

NeurIPS'24 & INFORMS Data  
Mining Paper Competition Finalist

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

On arXiv soon!

Qian Xie 谢倩 (Cornell ORIE)

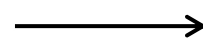
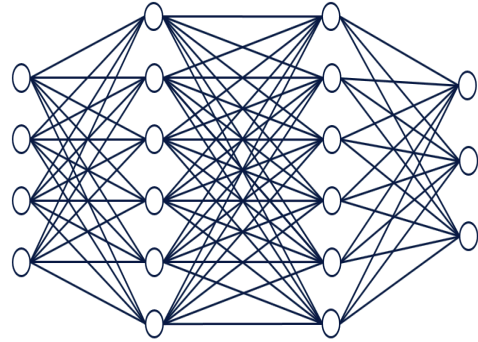
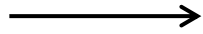
Joint work with Linda Cai (UC Berkeley), Theodore Brown (UCL), Raul Astudillo (MBZUAI), Peter Frazier, Alexander Terenin, and Ziv Scully (Cornell)

INFORMS Applied Probability Society Conference 2025

# World of Hyperparameter Optimization

Hyperparameter tuning:

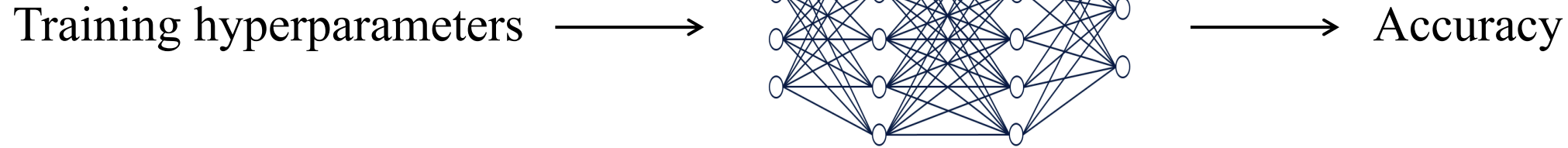
Training hyperparameters



Accuracy

# World of Hyperparameter Optimization

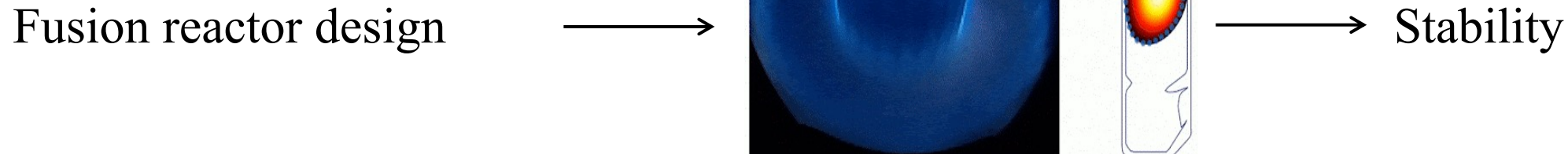
## Hyperparameter tuning:



## Control optimization:



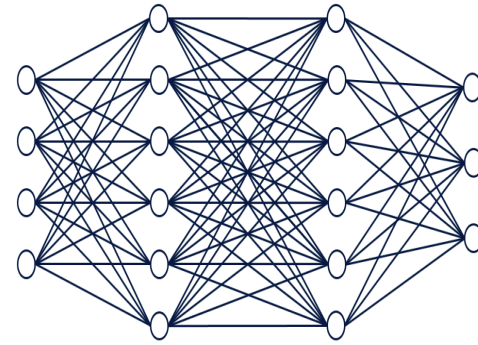
## Plasma physics:



# World of Hyperparameter Optimization

Hyperparameter tuning:

Training hyperparameters

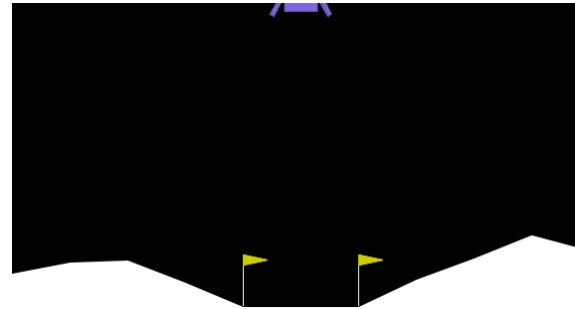


unknown &  
expensive-to-evaluate

Accuracy

Control optimization:

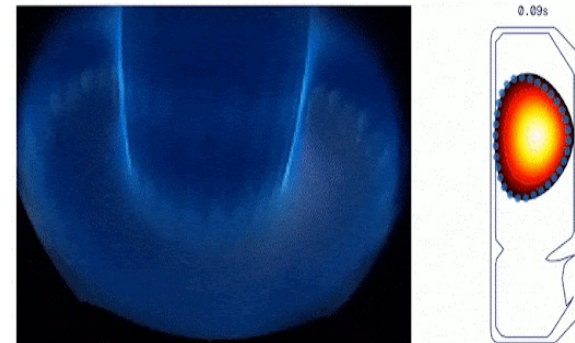
Control variables



Reward

Plasma physics:

Fusion reactor design



Stability

# Black-Box Optimization

Black-box optimization:

Input hyperparameters  $x$   $\longrightarrow$



$\longrightarrow$  Performance metric  $f(x)$

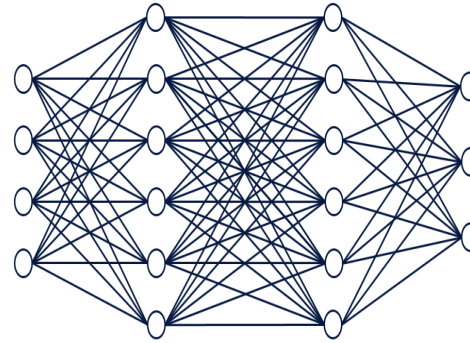
unknown &  
expensive-to-evaluate

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

# Naïve (Non-Adaptive) Approach: Grid Search

Hyperparameter tuning:

Training hyperparameters →



unknown &  
expensive-to-evaluate

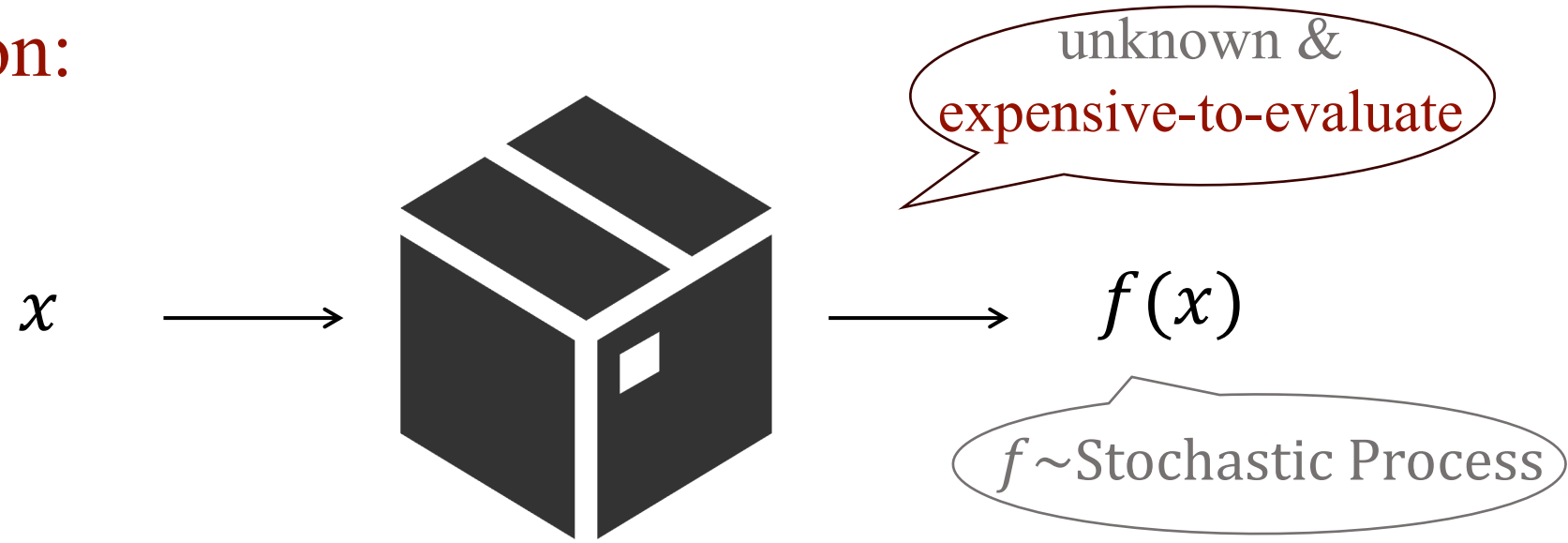
→ Accuracy

Training hyperparameter	Range	Number of Options
Batch size	[16, 512]	10
Learning rate	[1e-4, 1e-1]	10
Momentum	[0.1, 0.99]	10
Weight decay	[1e-5, 1e-1]	10
Number of layers	{1, 2, 3, 4}	4
Max units per layer	[64, 1024]	10
Dropout	[0.0, 1.0]	10

40,000,000  
combinations!

# Adaptive Approach: Bayesian Optimization

Black-box function:

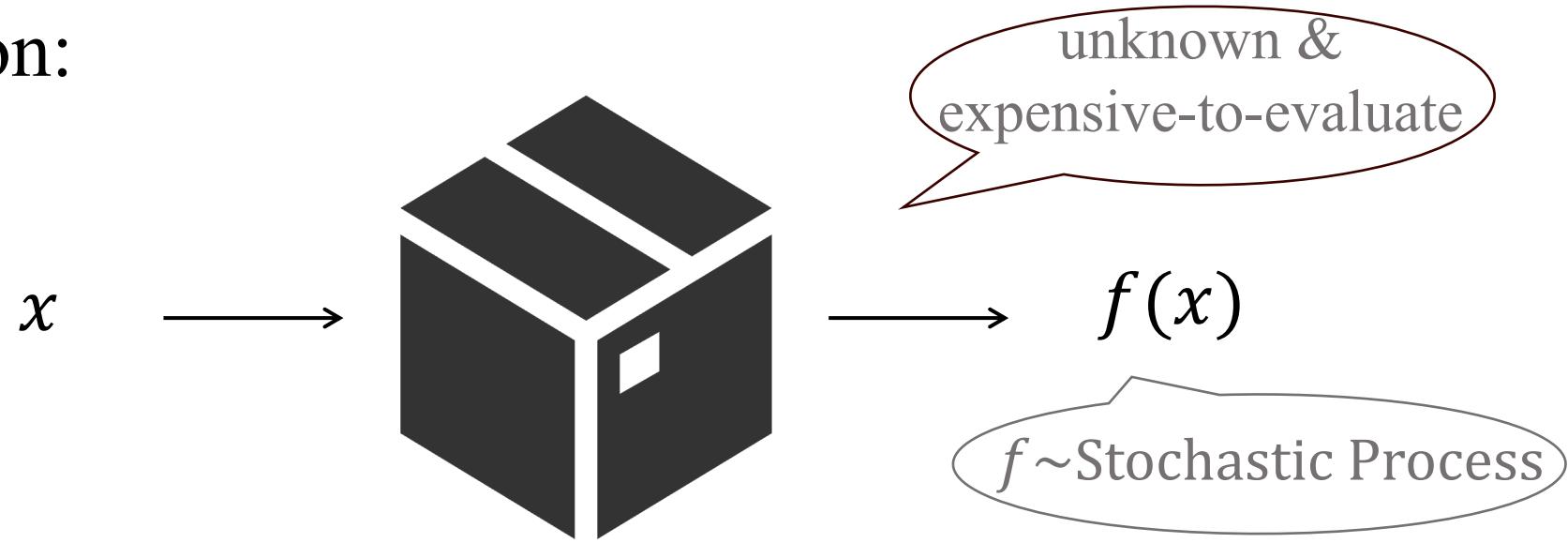


Goal:  $\sup_{\text{policy}} \mathbb{E} \max_{t=1,2,\dots,T} f(x_t)$

limited #evaluations

# Adaptive Approach: Bayesian Optimization

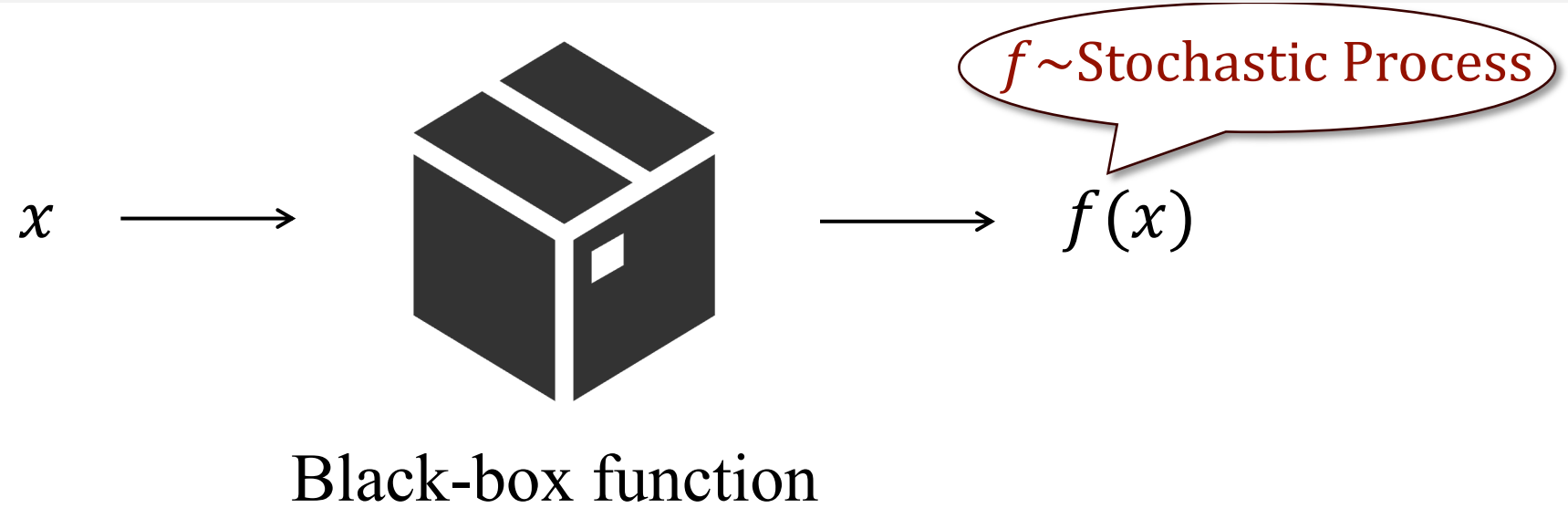
Black-box function:



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

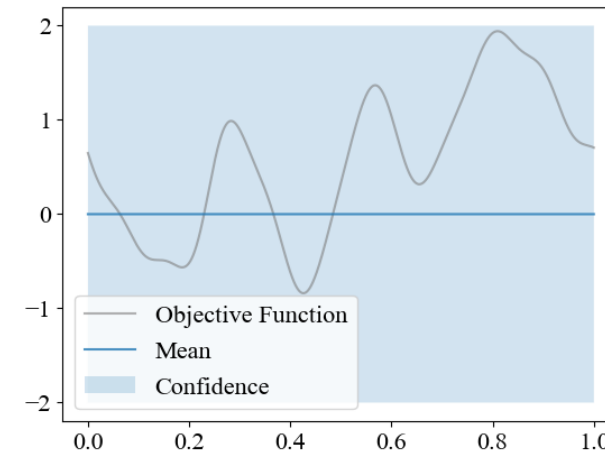
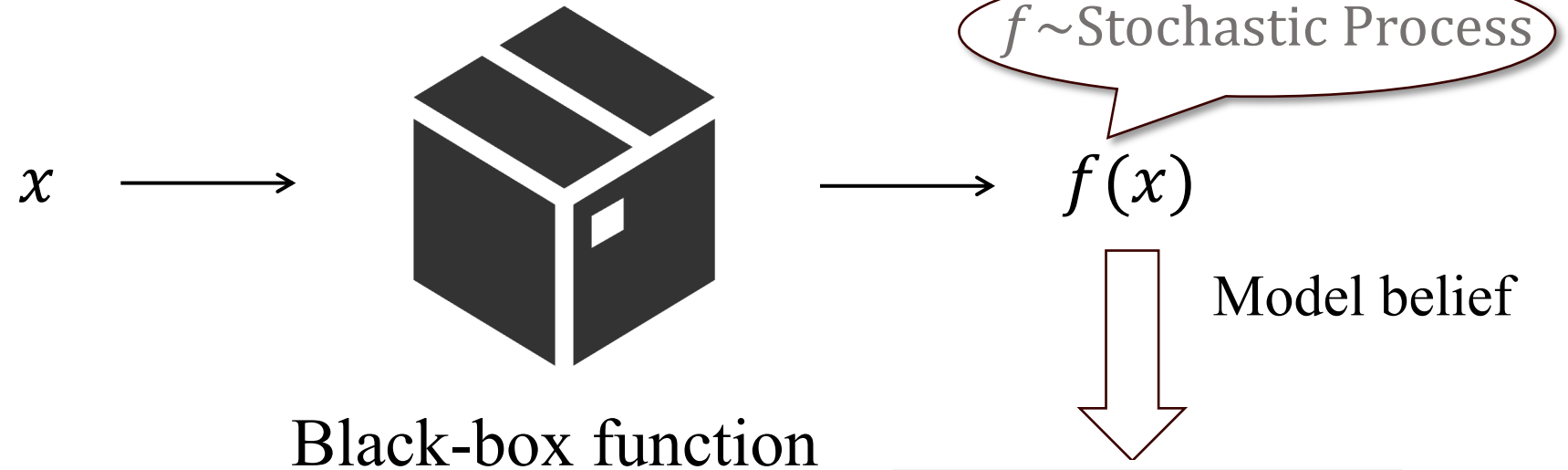
Key idea: maintain probabilistic belief about  $f$

