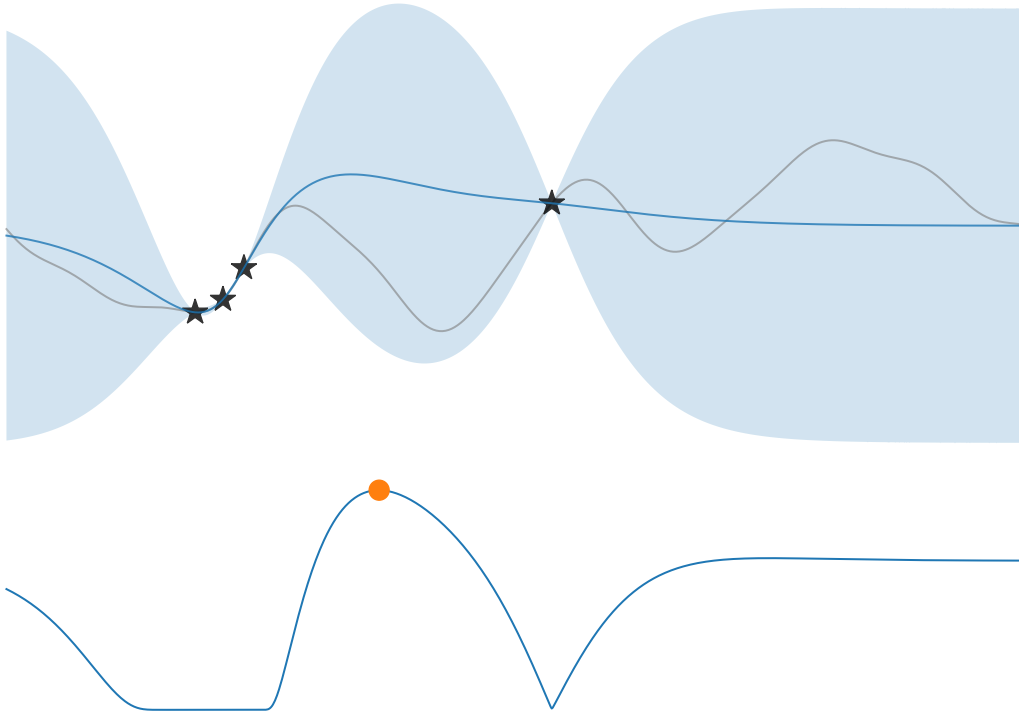
## Gittins Index



$$GI_{f|D}(x) = g \text{ s.t. } EI_{f|D}(x; g) = c(x)$$

$$\max_x GI_{f|D}(x)$$

## Expected Improvement

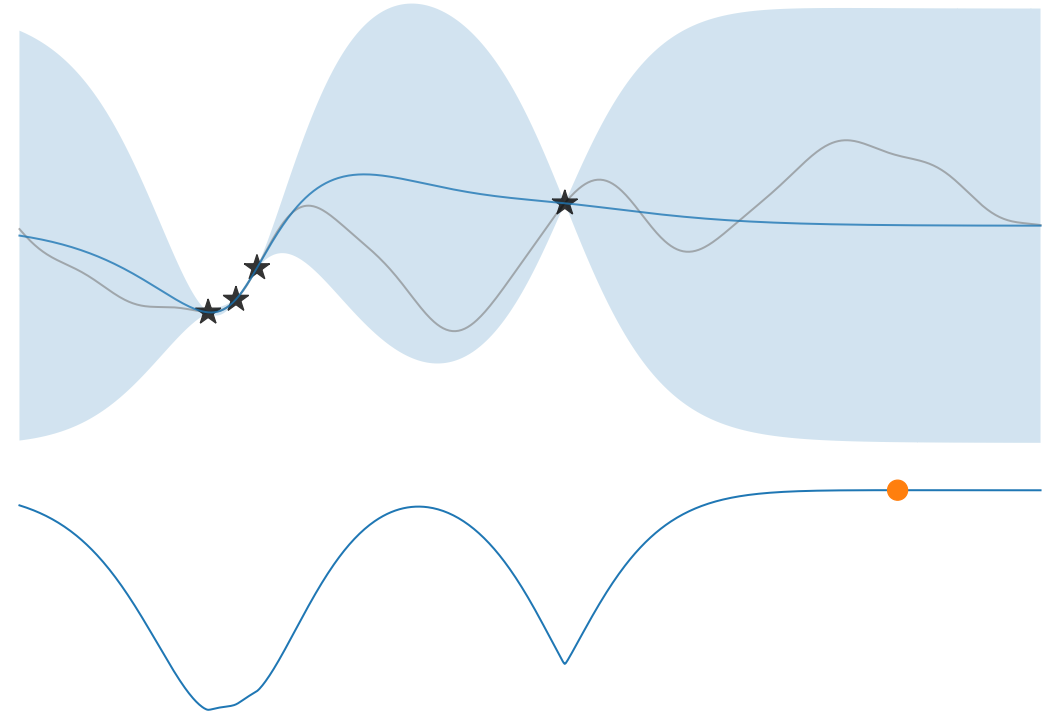


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One-step approximation to MDP

