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!

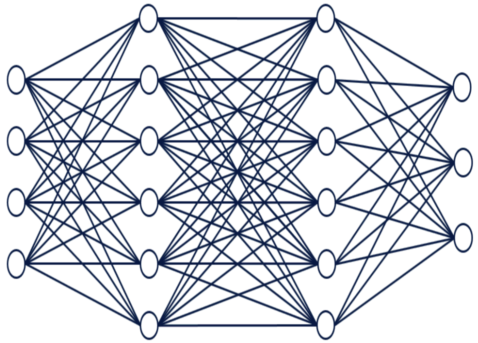
Qian Xie 谢倩 (Cornell ORIE)

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

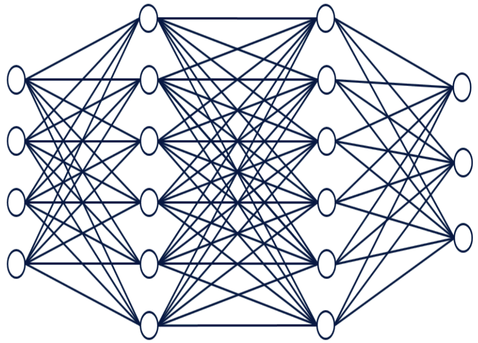
World of Hyperparameter Optimization

Hyperparameter tuning:

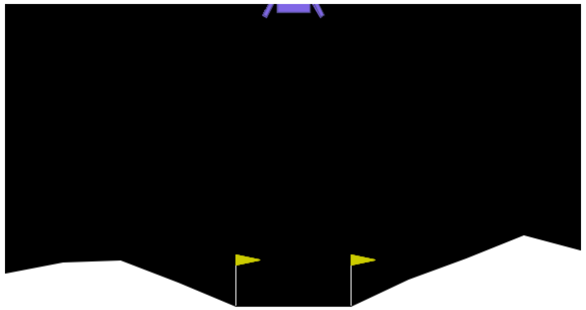
Training hyperparameters ⟶  ⟶ Accuracy

World of Hyperparameter Optimization

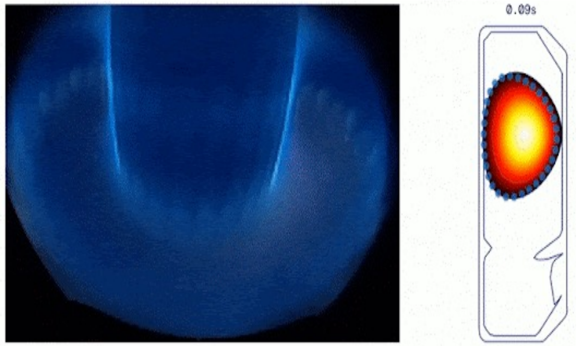
Hyperparameter tuning:

Training hyperparameters →  → Accuracy

Control optimization:

Control variables →  → Reward

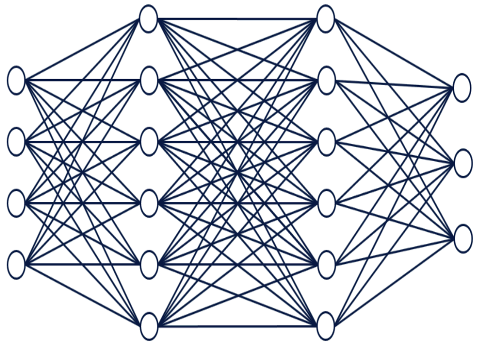
Plasma physics:

Fusion reactor design →  → Stability

World of Hyperparameter Optimization

unknown & expensive-to-evaluate

Hyperparameter tuning:

Training hyperparameters →  → Accuracy

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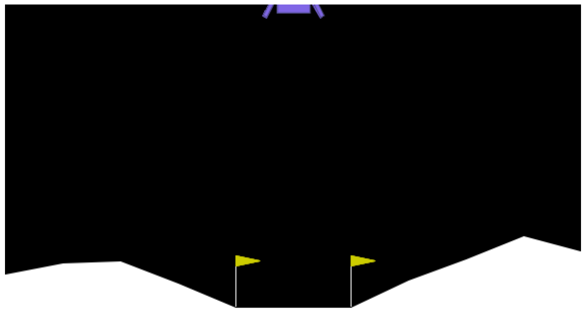
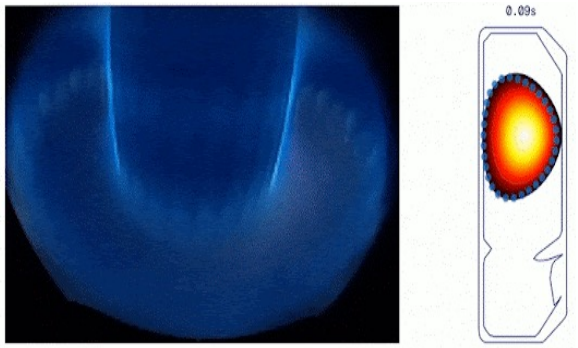
Control variables →  → Reward