# Bayesian Optimization



# Bayesian Optimization

Time 0



Probabilistic model  
(e.g., Gaussian process)

# Bayesian Optimization

Time  $t$

$x_1, \dots, x_t$



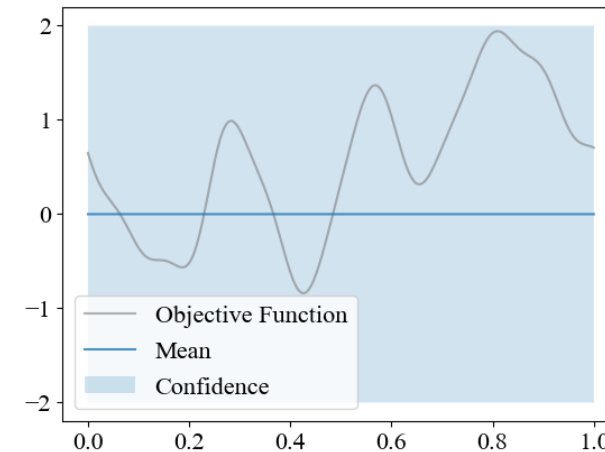
Black-box function



$f \sim \text{Stochastic Process}$

$f(x_1), \dots, f(x_t)$

Model belief

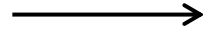


Probabilistic model  
(e.g., Gaussian process)

# Bayesian Optimization

Time  $t$

$x_1, \dots, x_t$



Black-box function

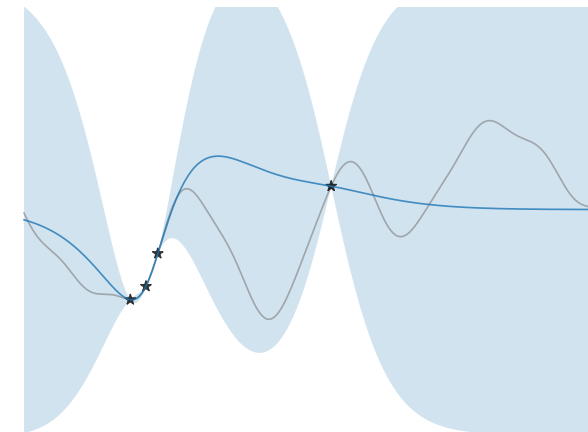


$f \sim \text{Stochastic Process}$

$f(x_1), \dots, f(x_t)$



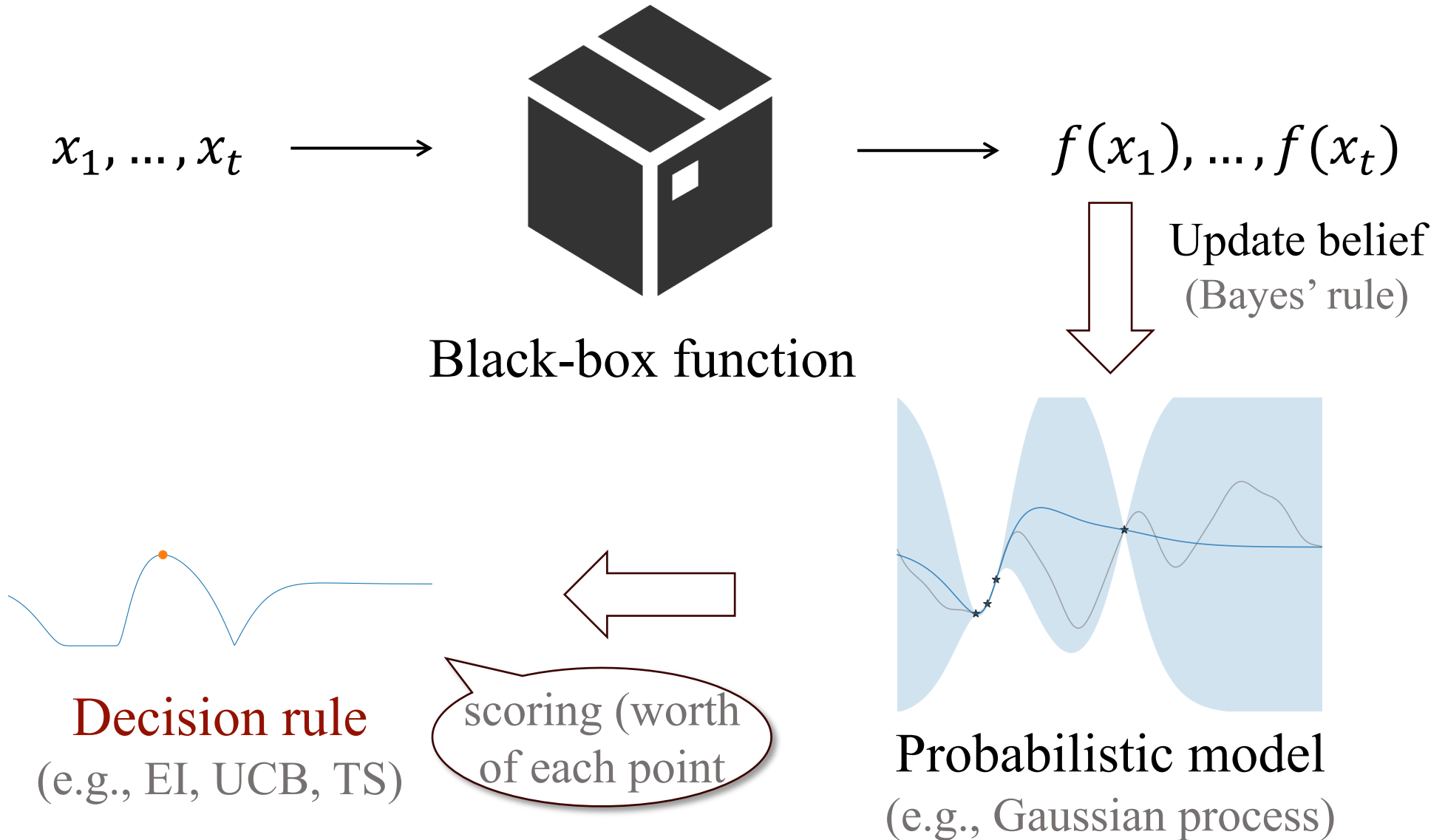
Update belief  
(Bayes' rule)



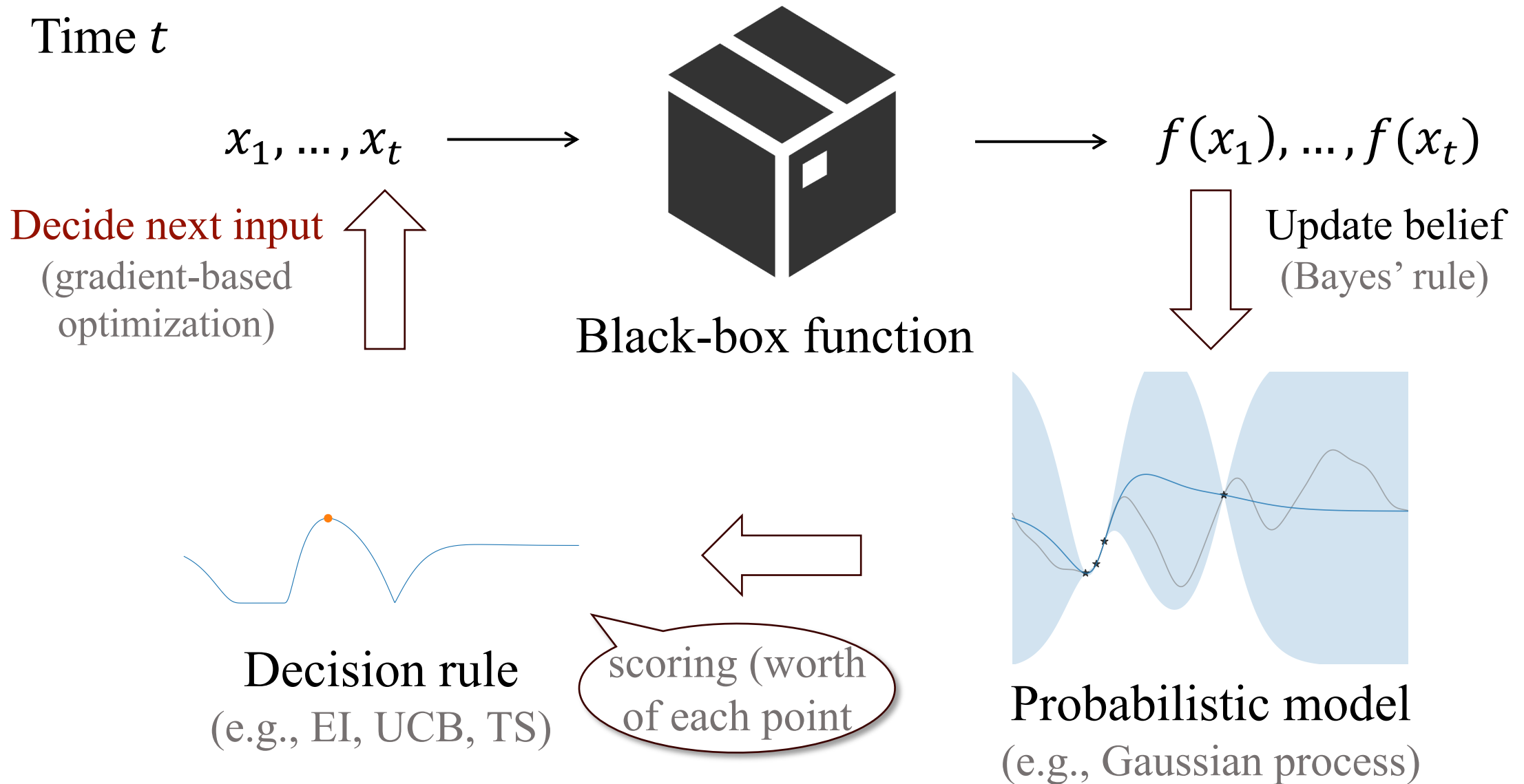
Probabilistic model  
(e.g., Gaussian process)

# Bayesian Optimization

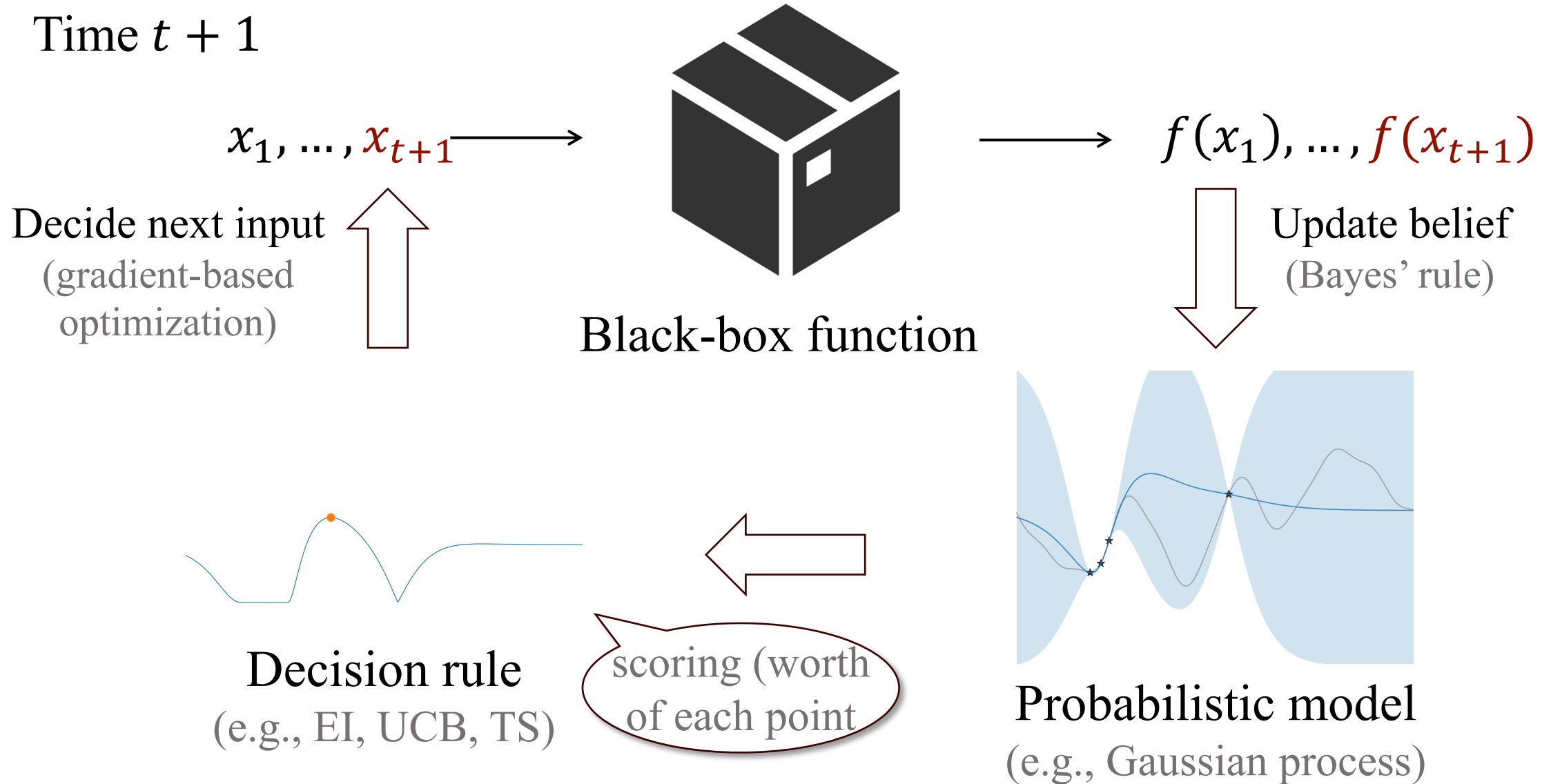
Time  $t$



# Bayesian Optimization



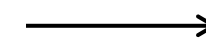
# Bayesian Optimization



# Bayesian Optimization

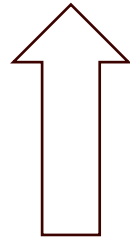
Time  $t + 1$

$x_1, \dots, x_{t+1}$



$f(x_1), \dots, f(x_{t+1})$

Decide next input  
(gradient-based  
optimization)

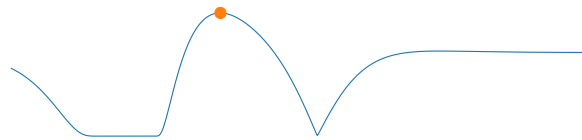


Black-box function

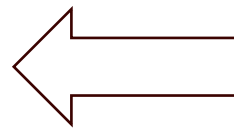
Update belief  
(Bayes' rule)



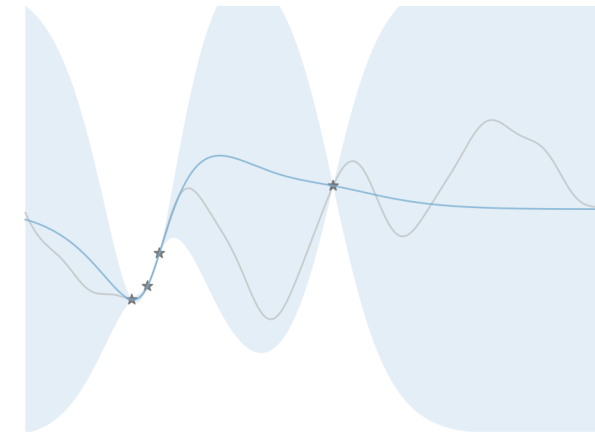
My focus



Decision rule  
(e.g., EI, UCB, TS)



scoring (worth  
of each point)



Probabilistic model  
(e.g., Gaussian process)