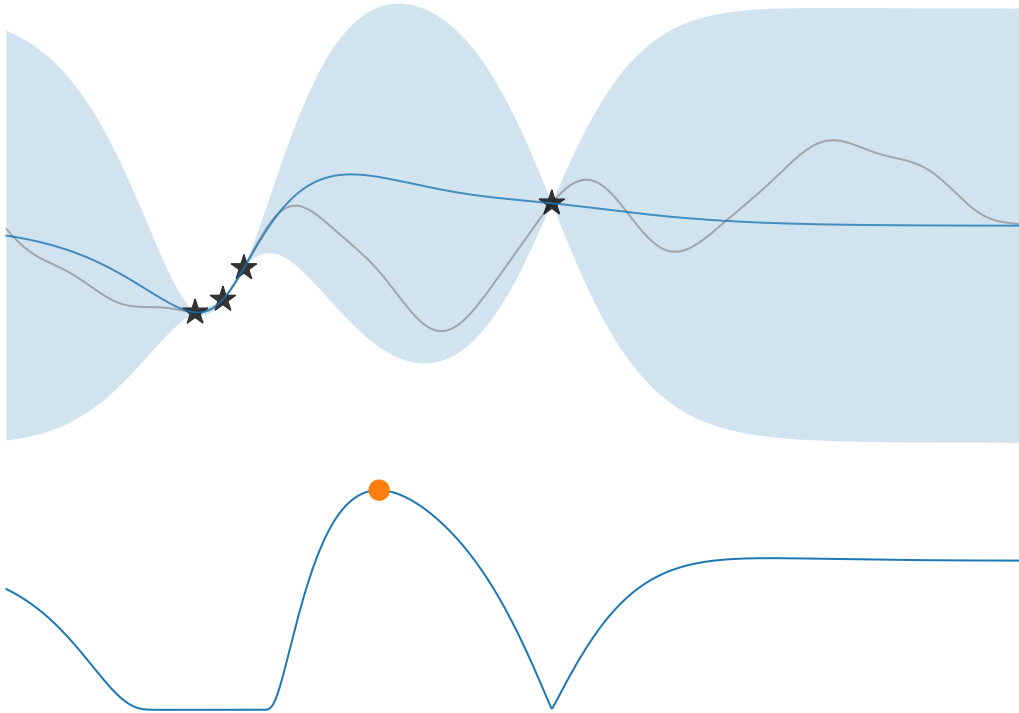
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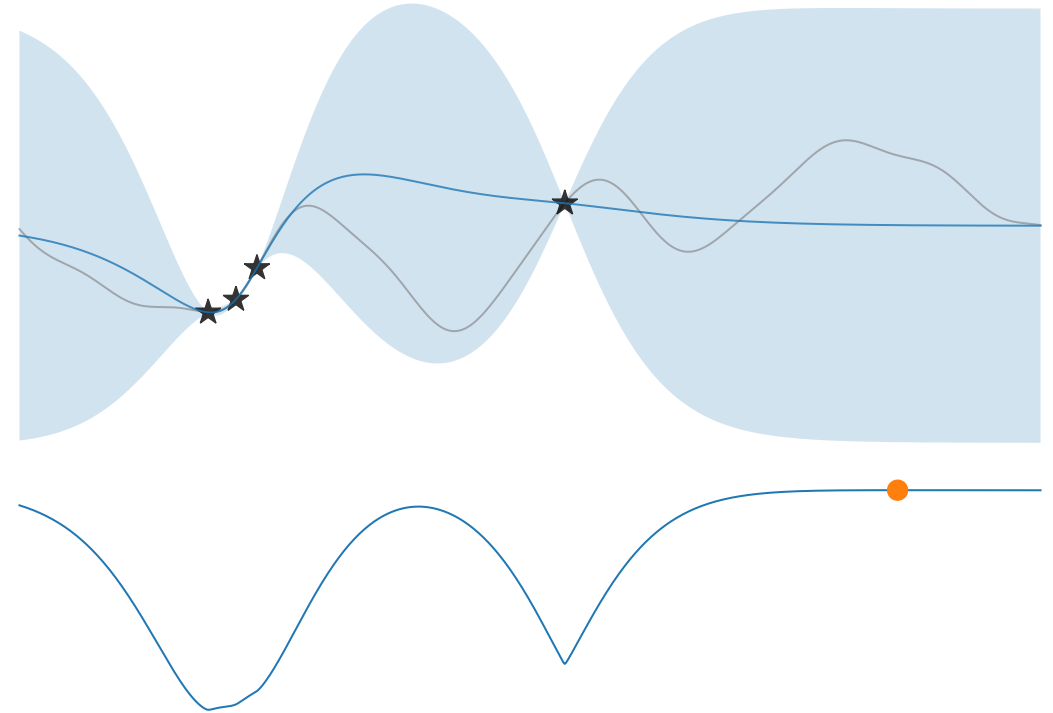


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**Temporal** simplification to MDP

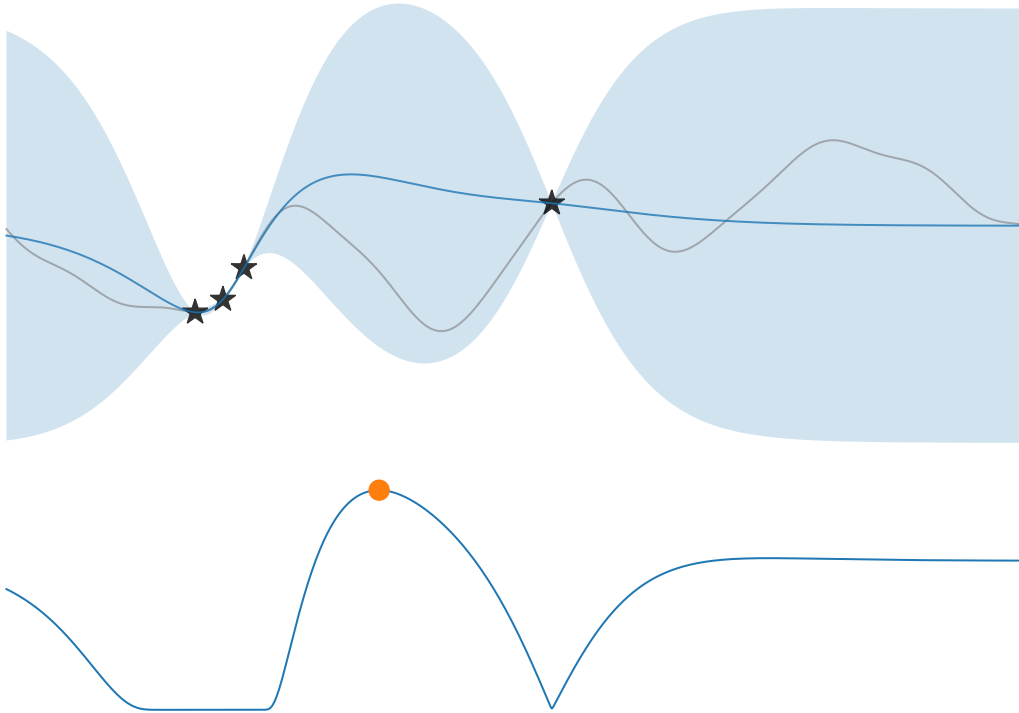
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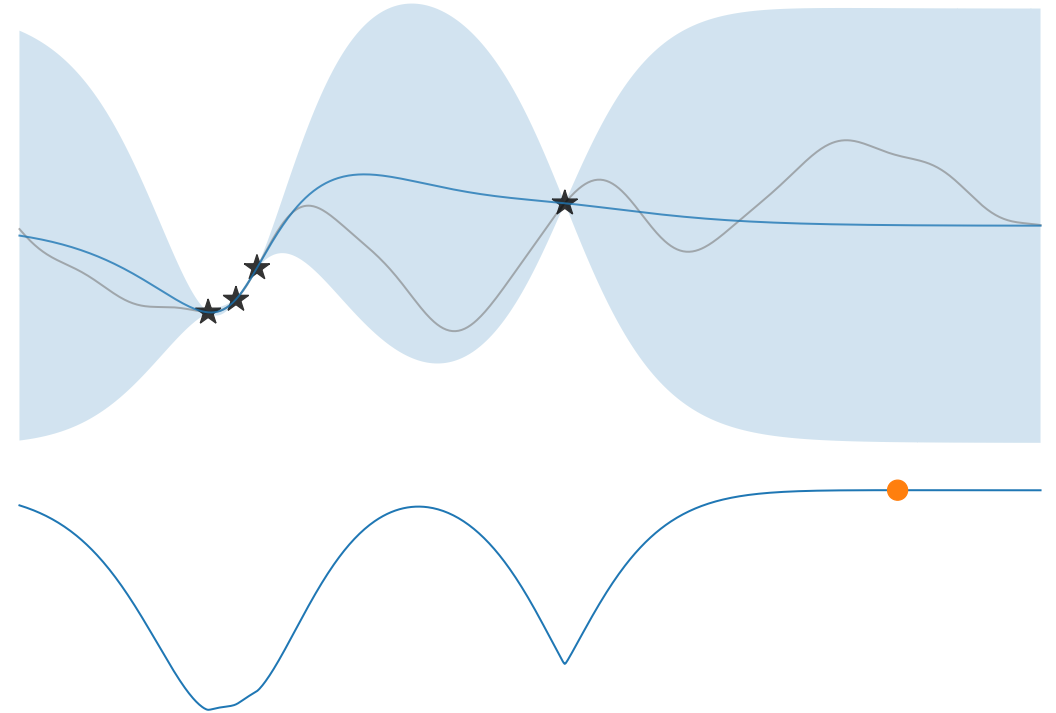