Plasma physics:

Fusion reactor design →  → Stability

Black-Box Optimization

Black-box optimization:

unknown &
expensive-to-evaluate

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

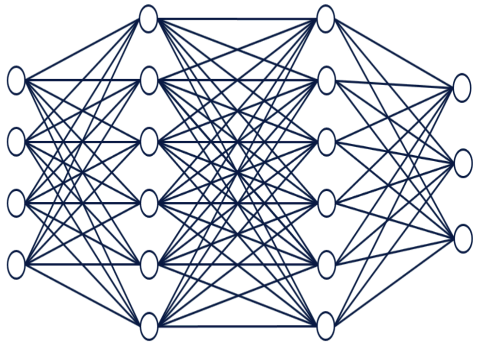
Goal: $\max_{x \in \mathcal{X}} f(x)$

Naïve (Non-Adaptive) Approach: Grid Search

Hyperparameter tuning:

unknown & expensive-to-evaluate

Training hyperparameters →



→ 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:

unknown &
expensive-to-evaluate

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

$f \sim$ Stochastic Process

limited #evaluations

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

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limited #evaluations

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

Key idea: maintain probabilistic belief about f

Bayesian Optimization

$f \sim$ Stochastic Process

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

Black-box function

Bayesian Optimization

Time 0

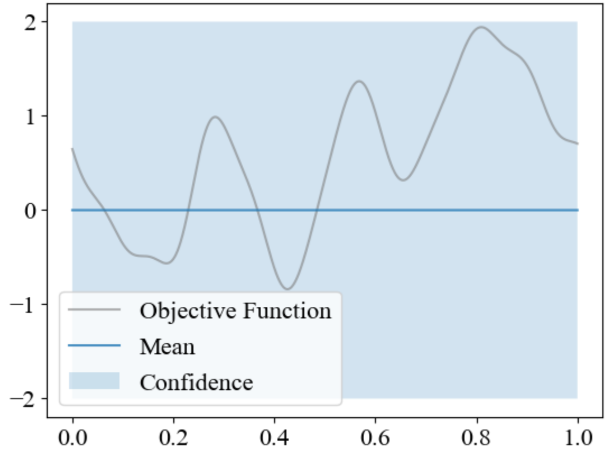
$f \sim$ Stochastic Process

$x \longrightarrow$

$\longrightarrow f(x)$

Model belief

Black-box function



Probabilistic model

(e.g., Gaussian process)

Bayesian Optimization

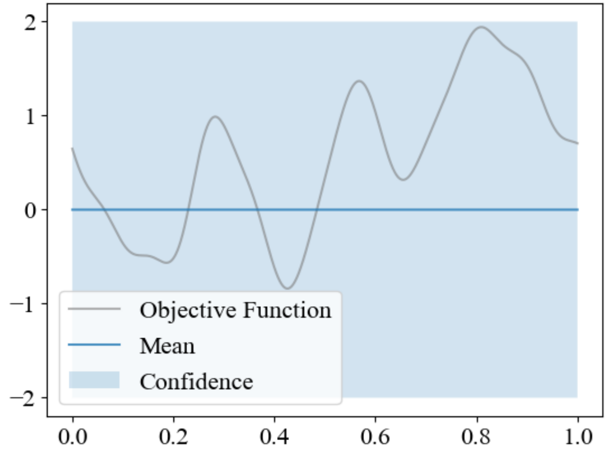
Time t

$f \sim$ Stochastic Process

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

Black-box function

Model belief



Probabilistic model
(e.g., Gaussian process)