# Popular Decision Rule: Expected Improvement

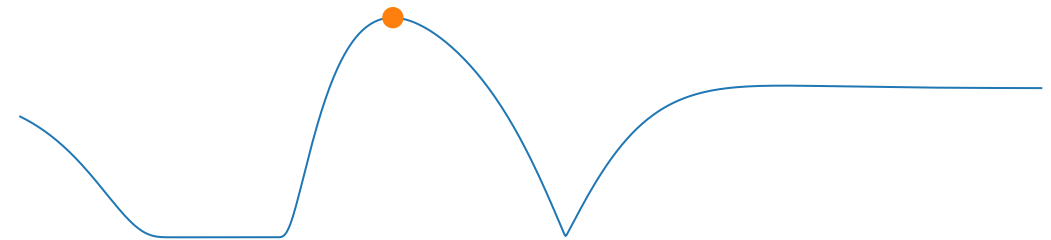
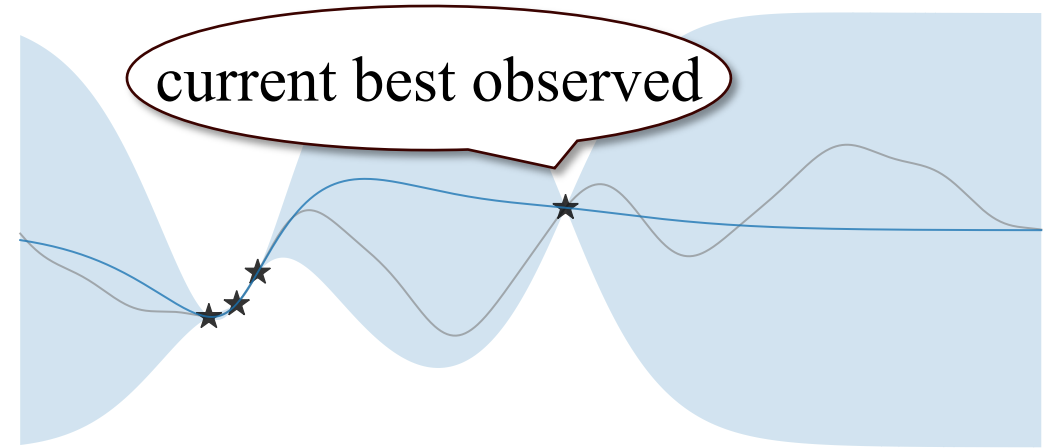
$$\text{EI}(x) = \mathbb{E}[\underbrace{\max(f(x) - y_{\text{best}}, 0)}_{\text{"improvement"}} \mid x_1, \dots, x_t]$$

Annotations: "current best observed" points to  $y_{\text{best}}$ ; "data" points to  $x_1, \dots, x_t$ .

$$x_{t+1} = \max_x \text{EI}_{f|D}(x; y_{\text{best}})$$

Annotation: "posterior distribution" points to  $f|D$ .

One-step approximation to MDP



Expected improvement  $\text{EI}(x)$

# Popular Decision Rule: Expected Improvement

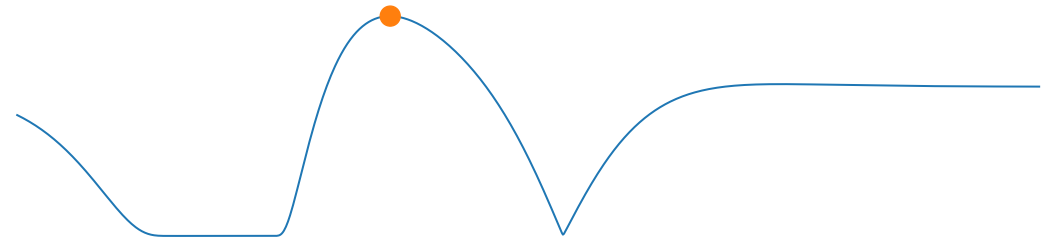
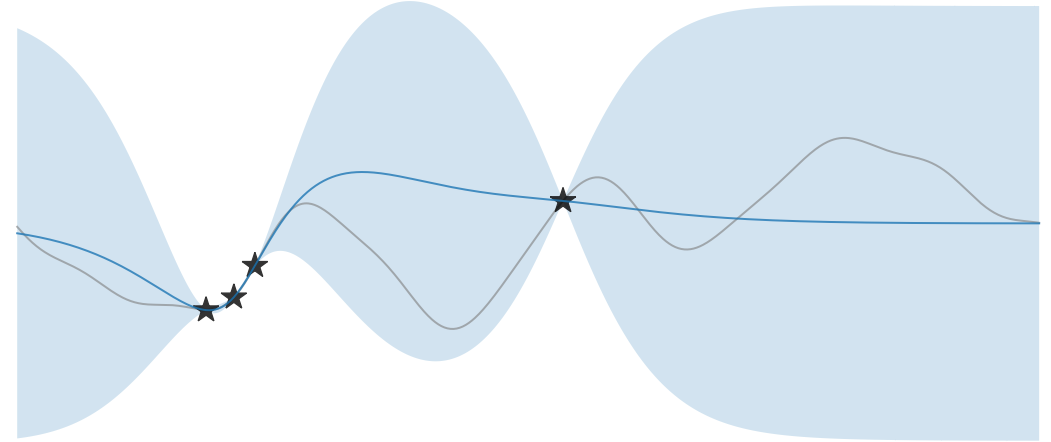
$$\text{EI}(x) = \mathbb{E}[\underbrace{\max(f(x) - y_{\text{best}}, 0)}_{\text{"improvement"}} \mid x_1, \dots, x_t]$$

current best observed      data

$$x_{t+1} = \max_x \text{EI}_{f|D}(x; y_{\text{best}})$$

posterior distribution

One-step approximation to MDP

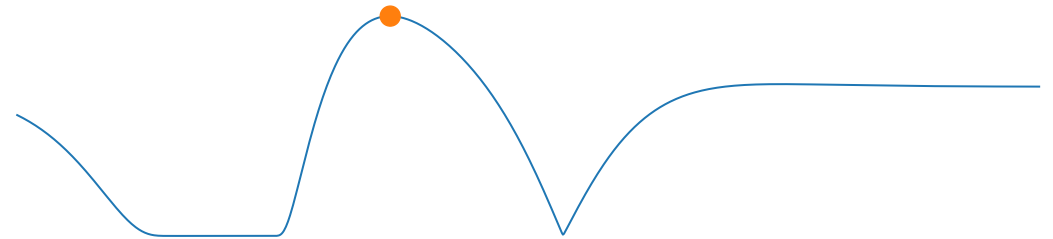
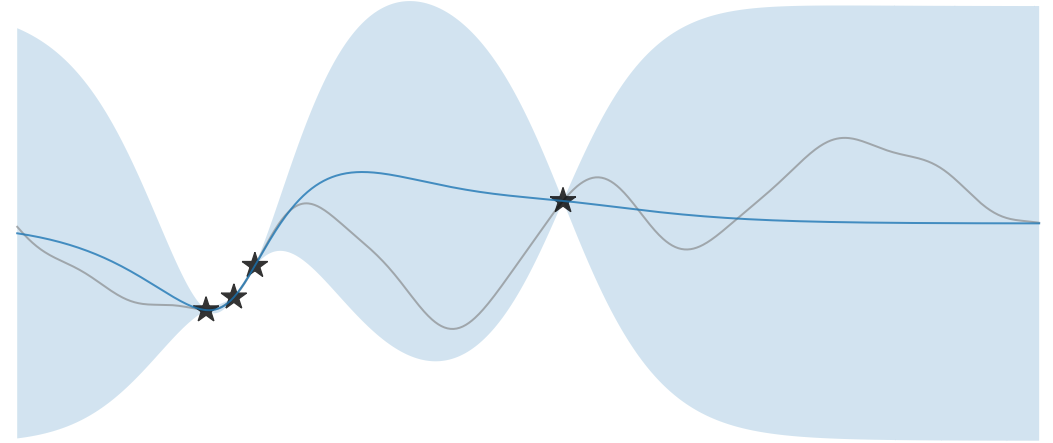


Expected improvement  $\text{EI}(x)$

Improvement-based  
design principle

# Existing Design Principles

- Improvement-based (e.g., EI)
- Entropy-based
- Confidence bounds (UCB/LCB)
- Thompson sampling (TS)

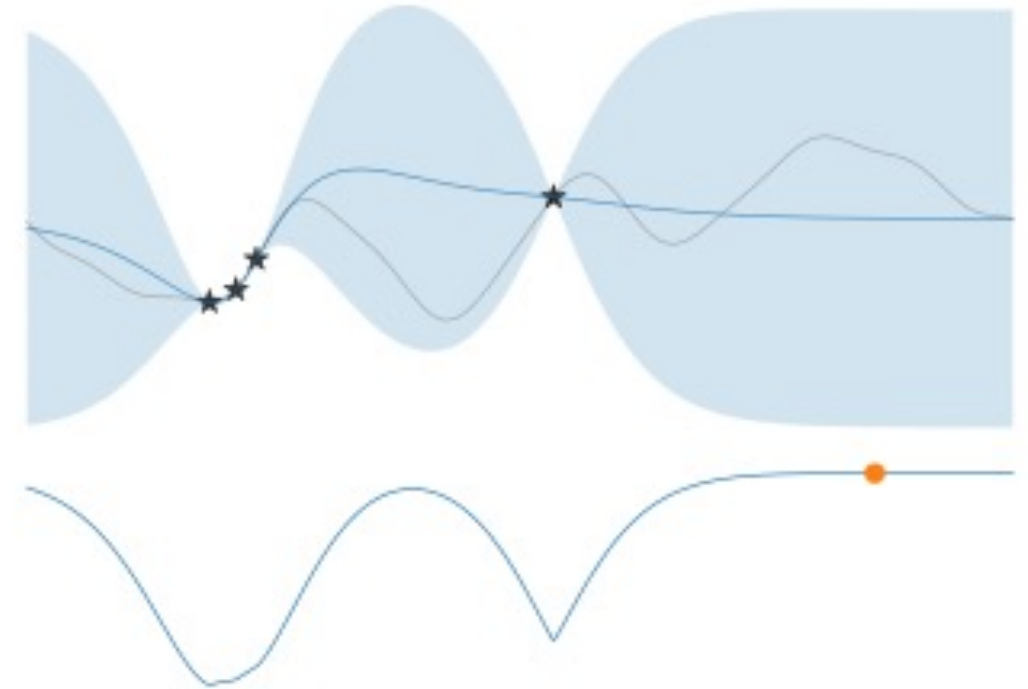


Expected improvement  $EI(x)$

Improvement-based  
design principle

# New Design Principle: Gittins Index

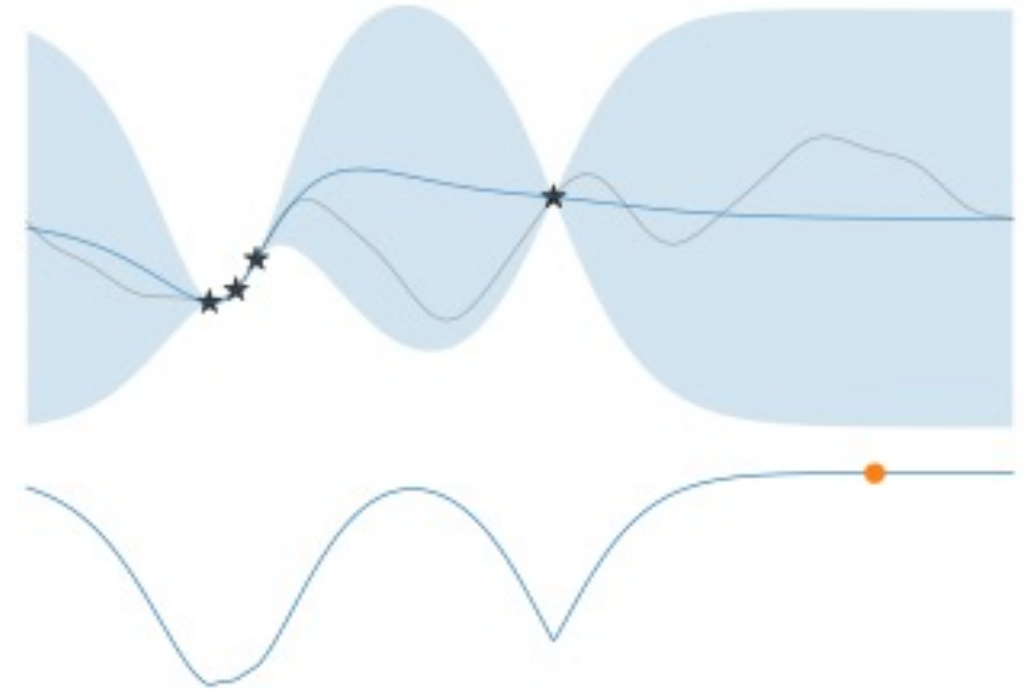
- Improvement-based (e.g., EI)
- Entropy-based
- Confidence bounds (UCB/LCB)
- Thompson sampling (TS)
- Gittins Index



Gittins index  $GI(x)$

# New Design Principle: Gittins Index

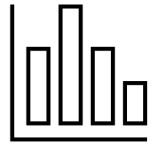
- Improvement-based (e.g., EI)
- Entropy-based
- Confidence bounds (UCB/LCB)
- Thompson sampling (TS)
- Gittins Index



Gittins index  $GI(x)$

? Why another principle?

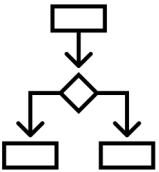
# Under-explored Side Info and Flexibility



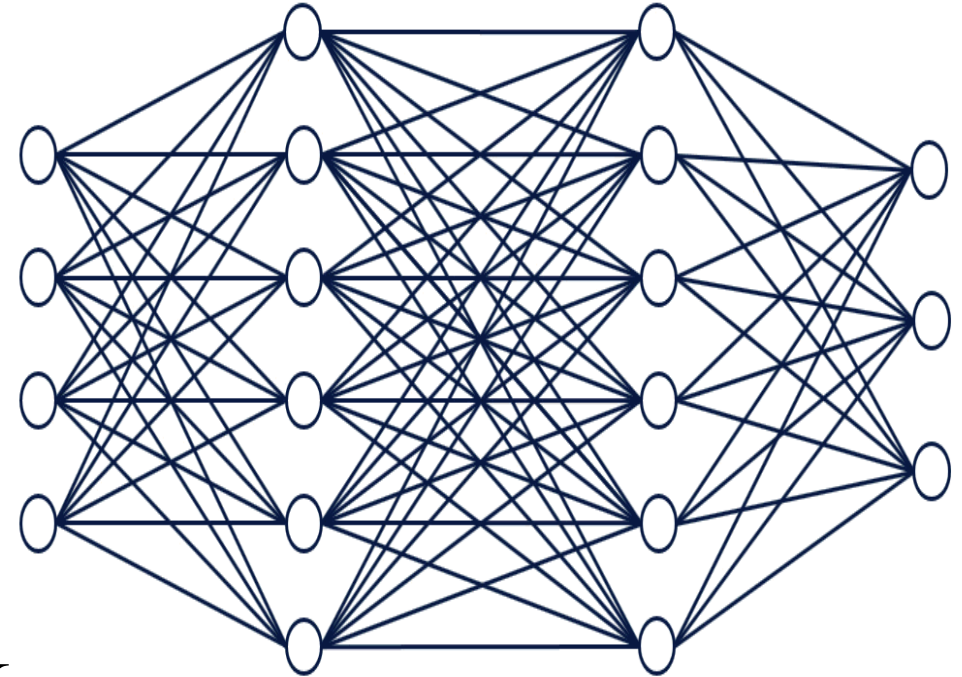
Varying evaluation costs



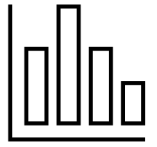
Smart stopping time



Observable multi-stage feedback



# How does existing principle incorporate them?



Varying evaluation costs

$$EI(x)/c(x)$$

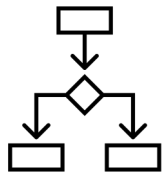
Why not subtraction?