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Temporal simplification to MDP

## Gittins Index



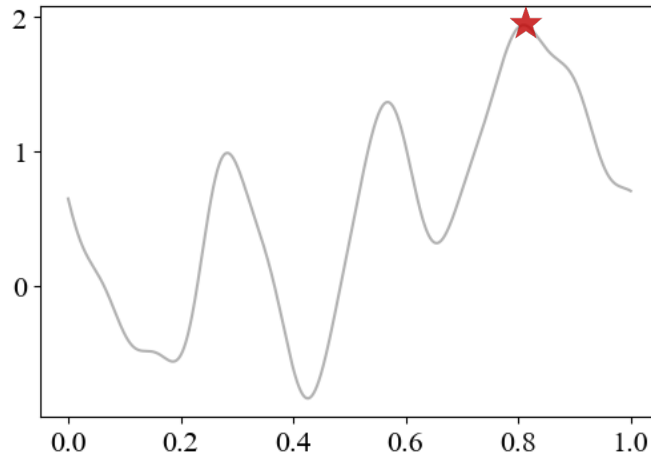
$$\text{GI}_{f|D}(x) = g \text{ s.t. } \text{EI}_{f|D}(x; g) = c(x)$$

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

**Spatial** simplification to MDP



# Our Approach: Spatial Simplification

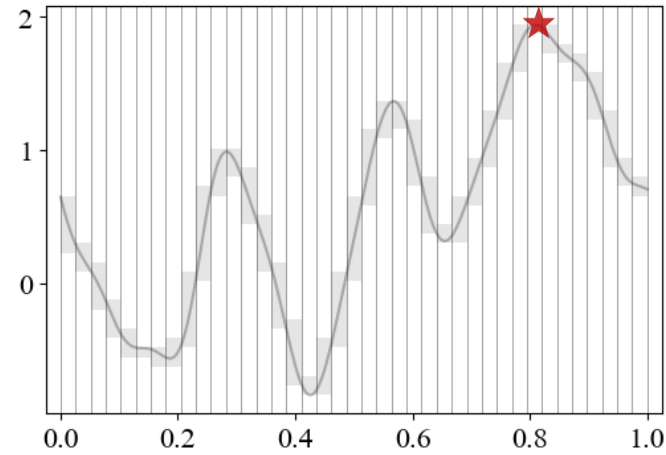
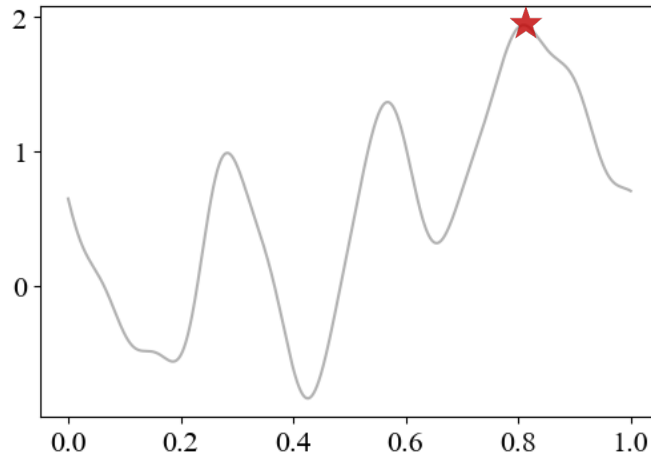