Bayesian Optimization

Time t

$x_1, \dots, x_t \longrightarrow$

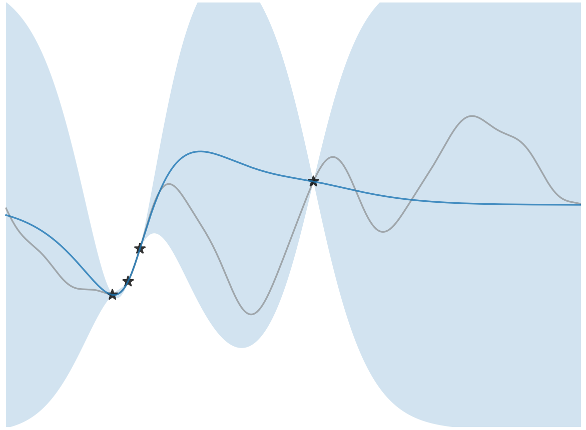
Black-box function

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

$f \sim$Stochastic Process

Update belief

(Bayes' rule)



Probabilistic model

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Bayesian Optimization

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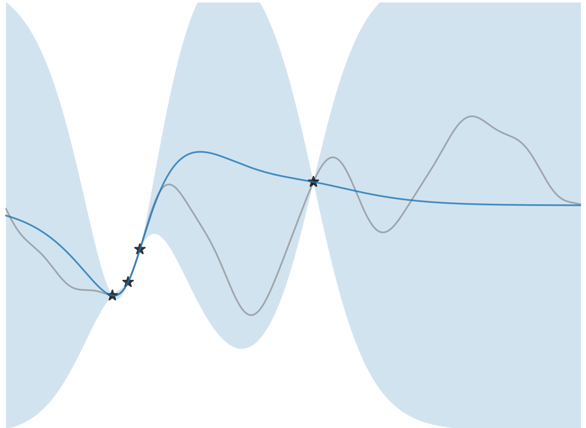
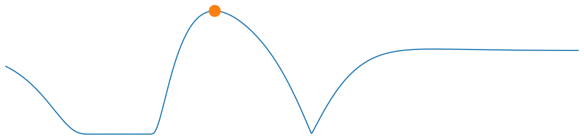


Probabilistic model
(e.g., Gaussian process)

scoring (worth of each point



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

Bayesian Optimization

Time t

$x_1, \ldots, x_t$ $\longrightarrow$

Black-box function

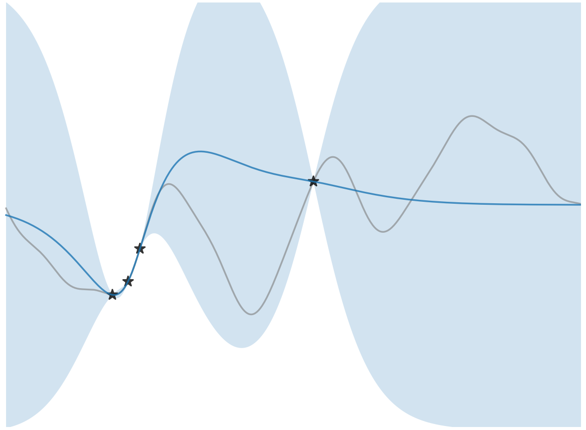
$\longrightarrow$ $f(x_1), \ldots, f(x_t)$

Decide next input

(gradient-based optimization)

Update belief

(Bayes' rule)