Smart stopping time

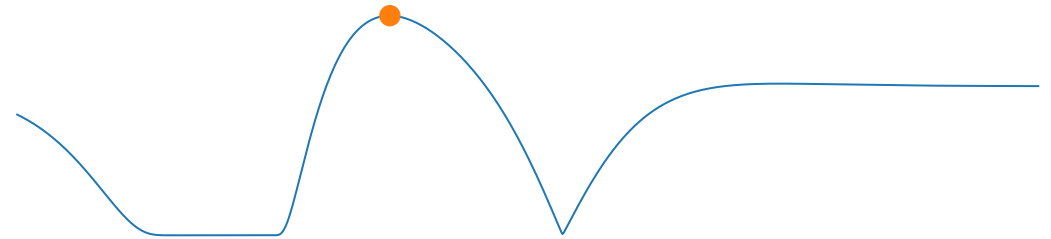
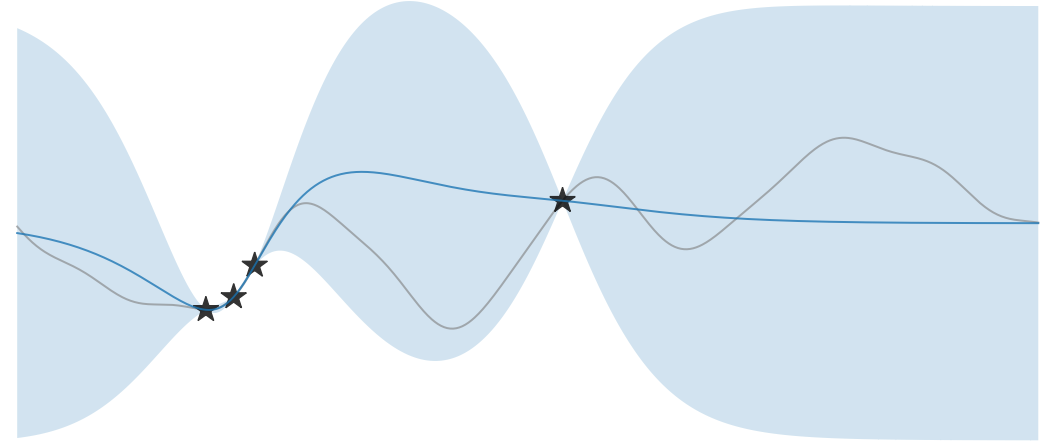
$$EI(x) \leq \theta$$

Which threshold?



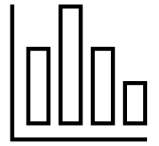
Observable multi-stage feedback

?



Expected improvement  $EI(x)$

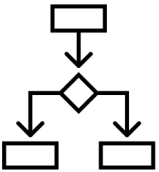
# Under-explored Side Info and Flexibility



Varying evaluation costs



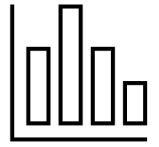
Smart stopping time



Observable multi-stage feedback

New design principle:  
**Gittins index**

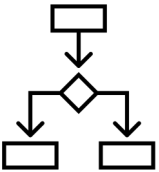
# Why Gittins index?



Varying evaluation costs



Smart stopping time

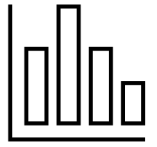


Observable multi-stage feedback

New design principle:  
Gittins index

**Optimal** in related sequential  
decision problems

# Why Gittins index?



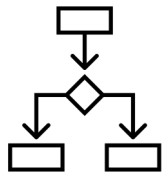
Varying evaluation costs

Features in Pandora's box



Smart stopping time

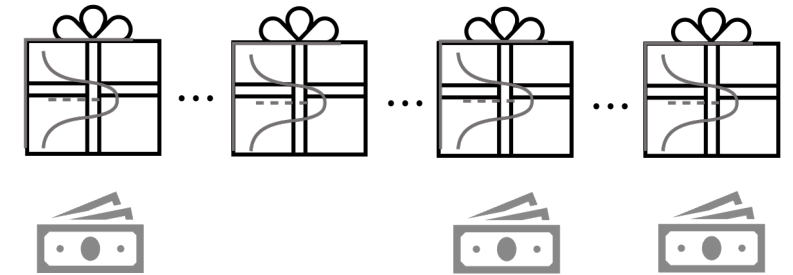
Features in Pandora's box



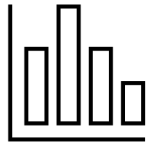
Observable multi-stage feedback

New design principle:  
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# Why Gittins index?



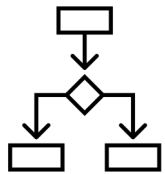
Varying evaluation costs

Features in Pandora's box



Smart stopping time

Features in Pandora's box

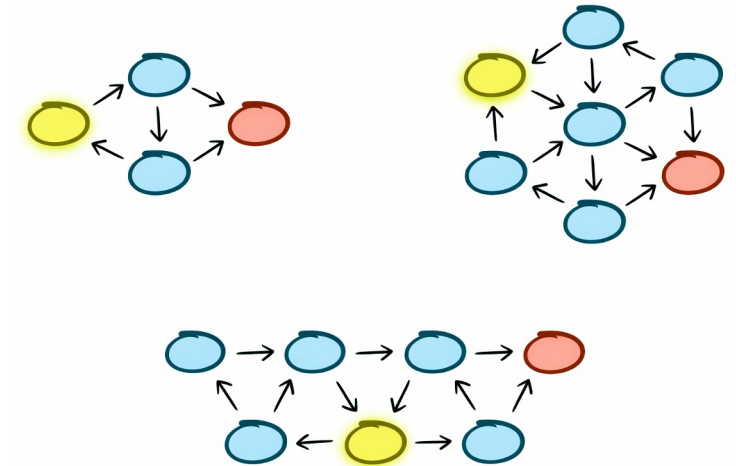


Observable multi-stage feedback

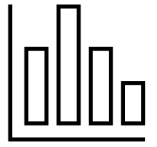
Features in **Markov chain selection**

New design principle:  
Gittins index

Optimal in related sequential  
decision problems



# Why Gittins index?



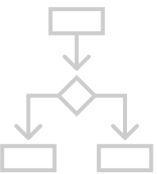
Varying evaluation costs

Features in Pandora's box



Smart stopping time

Features in Pandora's box



Observable multi-stage feedback

Features in Markov chain selection

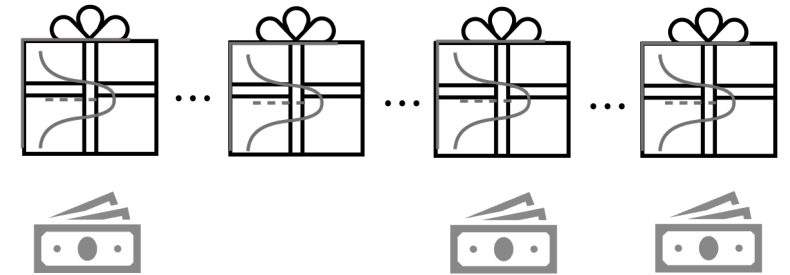


"Cost-aware Bayesian Optimization via the Pandora's Box Gittins Index." NeurIPS'24.

This talk's focus

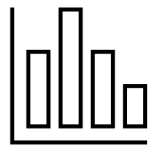
New design principle:  
Gittins index

Optimal in related sequential  
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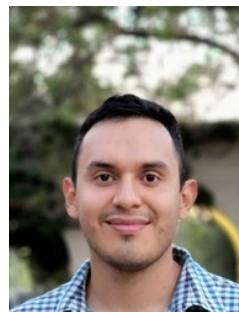


"Cost-aware Stopping for Bayesian Optimization." Under review.

# Coauthors



Varying evaluation costs  
[NeurIPS'24]



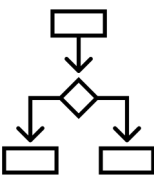
Raul Astudillo



Smart stopping time  
[Under review]



Linda Cai



Observable multi-stage feedback  
[Ongoing work]



Peter Frazier



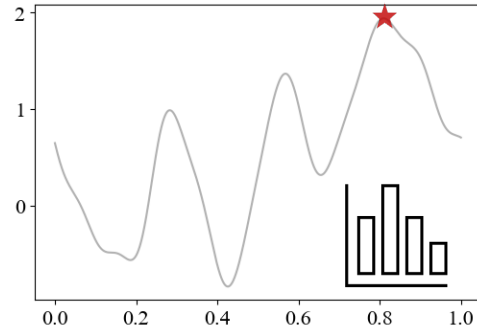
Alexander Terenin



Ziv Scully

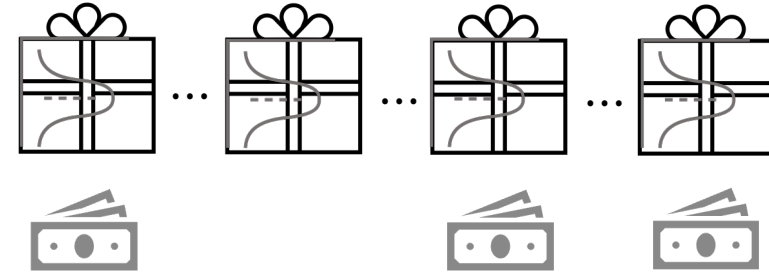
# Outline

## Studied Problem



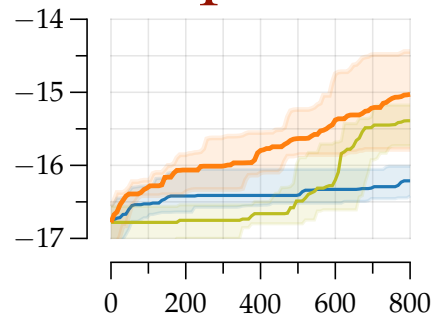
Cost-aware Bayesian optimization

## Key idea



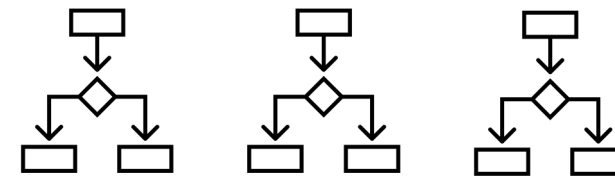
Link to simplified problem  
and Gittins index theory

## Impact



Competitive empirical performance

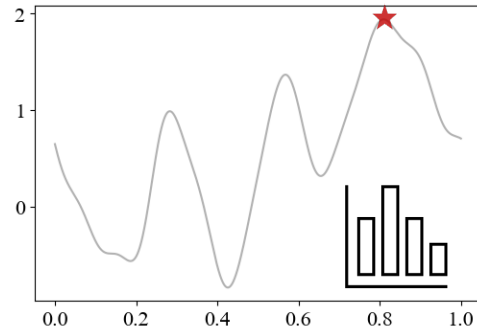
## Future direction



“Exotic” Bayesian optimization

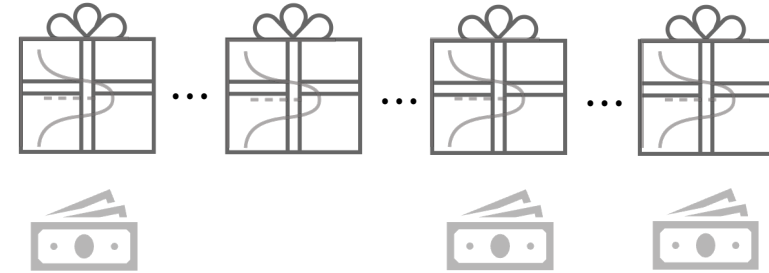
# Outline

## Studied Problem



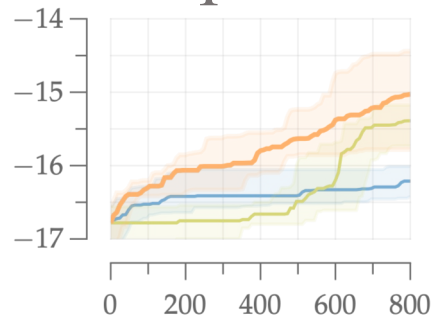
Cost-aware Bayesian optimization

## Key idea



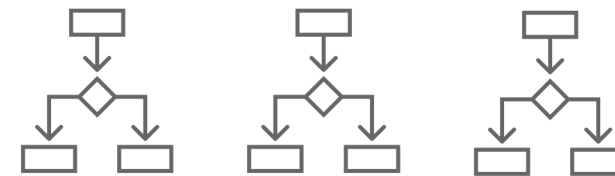
Link to simplified problem  
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Competitive empirical performance

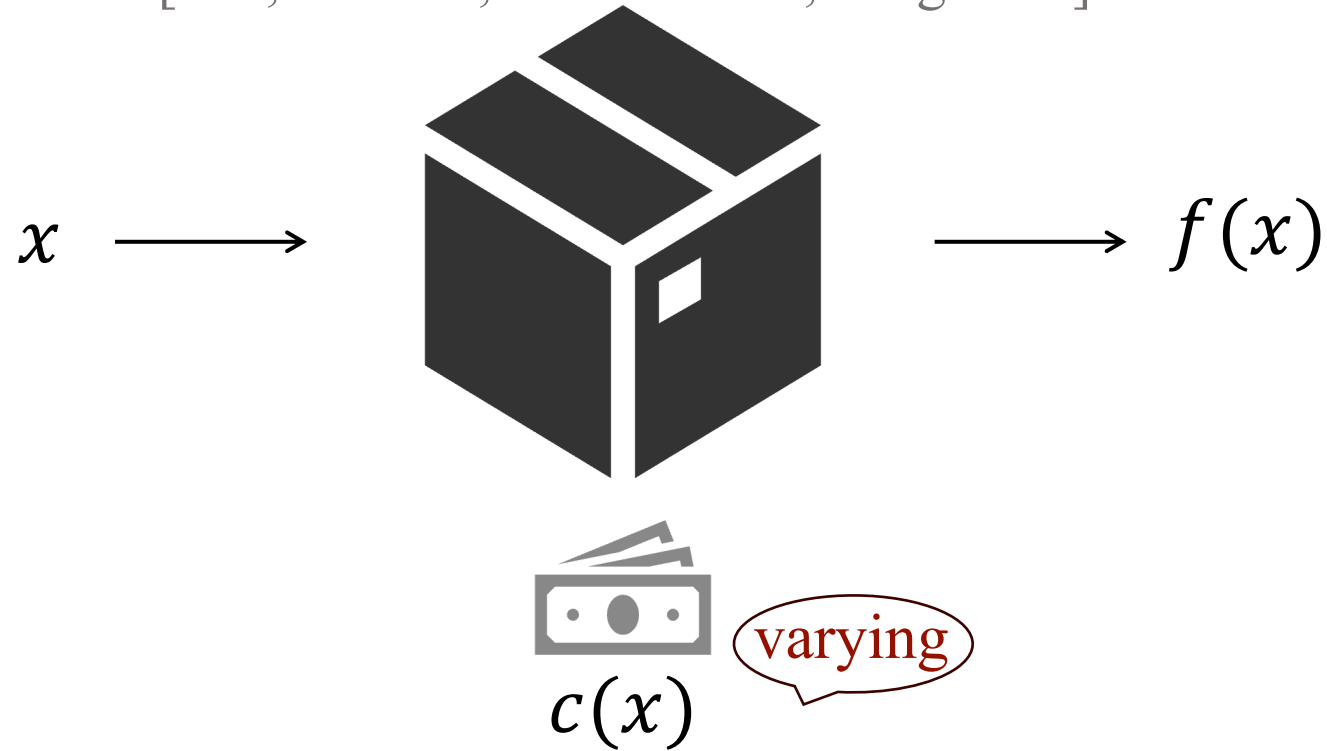
## Future direction



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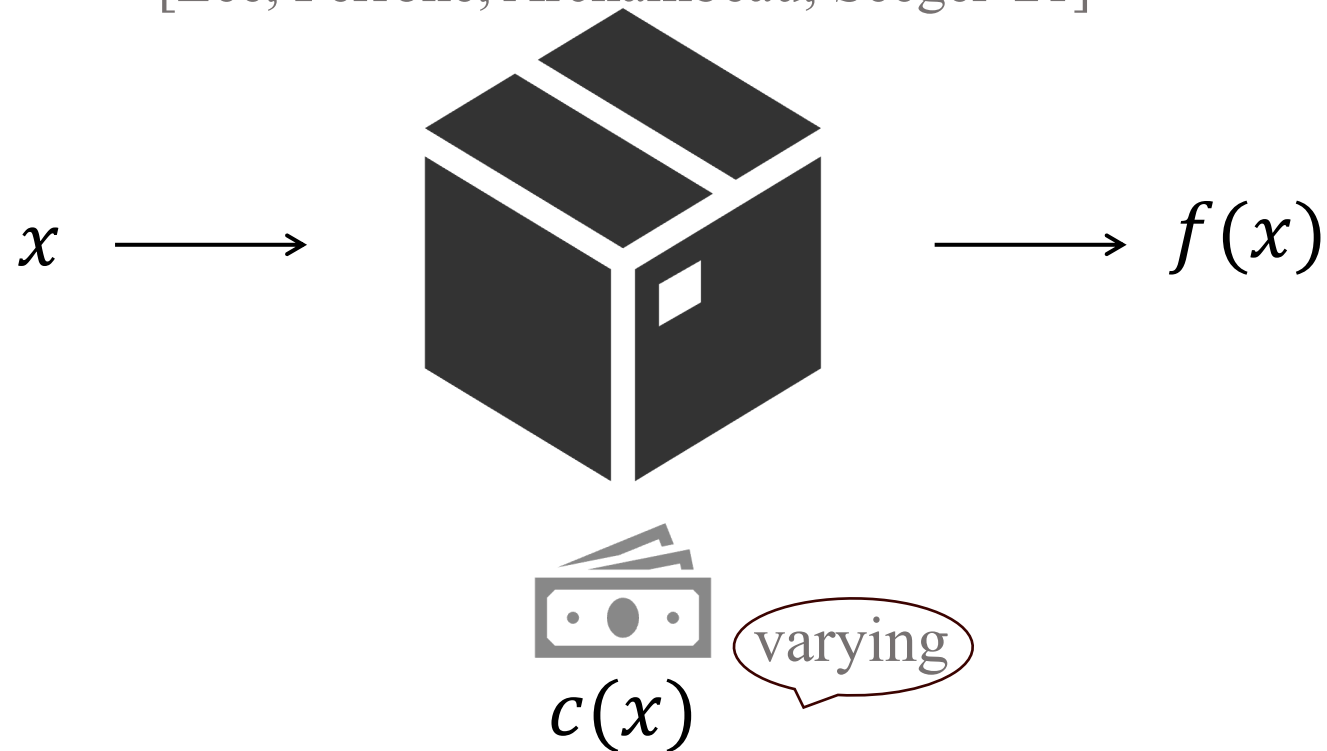
# Cost-aware Bayesian Optimization