Bayesian Optimization

Continuous

Correlated

# Our Approach: Spatial Simplification



Bayesian Optimization

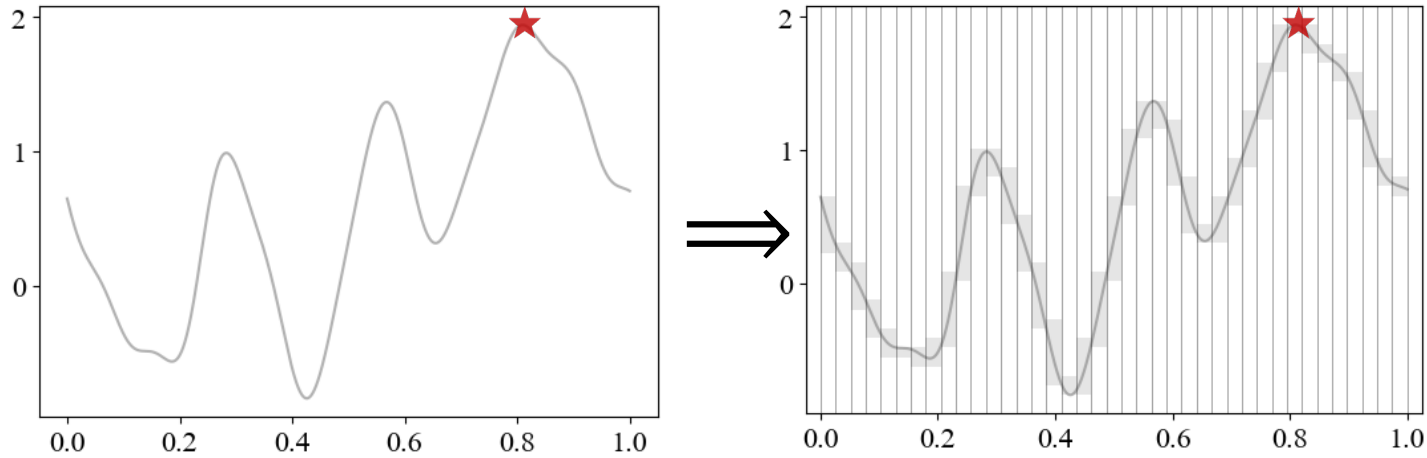
Continuous



Discrete

Correlated

# Our Approach: Spatial Simplification



Bayesian Optimization

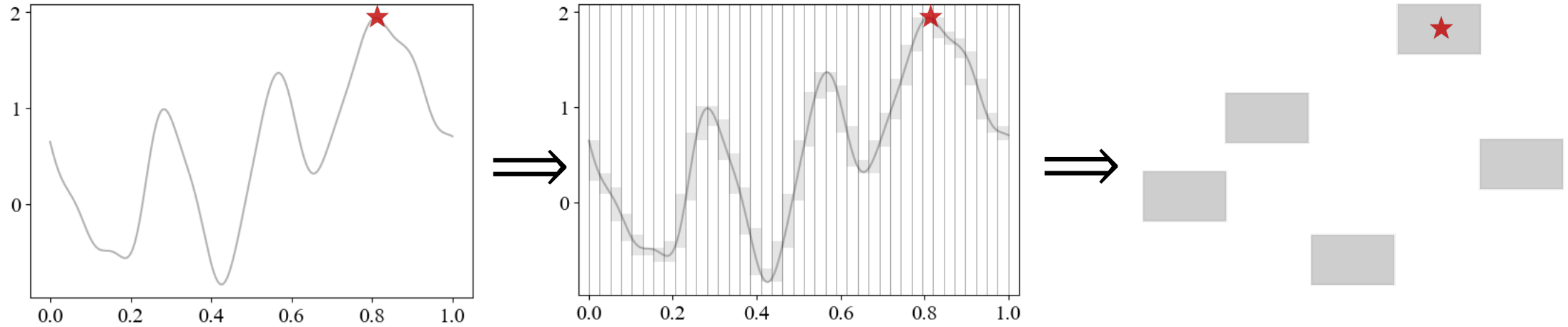
Continuous

$\Rightarrow$

Discrete

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# Our Approach: Spatial Simplification



## Bayesian Optimization

Continuous

$\Rightarrow$

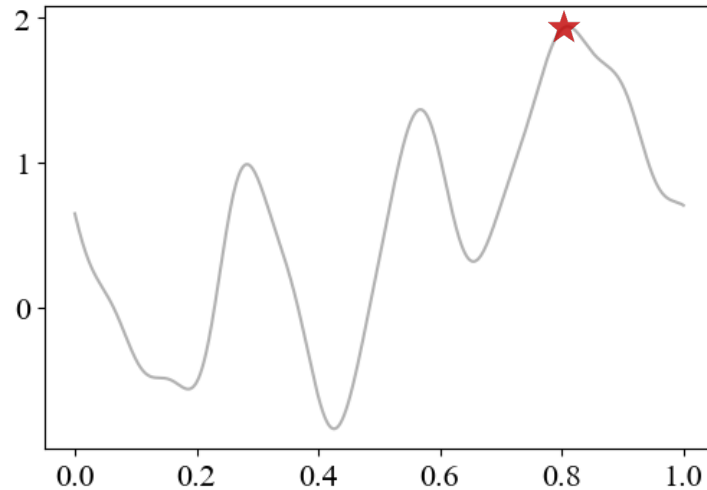
Discrete

Correlated

$\Rightarrow$

Independent

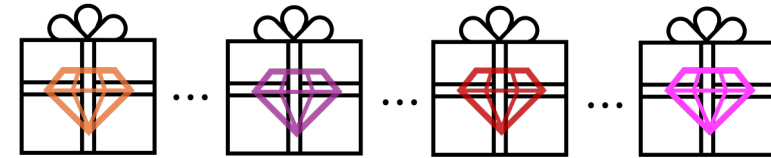
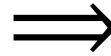
# Our Approach: Spatial Simplification



Bayesian Optimization

Continuous

Correlated



Pandora's Box [Weitzman'79]

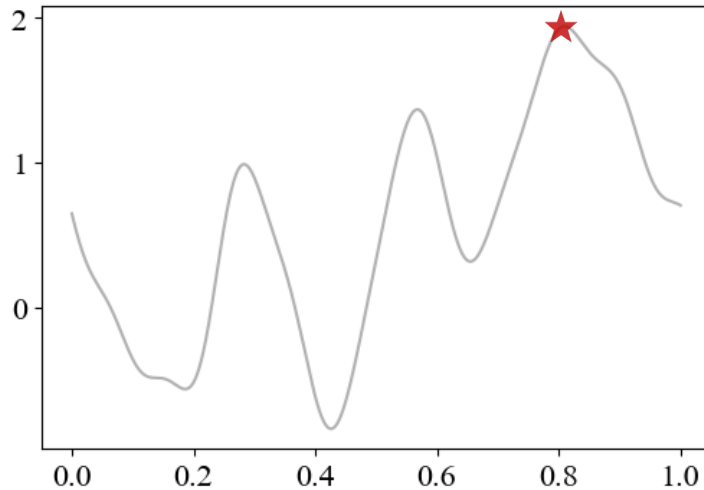


Discrete



Independent

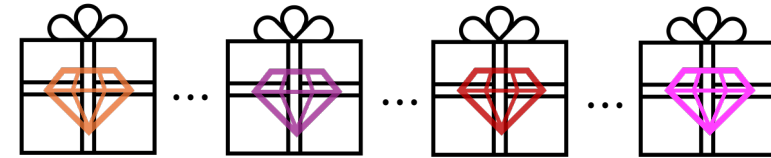
# Our Approach: Spatial Simplification



Bayesian Optimization

Continuous

Correlated



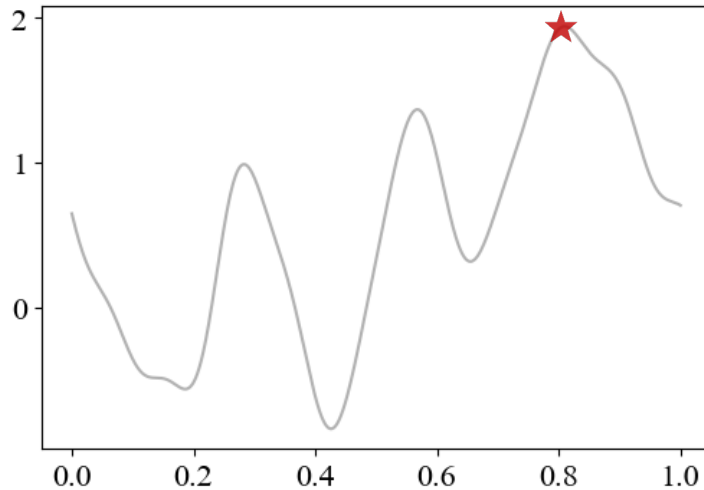
Pandora's Box [Weitzman'79]