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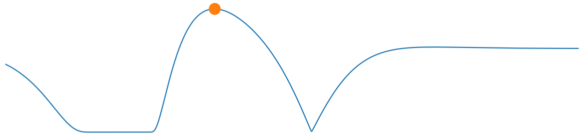
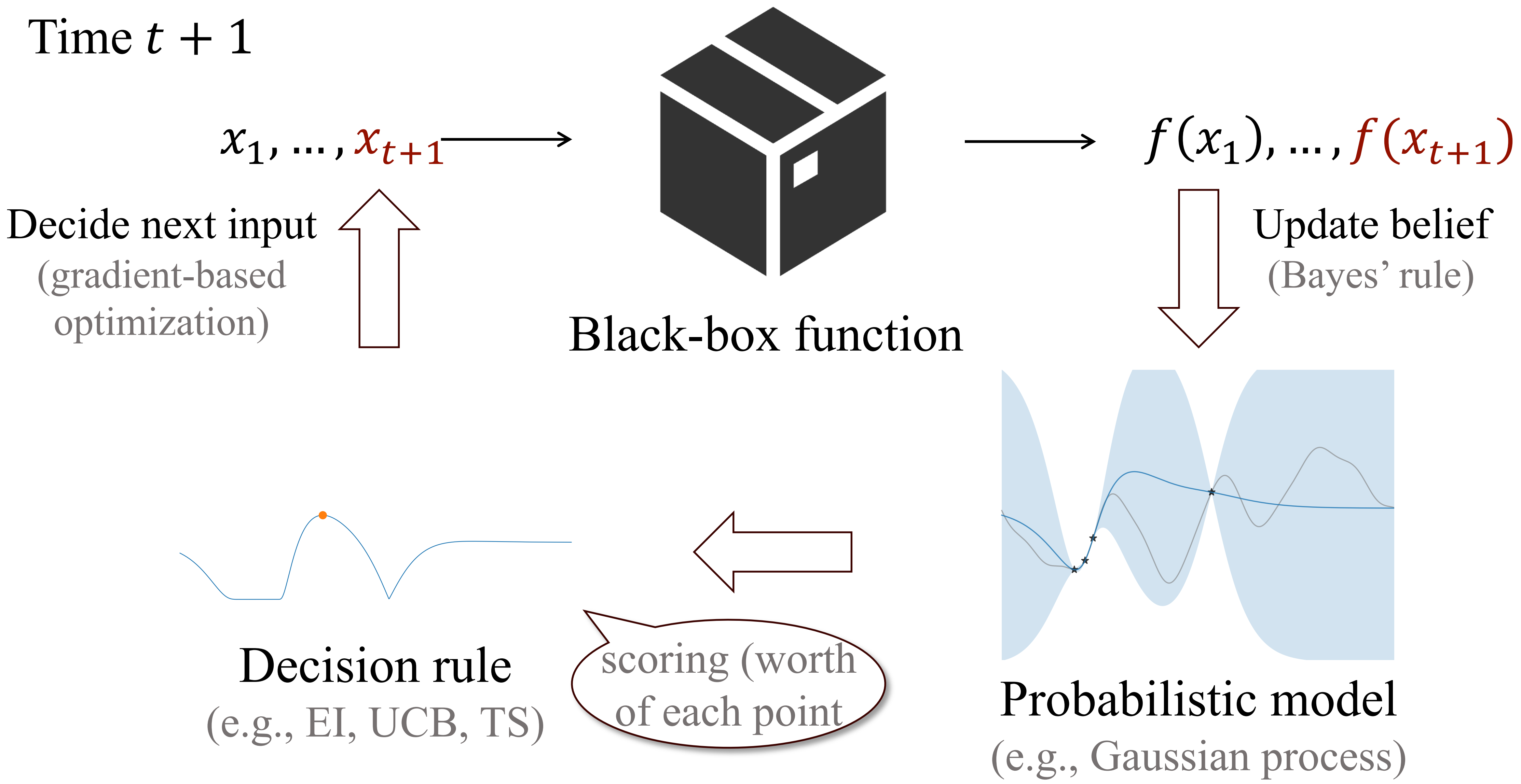


Decision rule

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

Bayesian Optimization



Bayesian Optimization

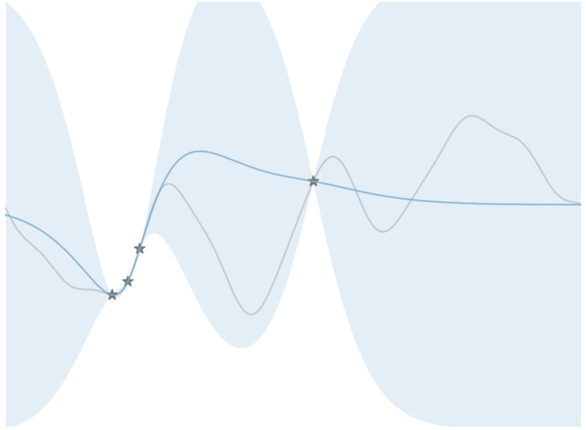
Time $t+1$

$x_1, \ldots, x_{t+1} \longrightarrow$

Black-box function

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

Update belief
(Bayes' rule)



Probabilistic model
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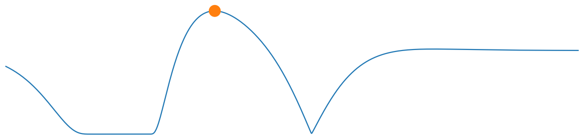


Decision rule
(e.g., EI, UCB, TS)

My focus

Decide next input
(gradient-based optimization)