[Lee, Perrone, Archambeau, Seeger'21]



# Cost-aware Bayesian Optimization

[Lee, Perrone, Archambeau, Seeger'21]

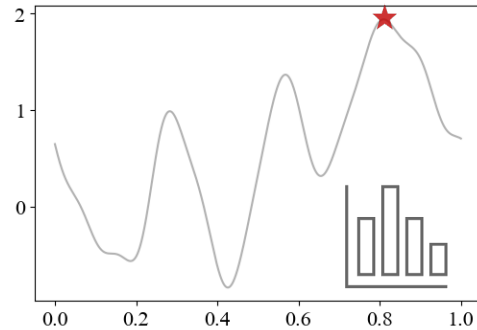


Goal:  $\sup_{\text{policy}} \mathbb{E} \max_{t=1,2,\dots,T} f(x_t)$

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

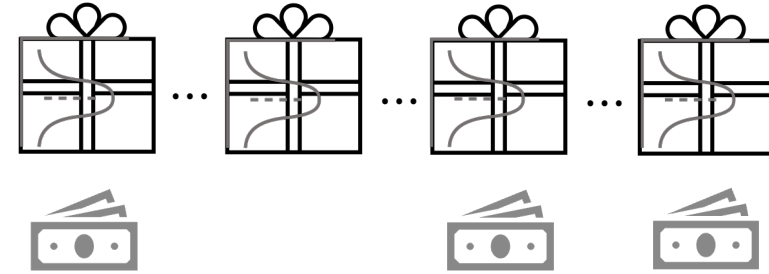
# Outline

## Studied Problem



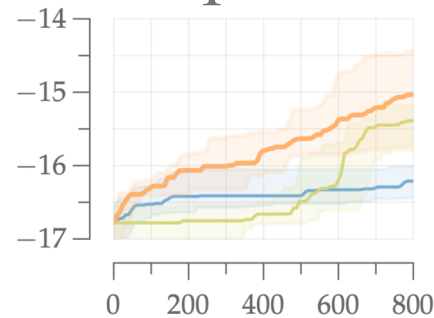
Cost-aware Bayesian optimization

## Key idea



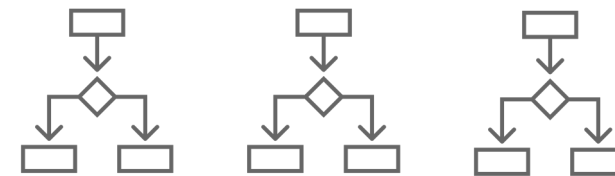
Link to simplified problem  
and Gittins index theory

## Impact



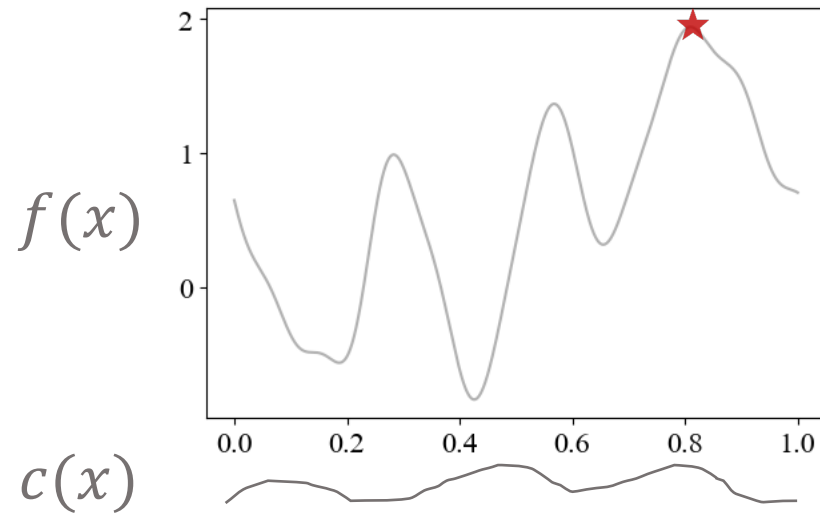
Competitive empirical performance

## Future direction

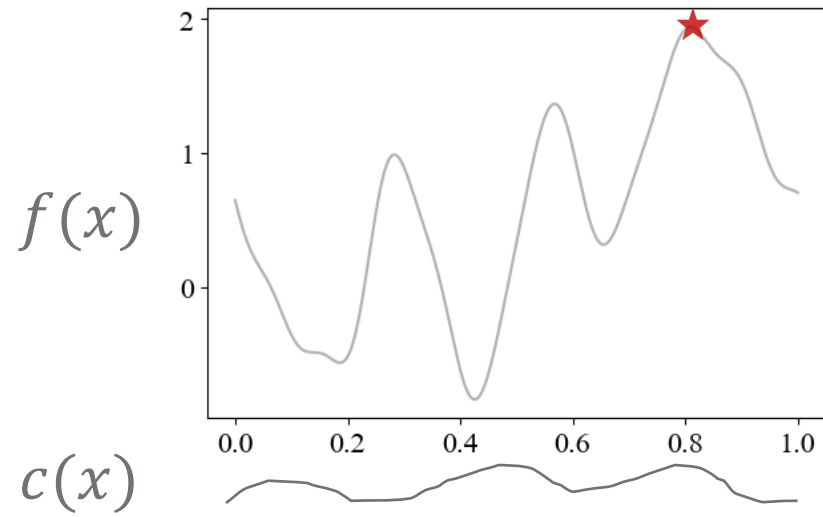


“Exotic” Bayesian optimization

# Cost-aware Bayesian Optimization



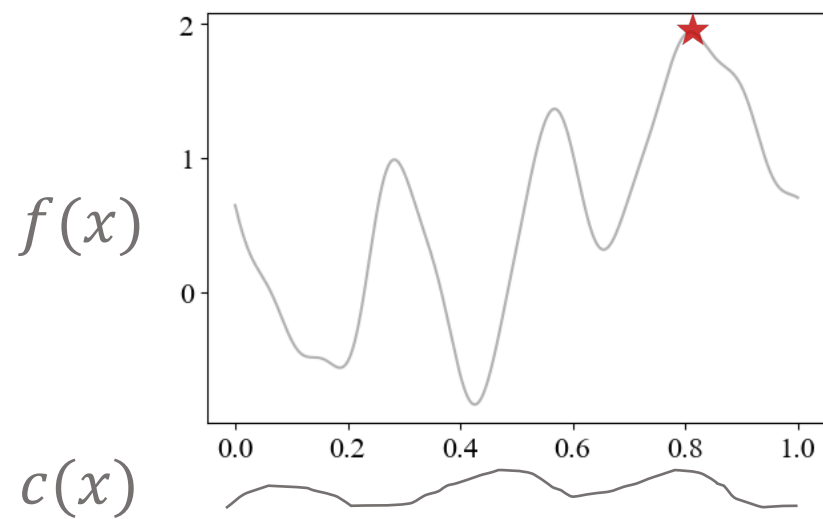
# Cost-aware Bayesian Optimization



Continuous

Correlated

# Cost-aware Bayesian Optimization



Continuous

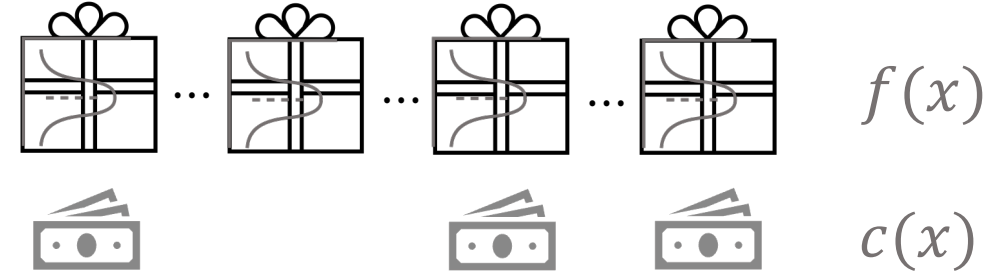
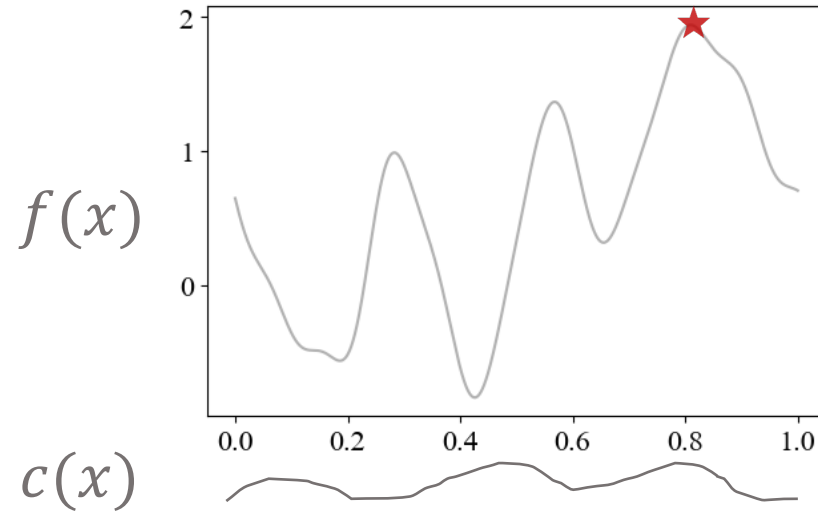
Correlated

**Intractable MDP!**

# Cost-aware Bayesian Optimization

## Pandora's Box

[Weitzman'79]



Continuous



Discrete

Correlated

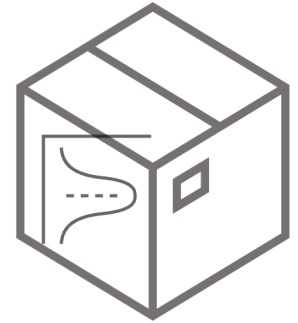
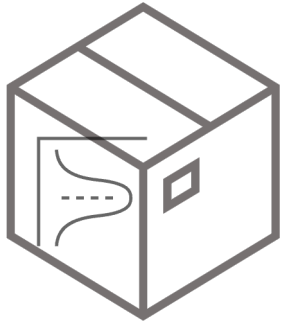


Independent

Intractable MDP!

# Pandora's Box

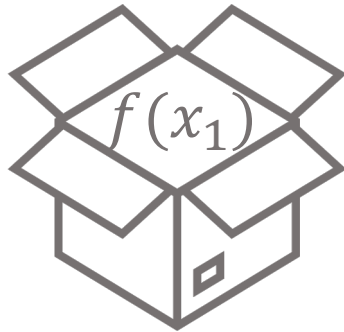
$t = 0$



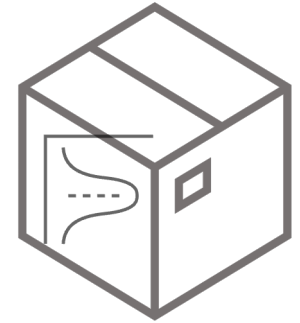
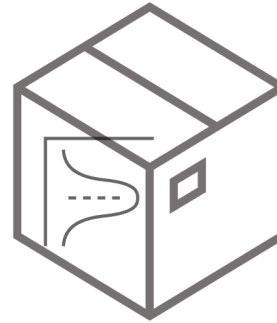
$$\sup_{\text{policy}} \mathbb{E} \left( \max_{t=1,2,\dots,T} f(x_t) - \sum_{t=1}^T c(x_t) \right)$$

# Pandora's Box

$t = 1$



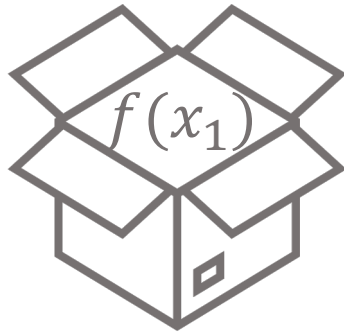
$c(x_1)$



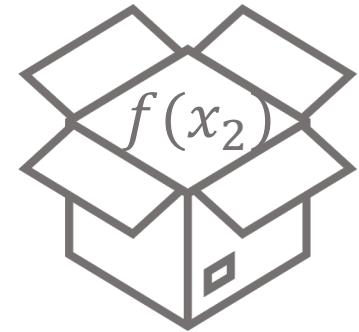
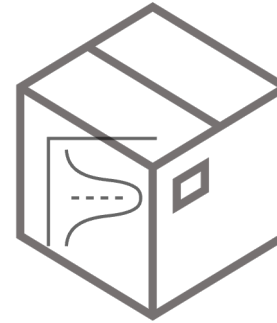
$$\sup_{\text{policy}} \mathbb{E} \left( \max_{t=1,2,\dots,T} f(x_t) - \sum_{t=1}^T c(x_t) \right)$$

# Pandora's Box

$t = 2$



$c(x_1)$

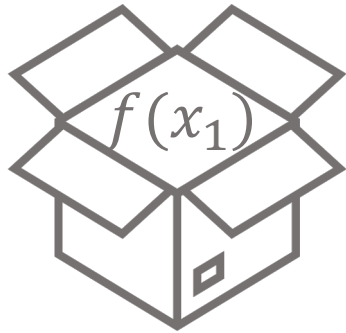


$c(x_2)$

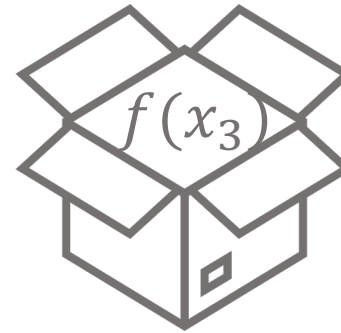
$$\sup_{\text{policy}} \mathbb{E} \left( \max_{t=1,2,\dots,T} f(x_t) - \sum_{t=1}^T c(x_t) \right)$$

# Pandora's Box

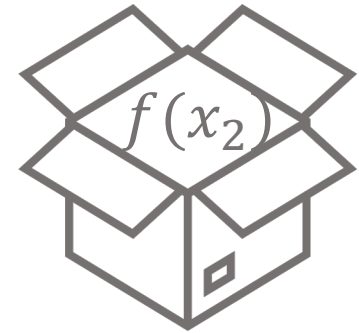
$t = 3$



$c(x_1)$



$c(x_3)$

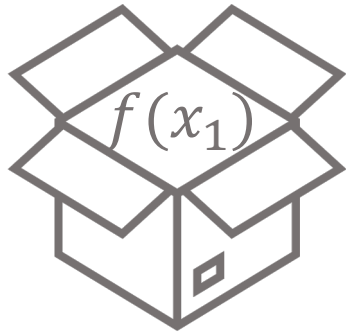


$c(x_2)$

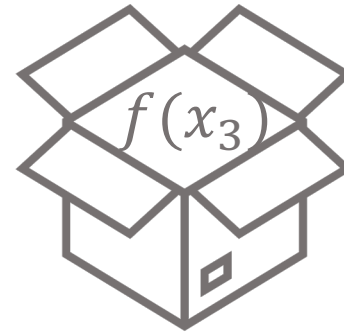
$$\sup_{\text{policy}} \mathbb{E} \left( \max_{t=1,2,\dots,T} f(x_t) - \sum_{t=1}^T c(x_t) \right)$$