Discrete

Independent

Optimal policy: Gittins index

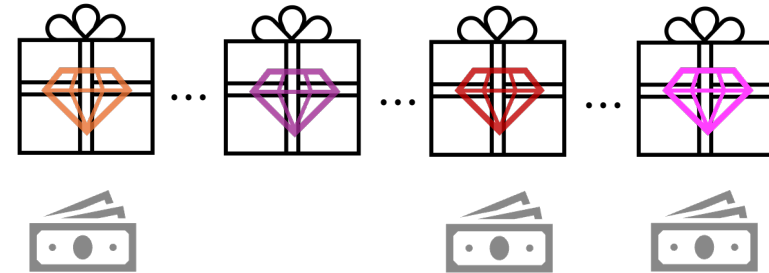
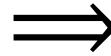
# Our Approach: Spatial Simplification



Bayesian Optimization

Continuous

Correlated



Pandora's Box

Discrete

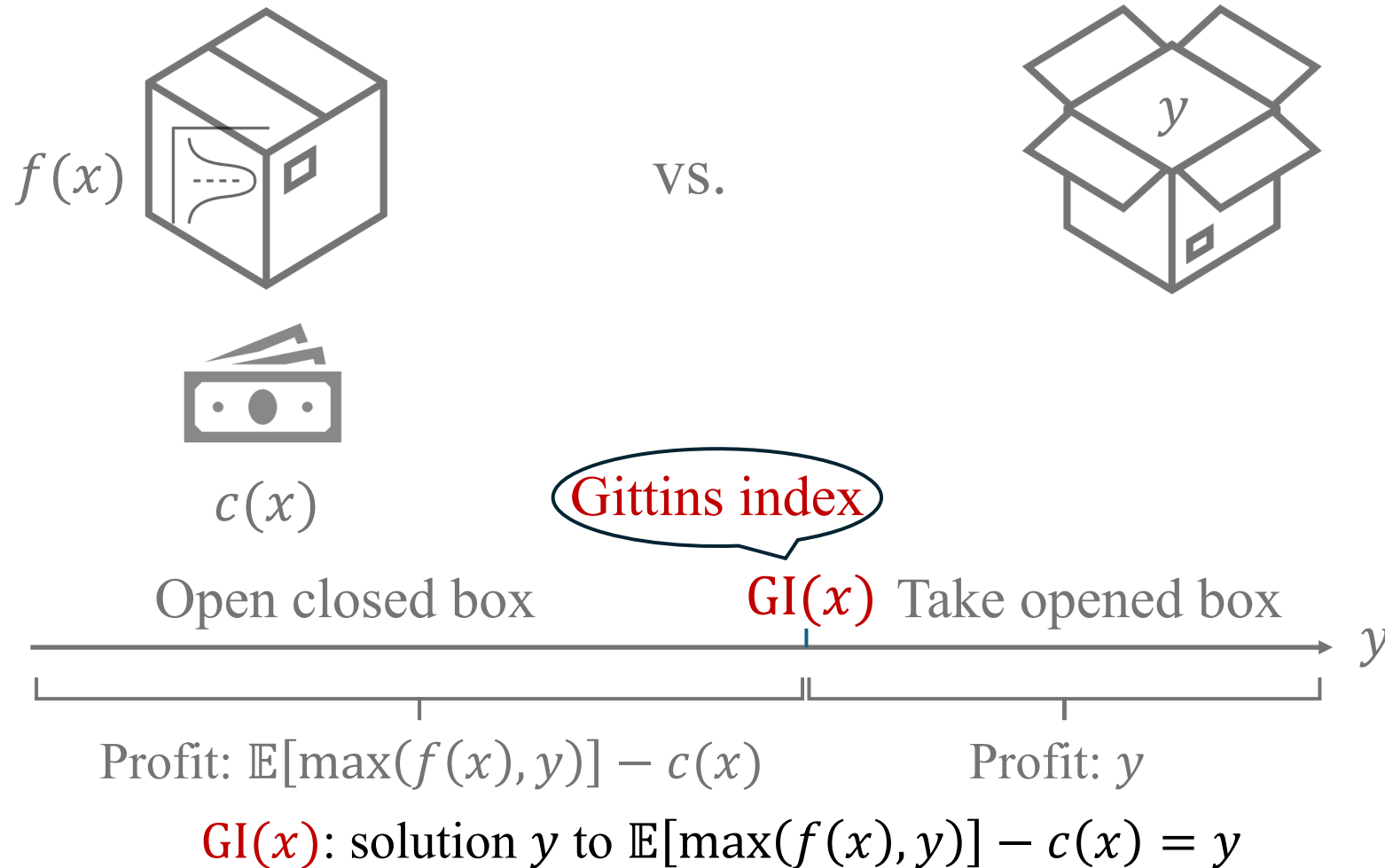
Independent

allow varying costs

Optimal policy: Gittins index

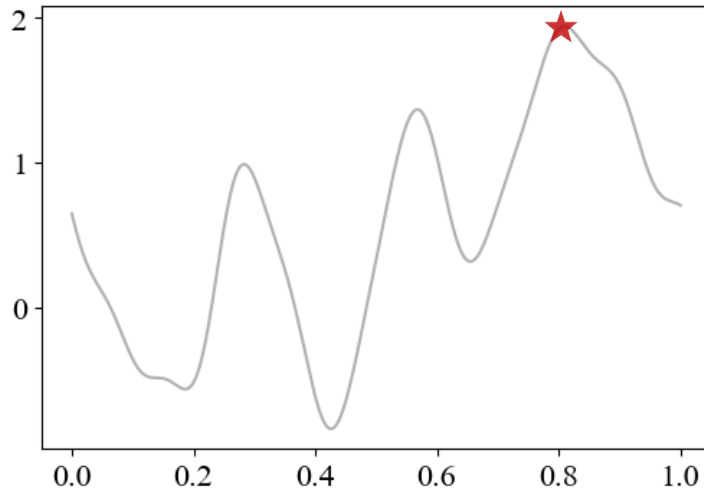
# Intuition Behind Pandora's Box Gittins Index