Popular Decision Rule: Expected Improvement

current best observed

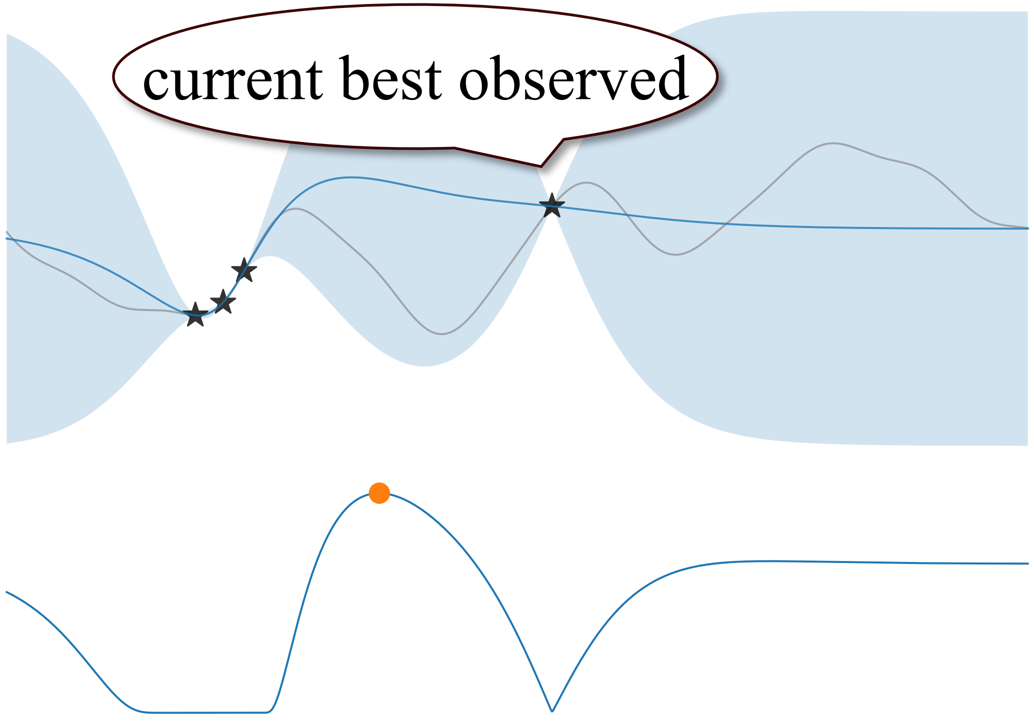
data

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

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

posterior distribution