# Pandora's Box

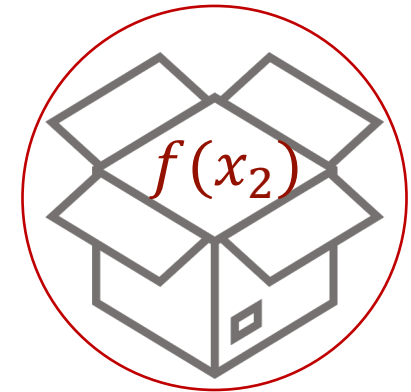
$t = T$ , stop



$c(x_1)$



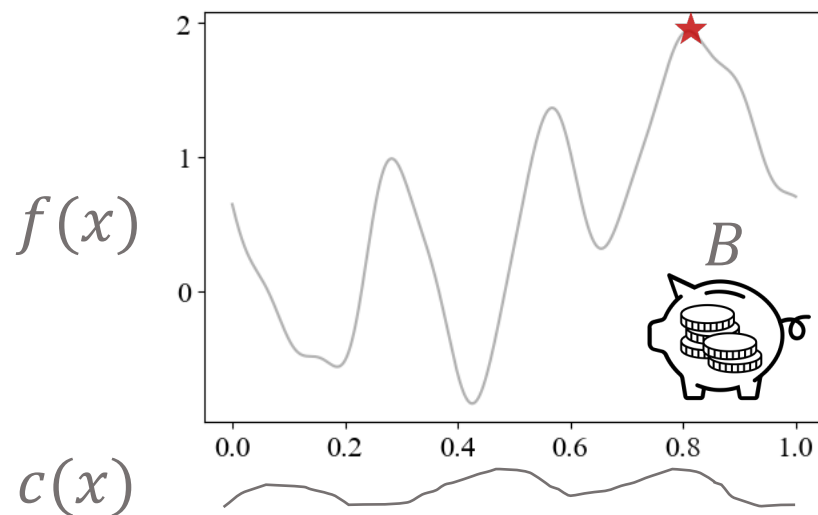
$c(x_3)$



$c(x_2)$

$$\sup_{\text{policy}} \mathbb{E} \left( \max_{t=1,2,\dots,T} f(x_t) - \sum_{t=1}^T c(x_t) \right)$$

# Cost-aware Bayesian Optimization



Continuous

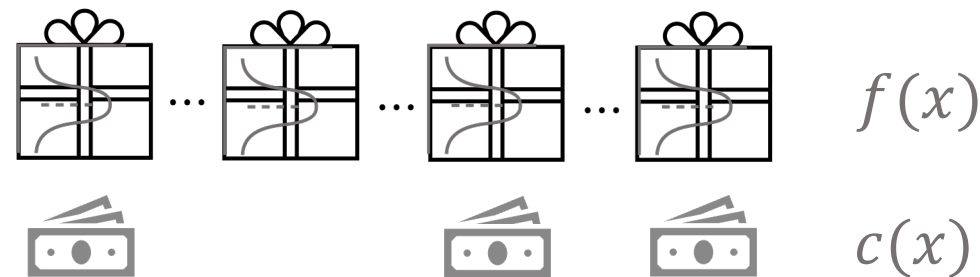
Correlated

Budget-constrained

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

# Pandora's Box

[Weitzman'79]



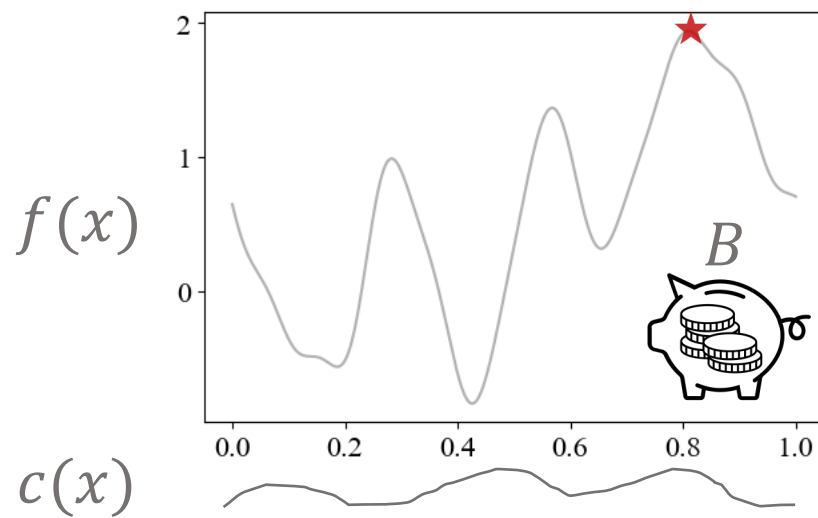
Discrete

Independent

Cost-per-sample

$$\sup_{\text{policy}} \mathbb{E} \left( \max_{t=1,2,\dots,T} f(x_t) - \sum_{t=1}^T c(x_t) \right)$$

# Cost-aware Bayesian Optimization



Continuous

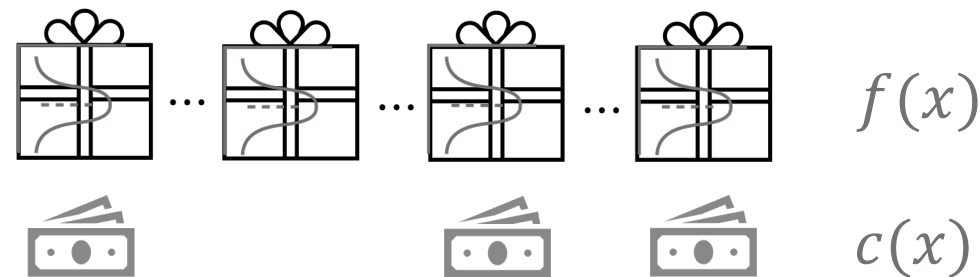
Correlated

**Expected**-budget-constrained

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

# Pandora's Box

[Weitzman'79]



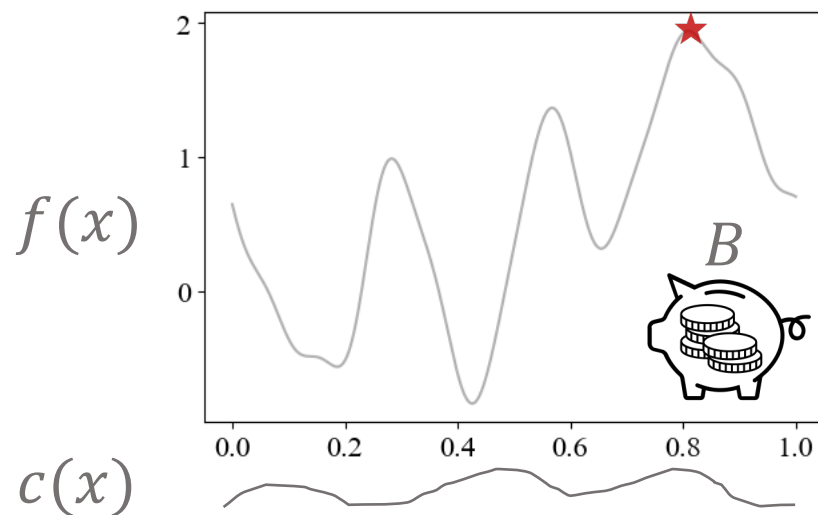
Discrete

Independent

Cost-per-sample

$$\sup_{\text{policy}} \mathbb{E} \left( \max_{t=1,2,\dots,T} f(x_t) - \sum_{t=1}^T c(x_t) \right)$$

# Cost-aware Bayesian Optimization



Continuous

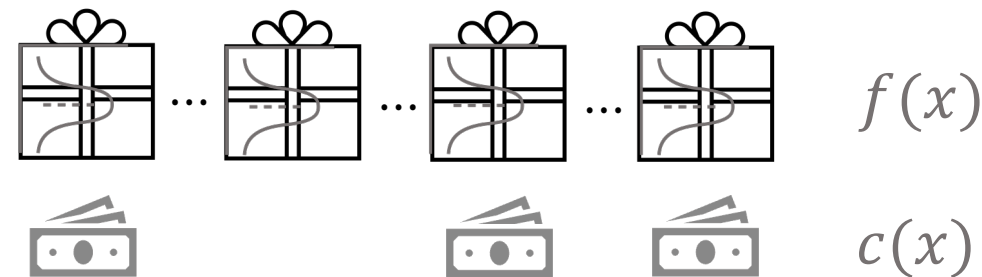
Correlated

**Ebc & Cps**

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

# Pandora's Box

[Weitzman'79]



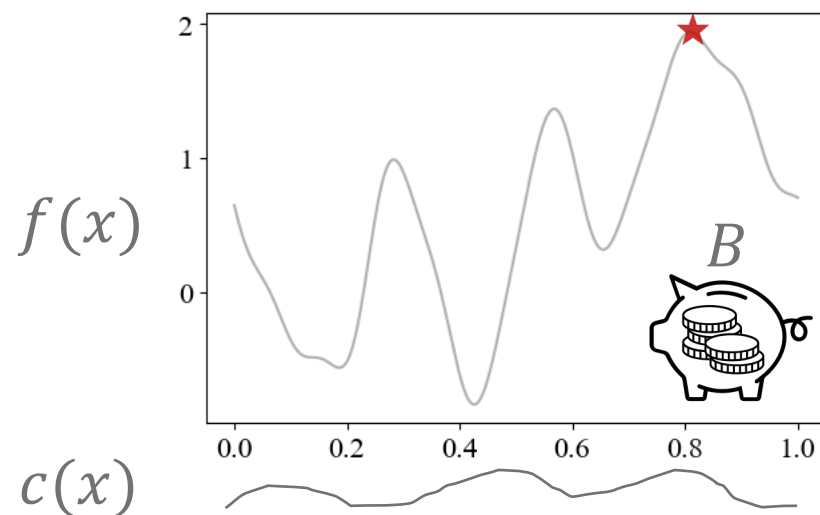
Discrete

Independent

Cost-per-sample

$$\sup_{\text{policy}} \mathbb{E} \left( \max_{t=1,2,\dots,T} f(x_t) - \sum_{t=1}^T c(x_t) \right)$$

# Cost-aware Bayesian Optimization



Continuous

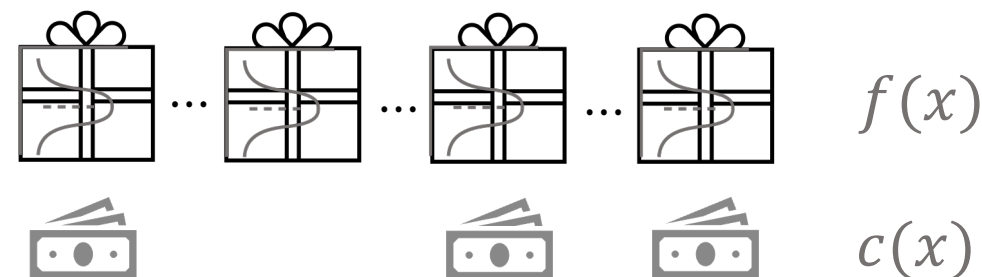
Correlated

Ebc & Cps

Intractable MDP!

# Pandora's Box

[Weitzman'79]



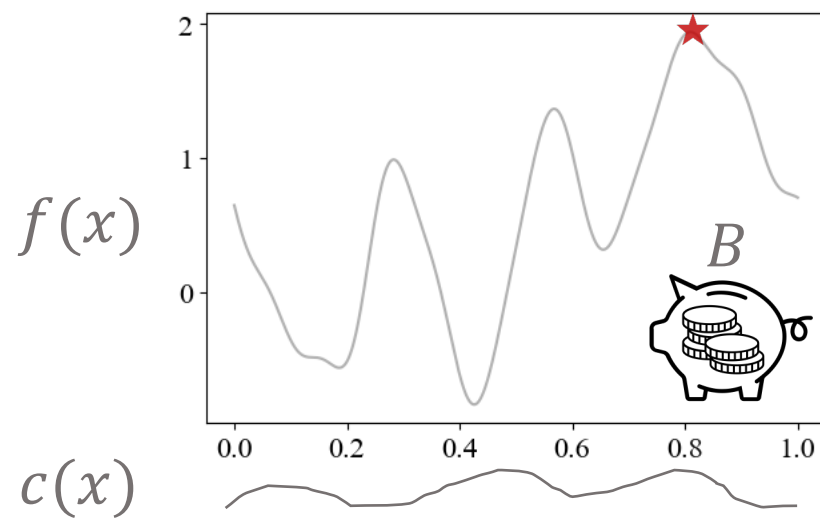
Discrete

Independent

Cost-per-sample

Optimal policy: Gittins index

# Cost-aware Bayesian Optimization



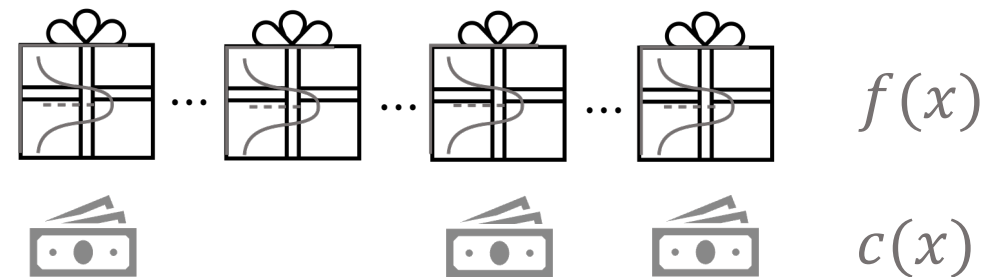
Continuous

Correlated

Ebc & Cps

# Pandora's Box

[Weitzman'79]



Discrete

Independent

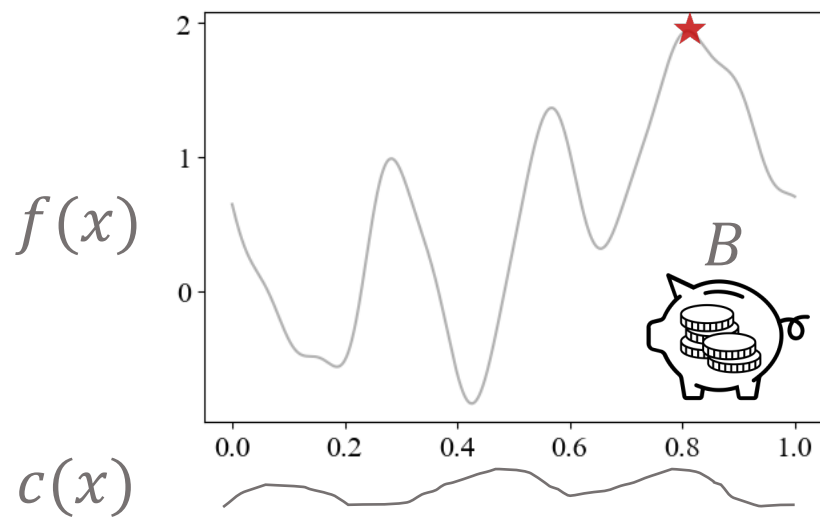
Cost-per-sample

How to translate?



Optimal policy: Gittins index

# Cost-aware Bayesian Optimization



Continuous

Correlated

Ebc & Cps

Acquisition function  
+ stopping rule

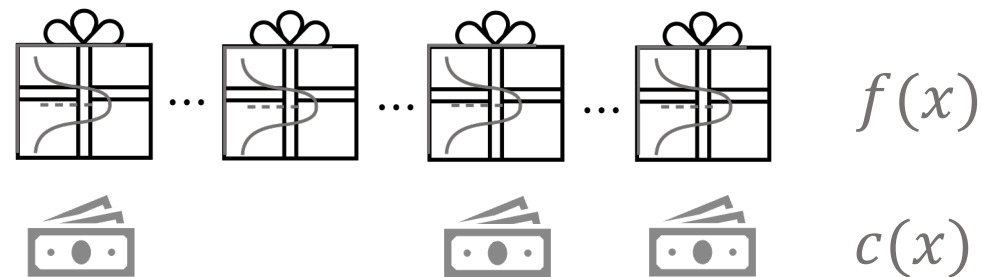
incorporate posterior



Optimal policy: Gittins index

# Pandora's Box

[Weitzman'79]

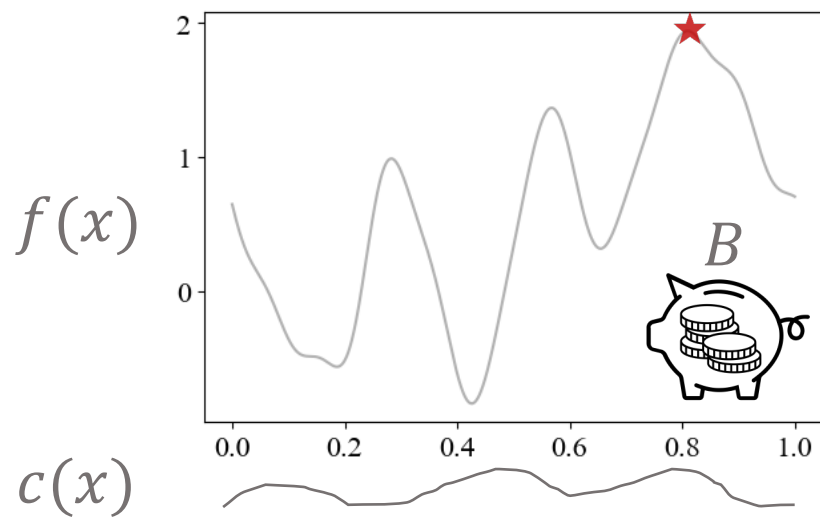


Discrete

Independent

Cost-per-sample

# Cost-aware Bayesian Optimization

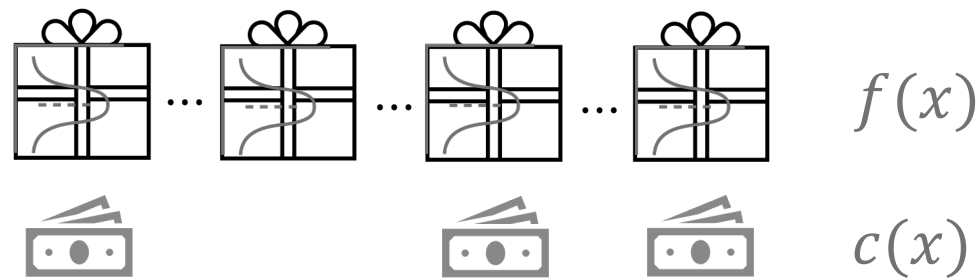


Continuous

Correlated

# Pandora's Box

[Weitzman'79]