1.5-box problem:

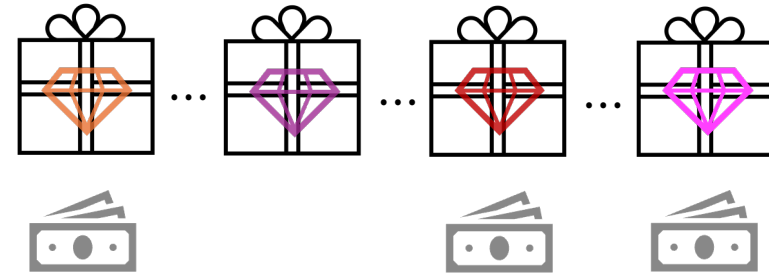




# How to translate Gittins index?



Bayesian Optimization



Pandora's Box

Continuous



Discrete

Correlated

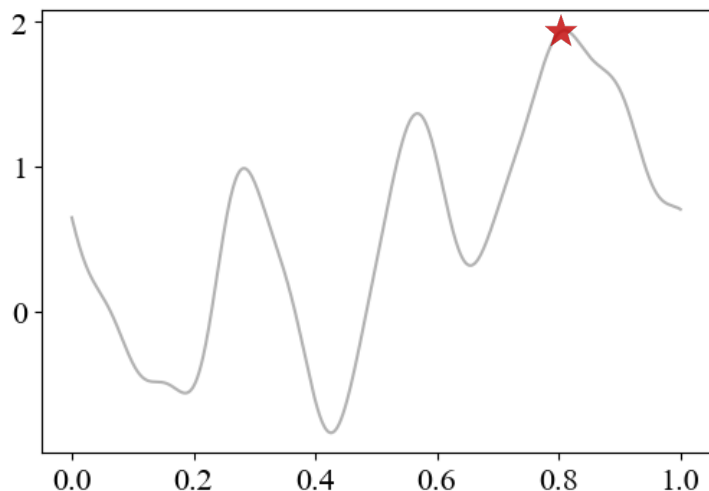


Independent

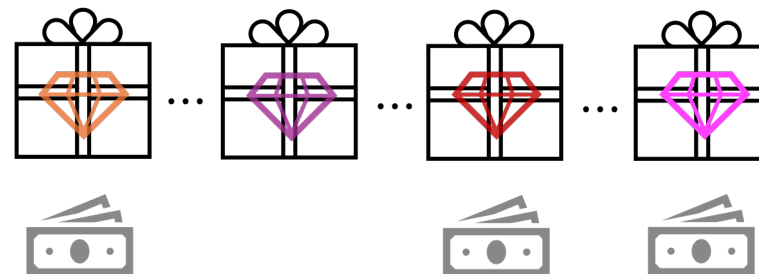
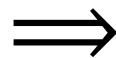
How to translate?

⇐ Optimal policy: Gittins index

# How to translate Gittins index?



Bayesian Optimization



Pandora's Box

Continuous



Discrete

Correlated



Independent

incorporate posterior

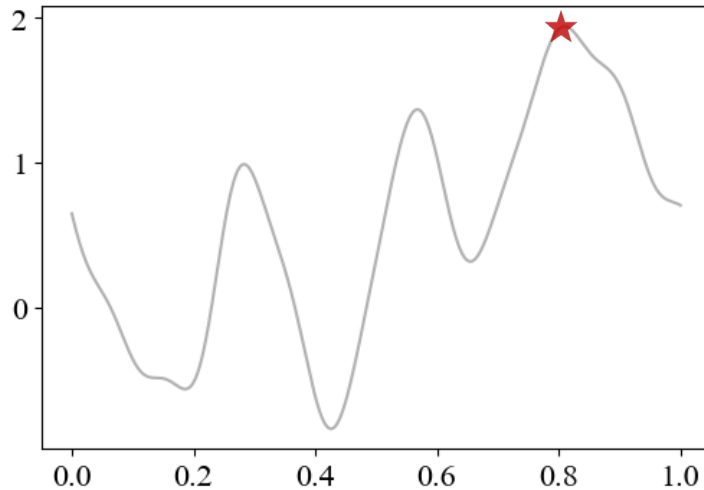
**Our policy**

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

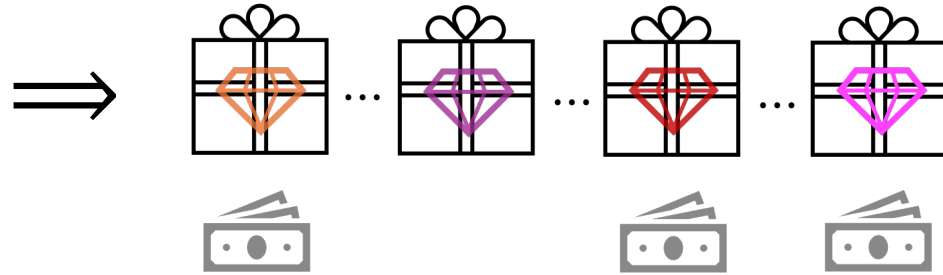
Optimal policy: Gittins index

$$\max_x \text{GI}(x)$$

# Is Gittins good in Bayesian Optimization?



Bayesian Optimization



Pandora's Box [Weitzman'79]

Continuous



Discrete

Correlated



Independent

incorporate posterior

Is Gittins index good?