One-step approximation to MDP



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

Popular Decision Rule: Expected Improvement

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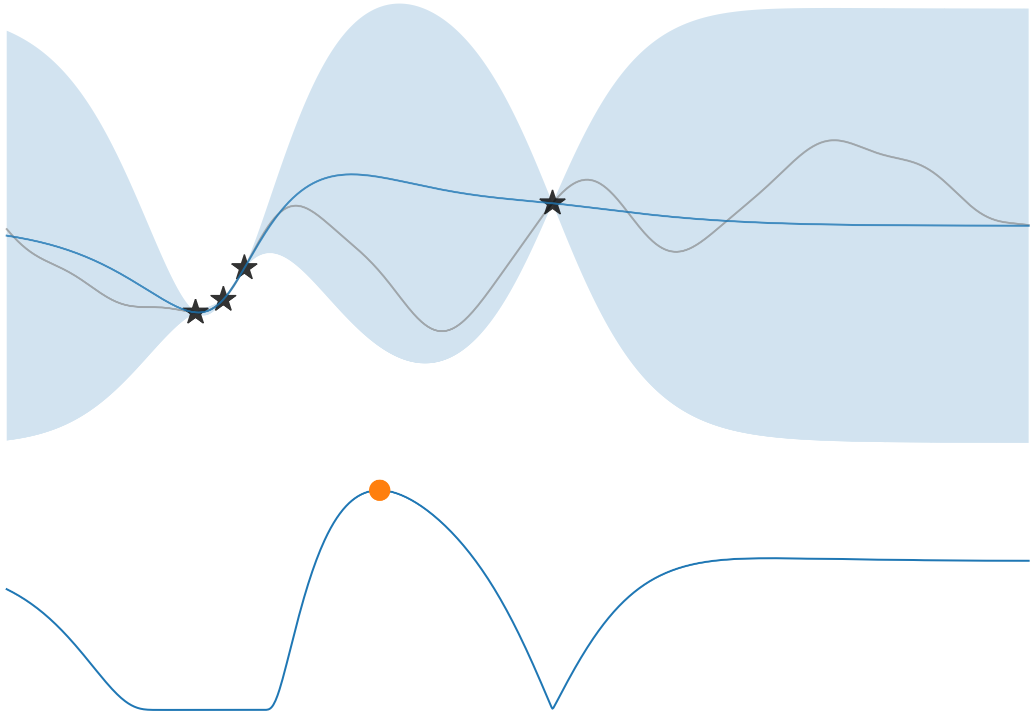
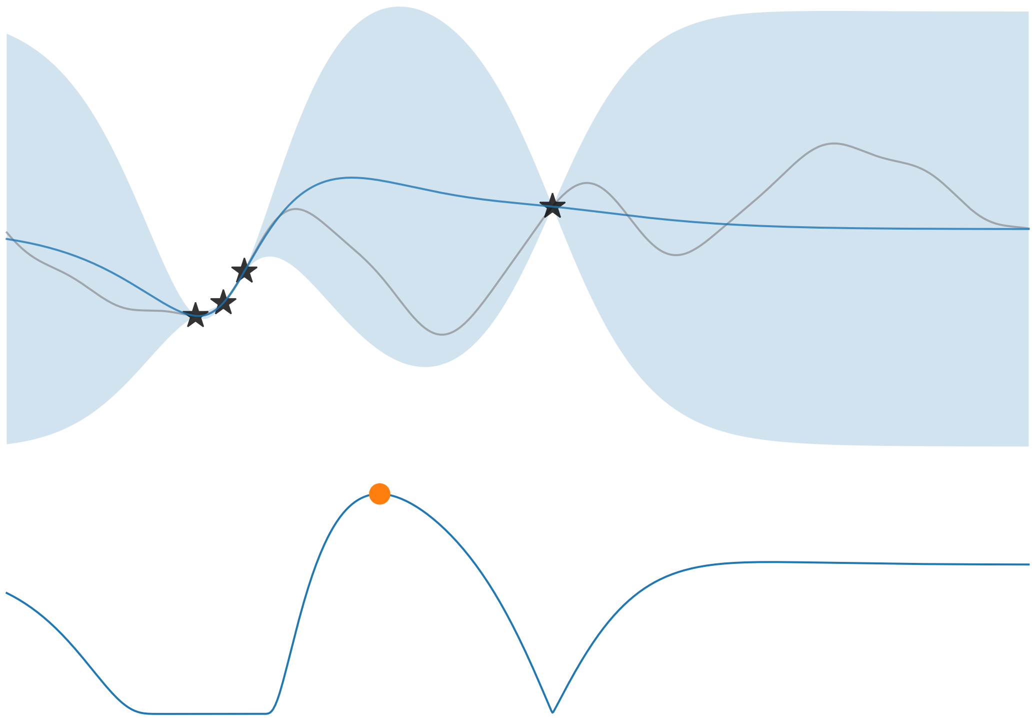