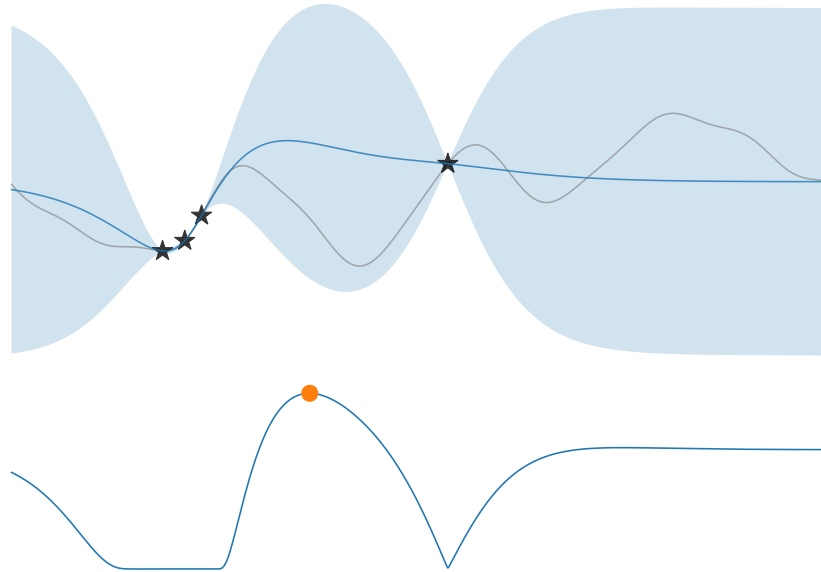
Discrete

Independent

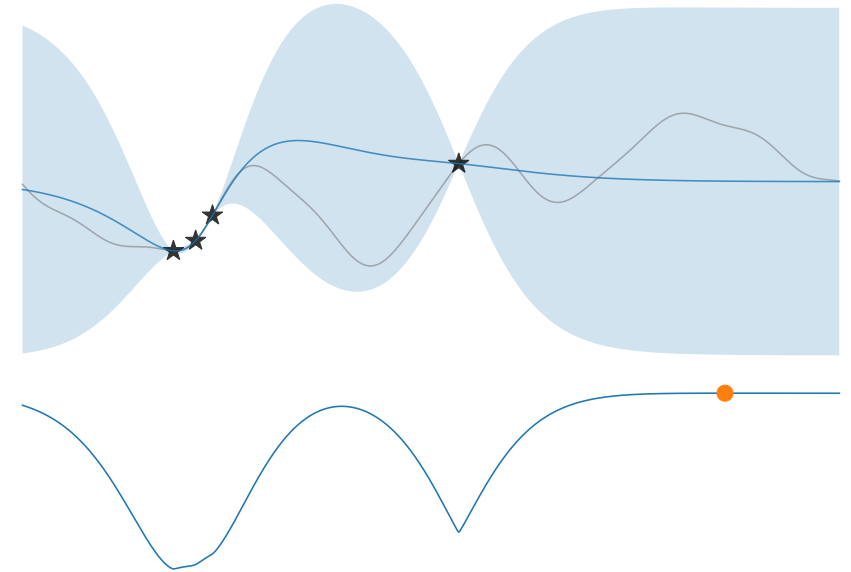
Acquisition function  $\xleftarrow{\text{incorporate posterior}}$  Optimal policy: Gittins index  
+ stopping rule

How to compute?

## Expected Improvement



## Gittins Index



$$\text{EI}_{f|D}(x; g) := \mathbb{E}[\max(f(x) - g, 0) \mid D] \quad \text{GI}_{f|D}(x) = g \text{ s.t. } \text{EI}_{f|D}(x; g) = c(x)$$

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

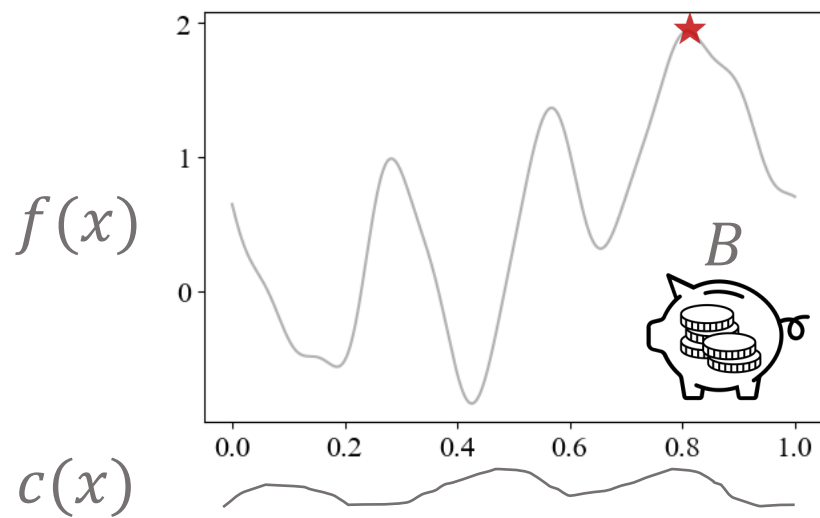
$\max_x \text{GI}_{f|D}(x; c(x))$

Stopping rule:  $\text{EI}_{f|D}(x; y_{\text{best}}) \leq c$

$\text{GI}_{f|D}(x; c(x)) \leq y_{\text{best}}$

$\text{GI}_{f|D}$  is **easy to compute** using  $\text{EI}_{f|D}$  + bisection search!

# Cost-aware Bayesian Optimization



Continuous

Correlated

Ebc & Cps

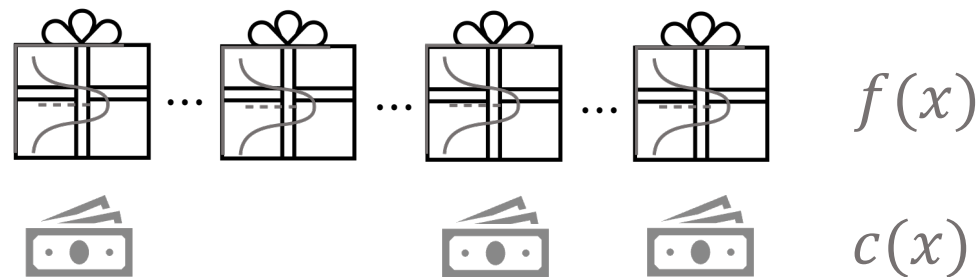
Acquisition function

+ stopping rule

Empirically good?

# Pandora's Box

[Weitzman'79]



Discrete

Independent

Cost-per-sample

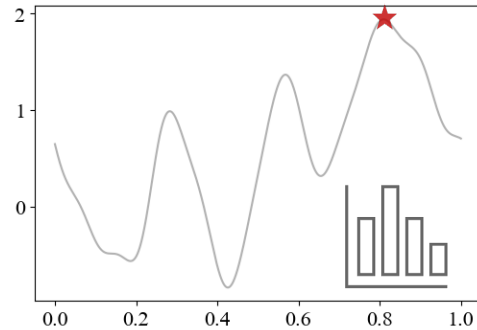
Gittins index is optimal

incorporate posterior

$\Leftarrow$

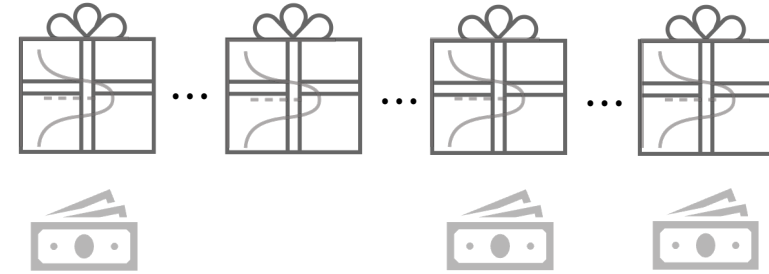
# Outline

## Studied Problem



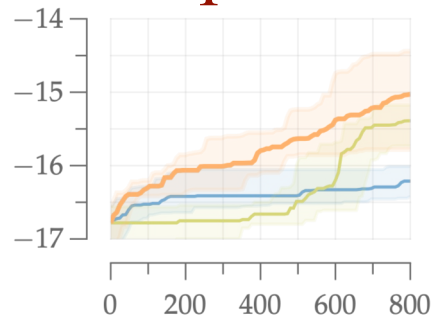
Cost-aware Bayesian optimization

## Key idea



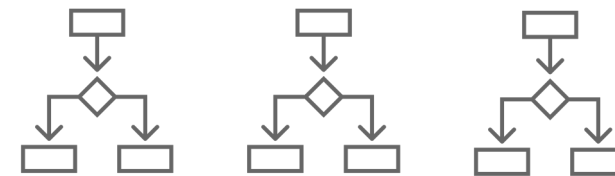
Link to Pandora's box and  
Gittins index theory