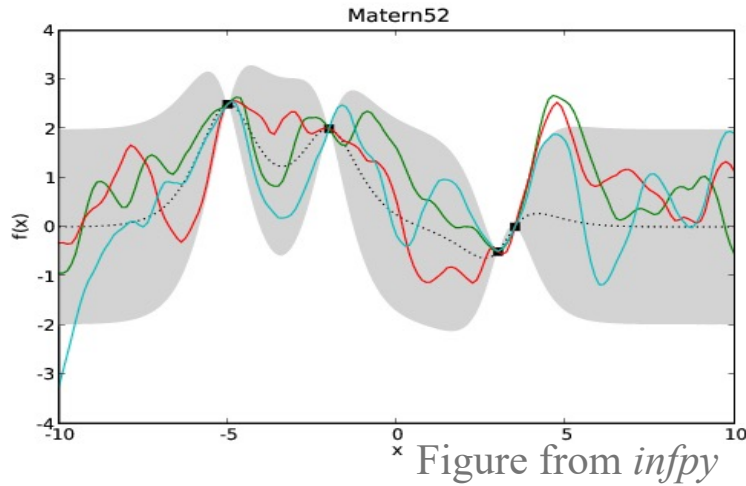
Gittins index is optimal

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

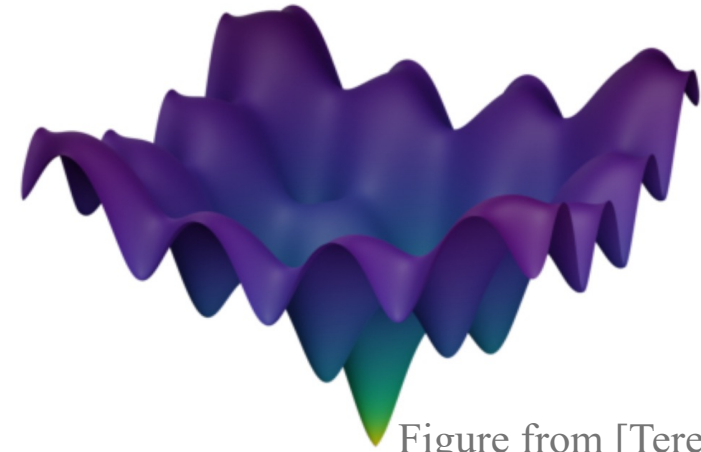
$$\max_x \text{GI}(x)$$

# Experiment Setup: Objective Functions

Samples from prior



Ackley function



Pest Control



Lunar Lander

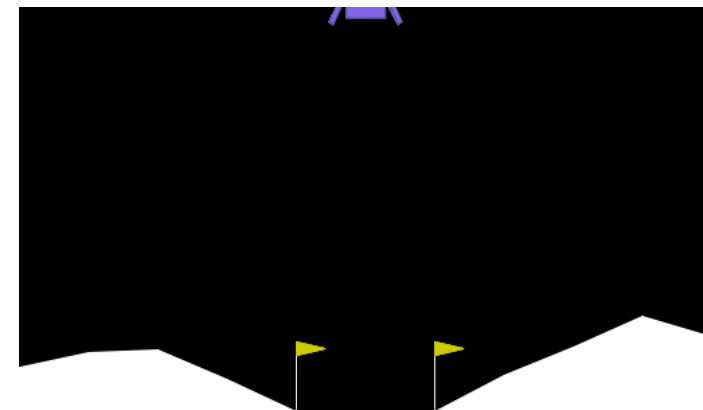
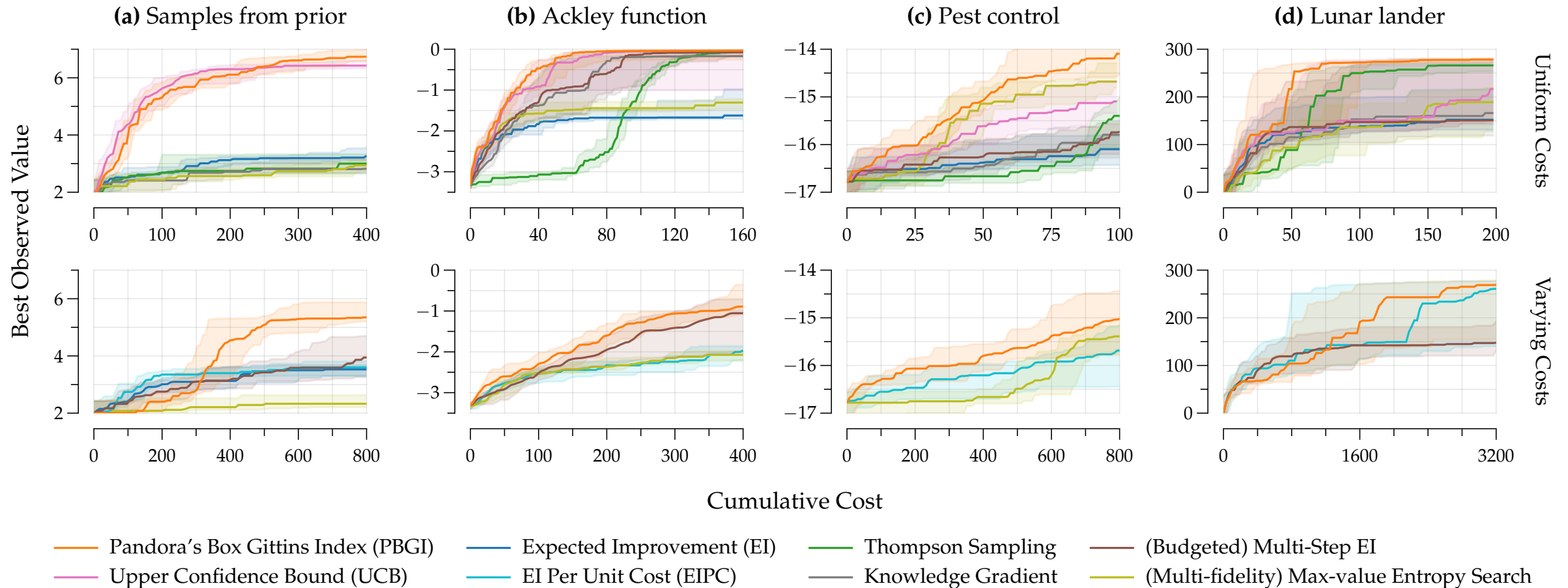


Figure from OpenAI Gym

# Experiment Results

Synthetic

Empirical



# 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?

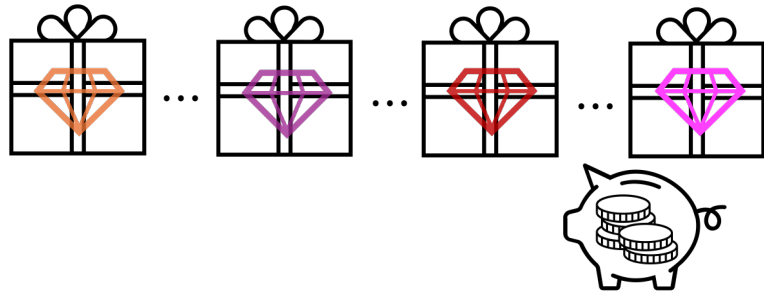
Yes, EI + bisection

- Any theoretical results?