Expected improvement $\mathrm{EI}(x)$

Improvement-based design principle

Existing Design Principles

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

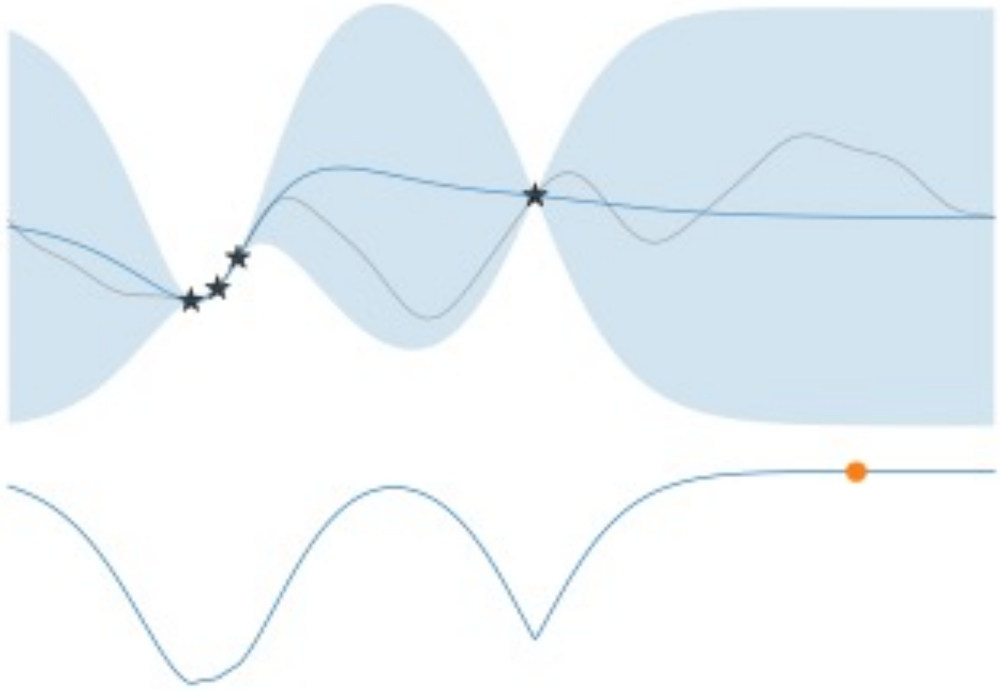


Expected improvement $\mathrm{EI}(x)$

Improvement-based design principle

New Design Principle: Gittins Index

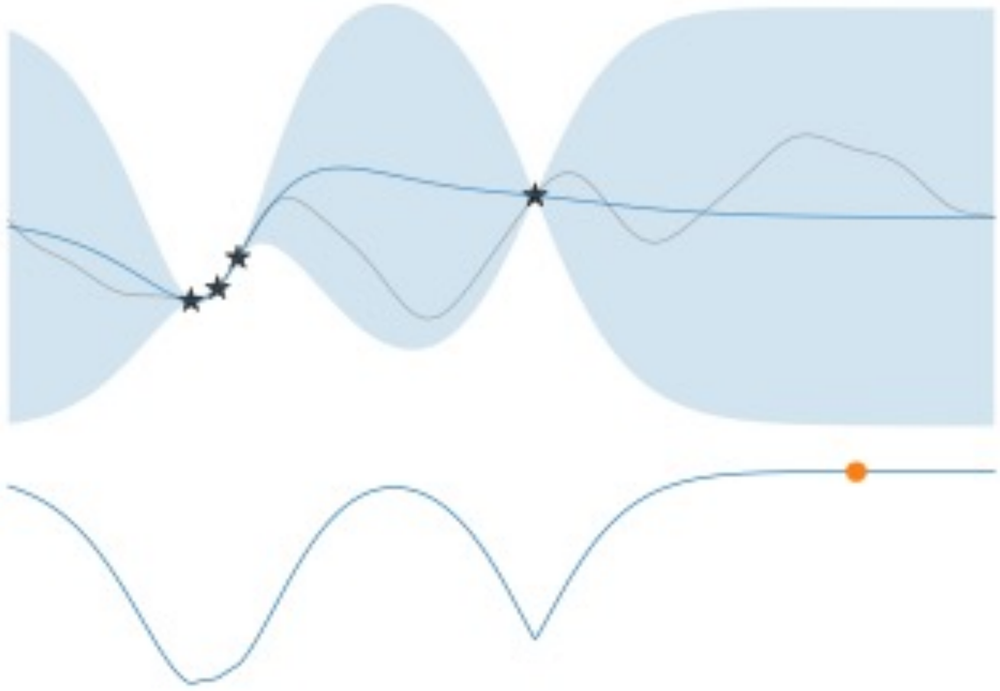
- Improvement-based (e.g., EI)
- Entropy-based
- Confidence bounds (UCB/LCB)
- Thompson sampling (TS)
- Gittins Index