## Impact



Competitive empirical performance

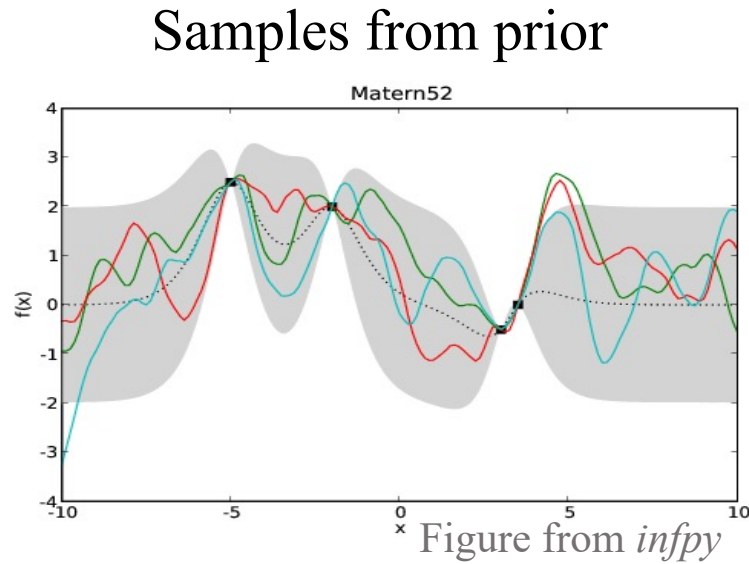
## Future direction



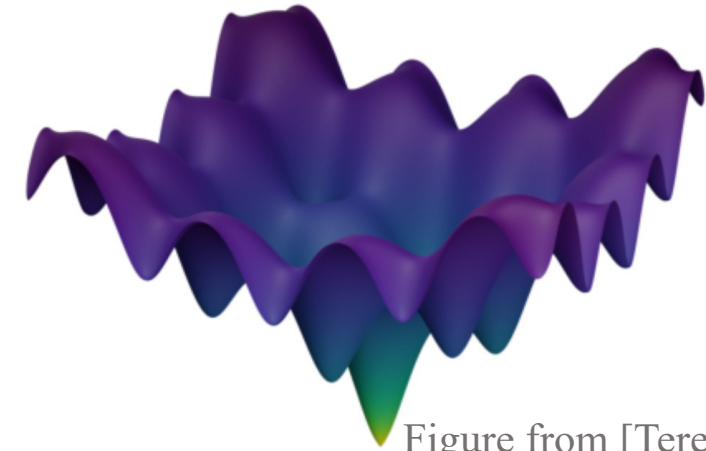
“Exotic” Bayesian optimization

# Experiment Setup: Objective Functions

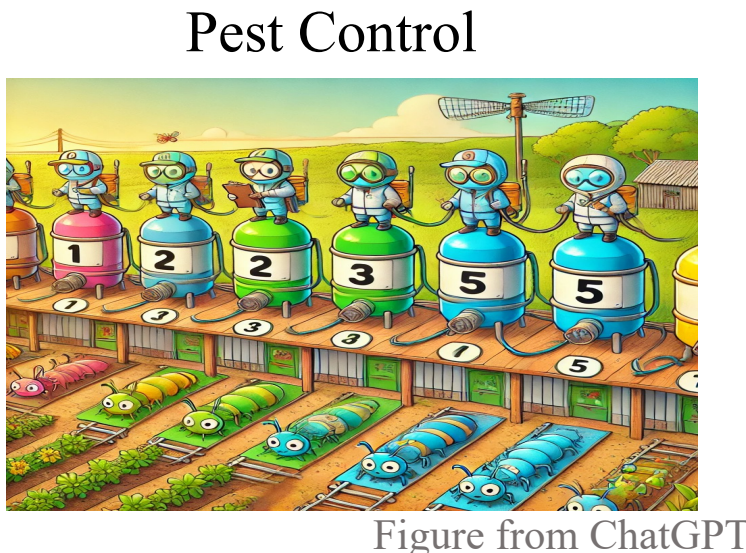
Synthetic



Ackley function



Empirical



Lunar Lander

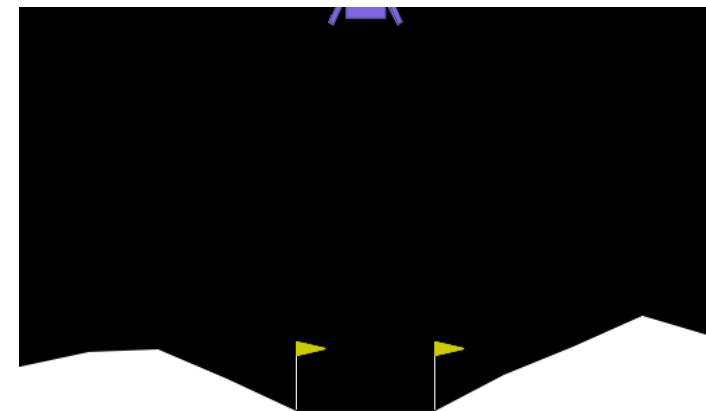
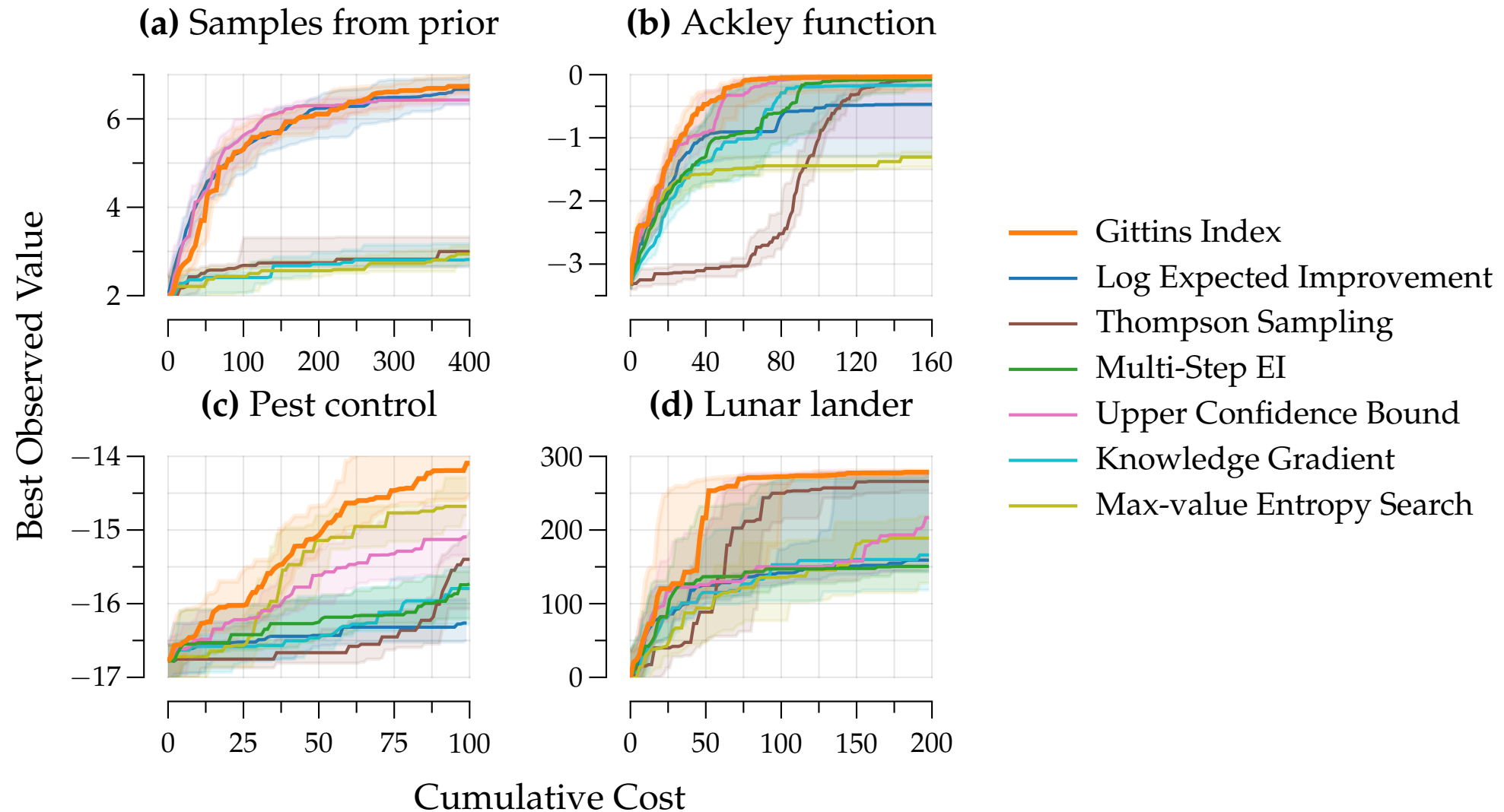
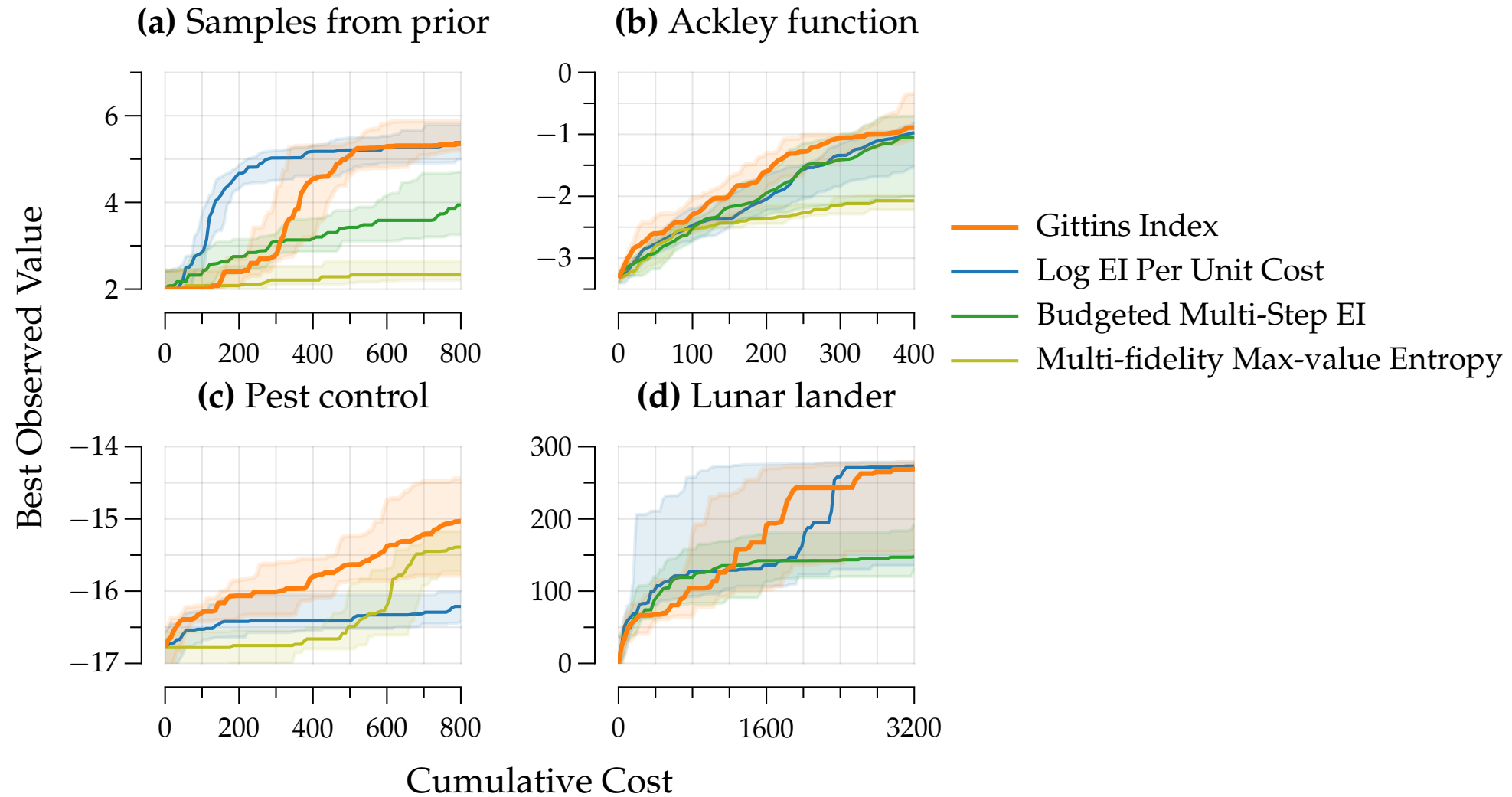


Figure from OpenAI Gym

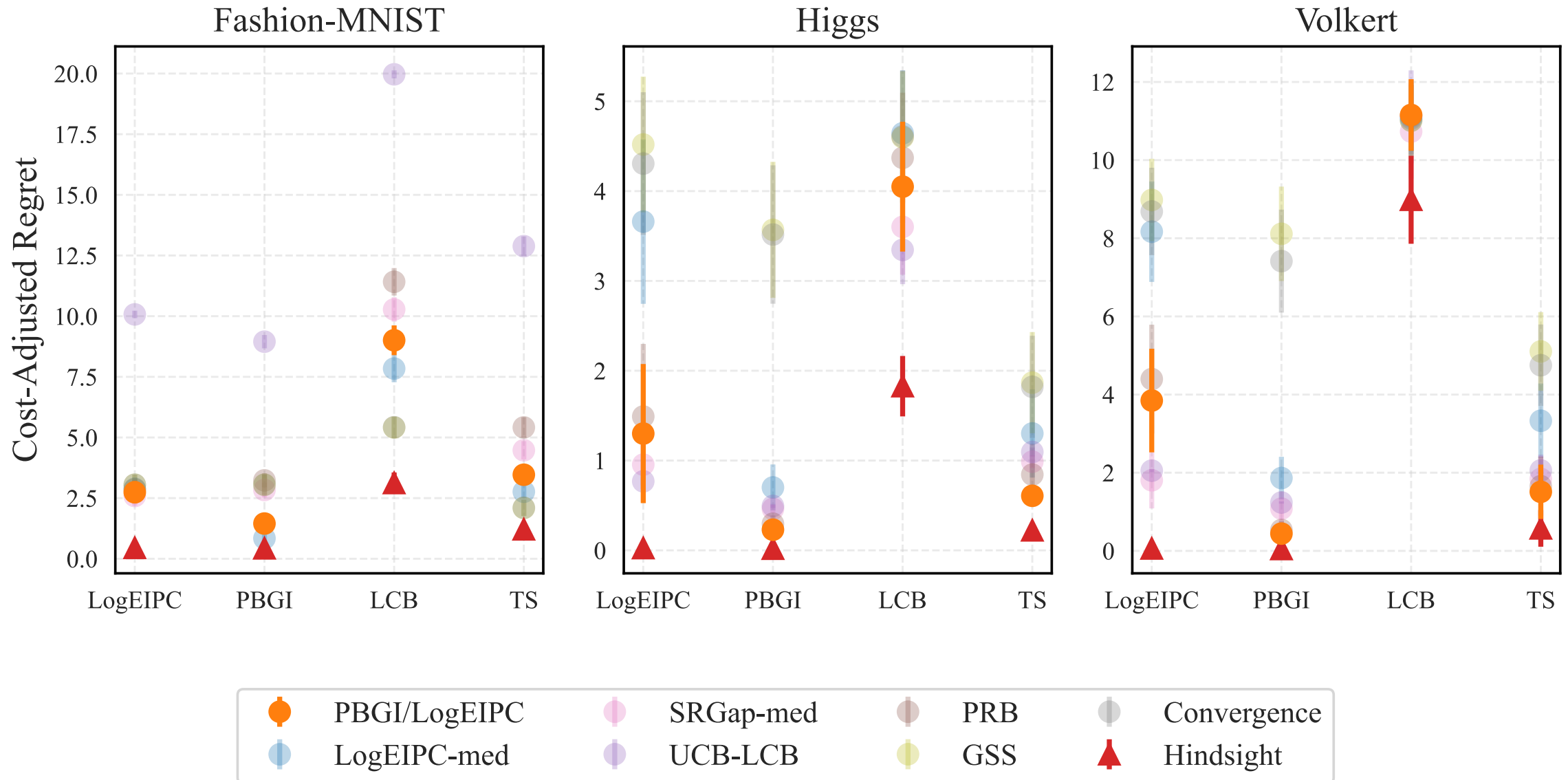
# Uniform-cost: Gittins Index vs Baselines



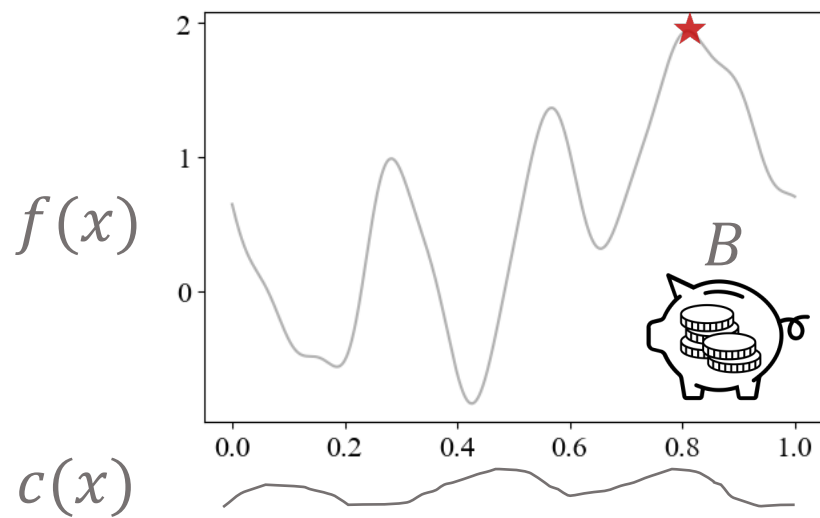
# Varying-cost: Gittins Index vs Baselines



# Stopping Rule: Gittins Index vs Baselines



# Cost-aware Bayesian Optimization



Continuous

Correlated

Ebc & Cps

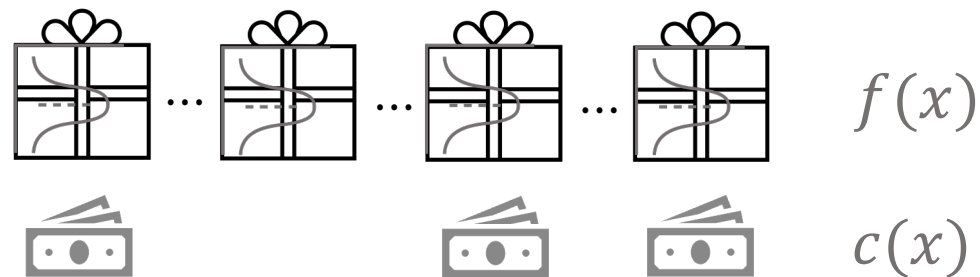
Acquisition function

+ stopping rule

Theoretical guarantee?

# Pandora's Box

[Weitzman'79]



Discrete

Independent

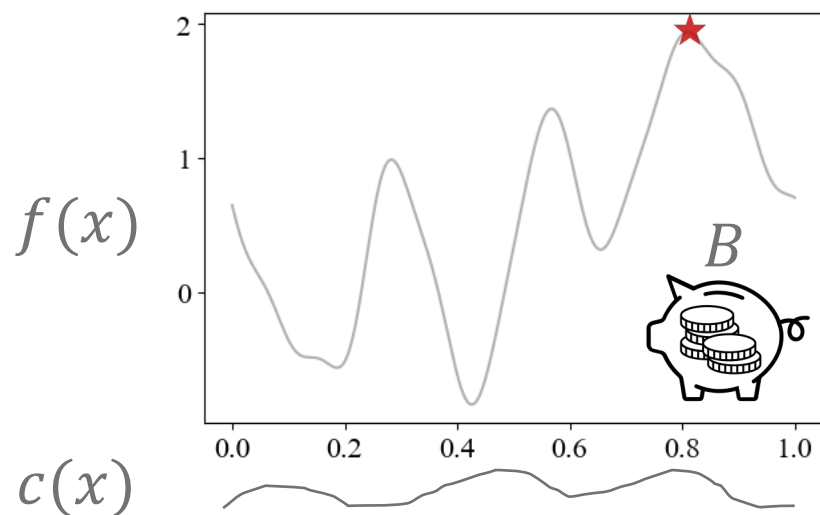
Cost-per-sample

Gittins index is optimal

incorporate posterior

⇐

# Cost-aware Bayesian Optimization



Continuous

Correlated

Ebc & Cps

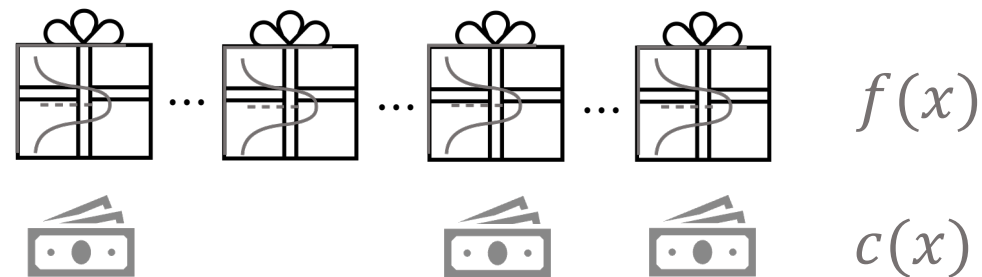
Acquisition function

+ stopping rule

Theoretical guarantee?

# Pandora's Box

[Weitzman'79]



Discrete

Independent

Cost-per-sample

Gittins index is optimal

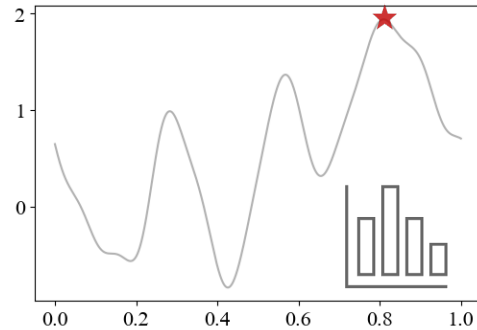
Yes! A bound on expected cost up to stopping

incorporate posterior

⇐

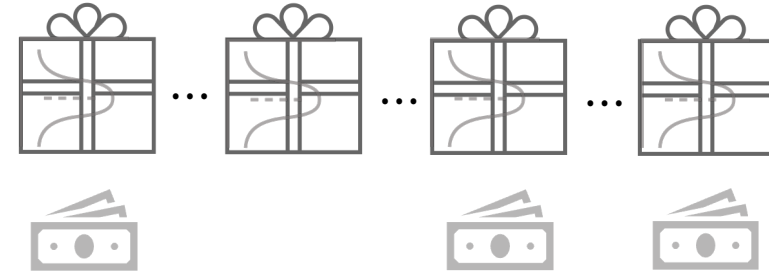
# Gittins Index: A New Design Principle

## Studied Problem



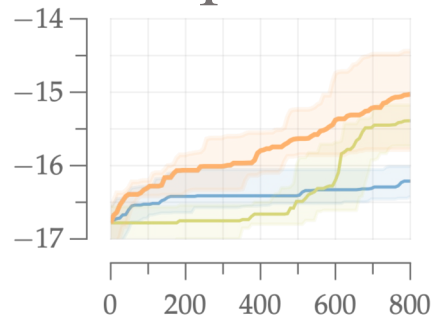
Cost-aware Bayesian optimization

## Key idea



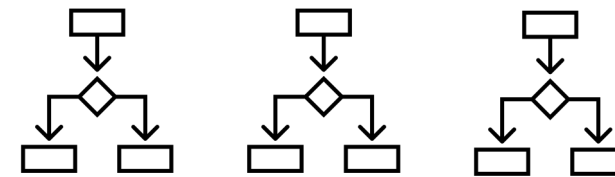
Link to Pandora's box and  
Gittins index theory

## Impact



Competitive empirical performance  
w/ theoretical guarantee

## Ongoing work



Bayesian optimization with  
multi-stage feedback

# Find our papers on arXiv!



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



"Cost-aware Stopping for  
Bayesian Optimization."