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

# Theoretical Result

**max** best observed under budget

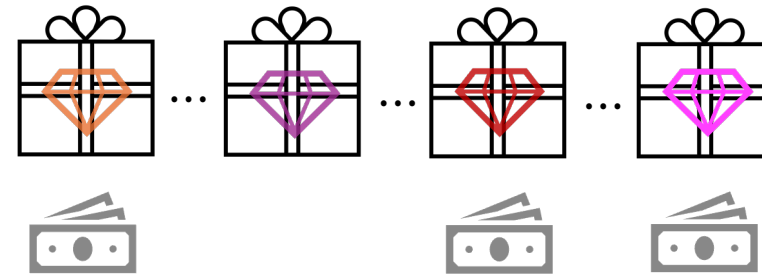


Budgeted Pandora's Box

Expected budget constraint

Optimal policy?

**max** (best observed – costs)



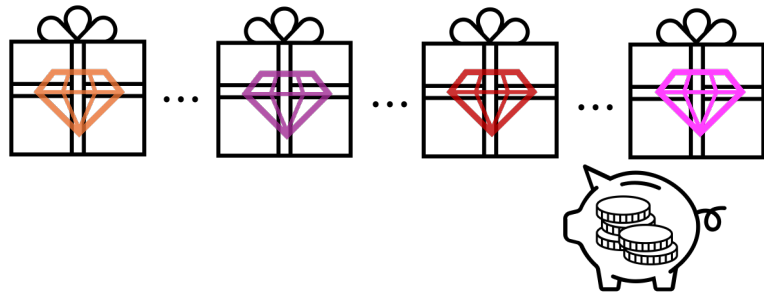
Pandora's Box

Cost per sample

Optimal policy: Gittins index

# Theoretical Result

**max** best observed under budget



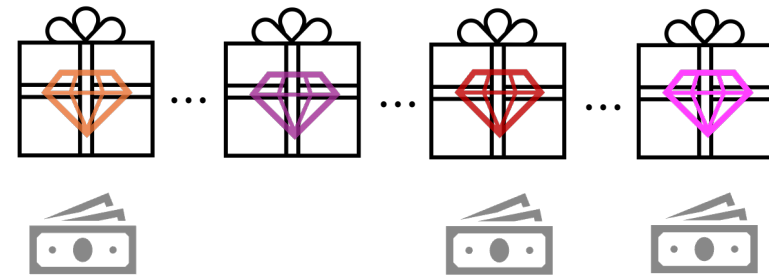
Budgeted Pandora's Box

Expected budget constraint

Optimal policy ✓

extension to [Aminian,  
Manshadi, Niazadeh'24]

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



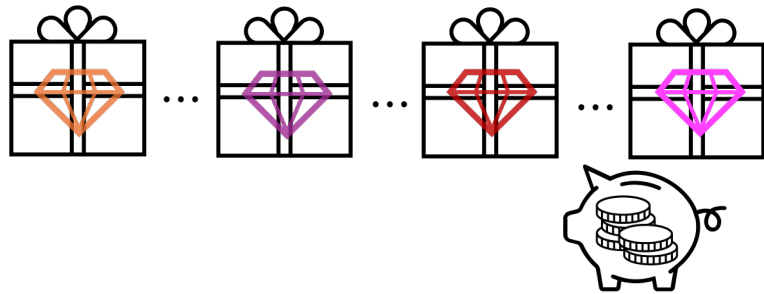
Pandora's Box

Cost per sample

Optimal policy: Gittins index

# Theoretical Result

**max** best observed under budget



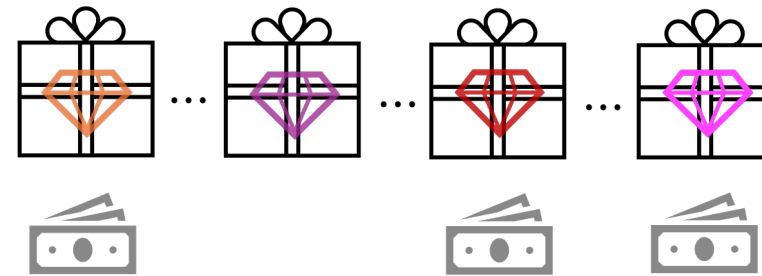
Budgeted Pandora's Box

Expected budget constraint

Optimal policy ✓

extension to [Aminian,  
Manshadi, Niazadeh'24]

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



Pandora's Box

Cost per sample

Optimal policy: Gittins index

budget-dependent

# 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?

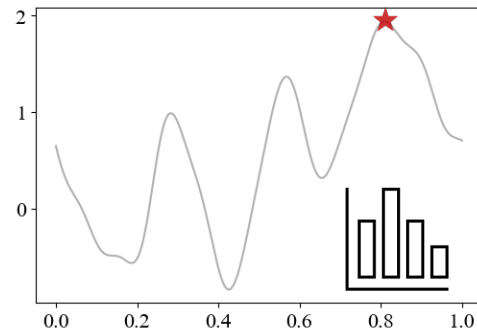
Yes, expected-budget-constrained  $\cong$  cost-per-sample

- Tuning parameters?

Yes, control unit conversion

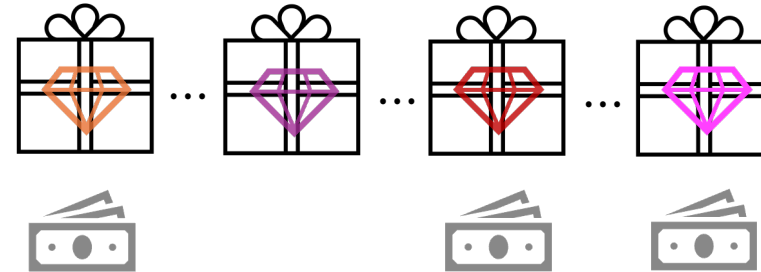
# New Design Principle: Gittins Index

## Problem



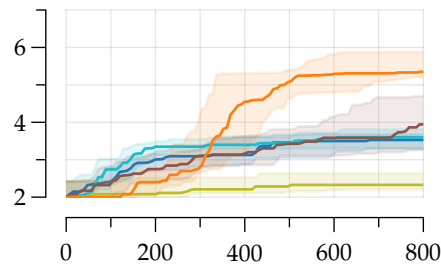
Bayesian optimization  
with varying costs

## Key idea



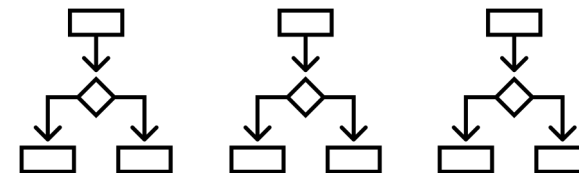
link to Pandora's box  
and Gittins index theory

## Impact



competitive performance

## Future potential



black-box processes  
with partial feedback