Gittins index $\mathrm{GI}(x)$

New Design Principle: Gittins Index

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

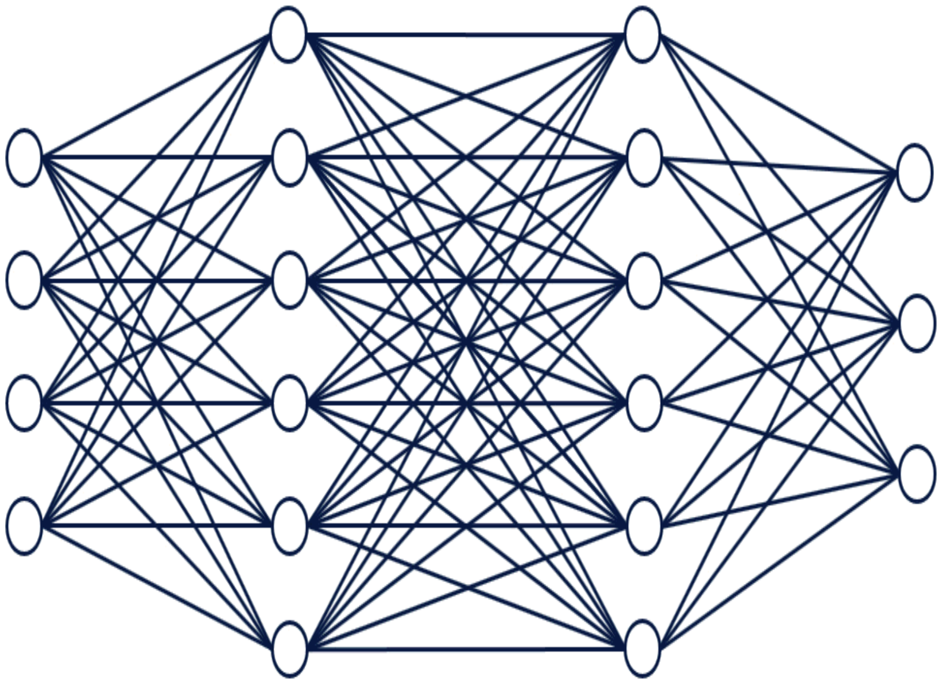


Gittins index $\mathrm{GI}(x)$

? 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

$\mathrm{EI}(x)/c(x)$

Why not subtraction?

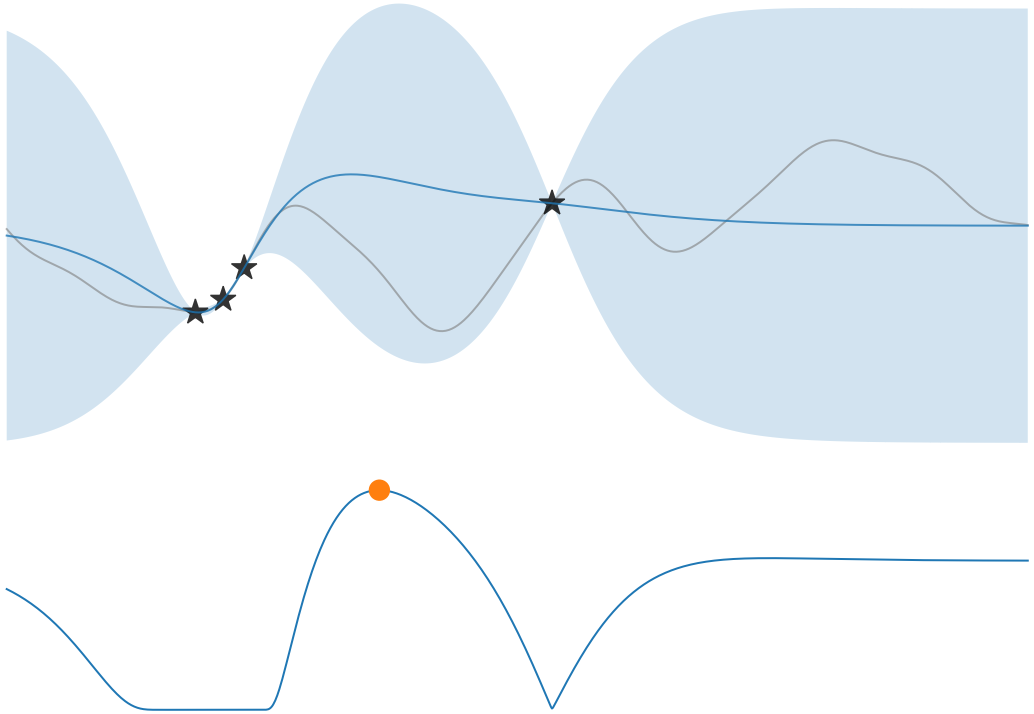
Smart stopping time

$\mathrm{EI}(x) \leq \theta$

Which threshold?

Observable multi-stage feedback

?



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

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

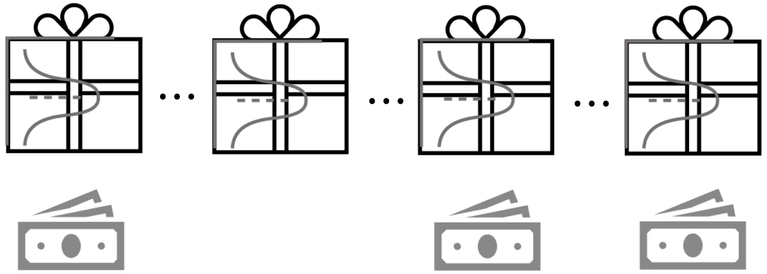
Smart stopping time

Features in Pandora's box

Observable multi-stage feedback

New design principle:
Gittins index

Optimal in related sequential decision problems



Why Gittins index?

Varying evaluation costs

Features in Pandora's box

Smart stopping time

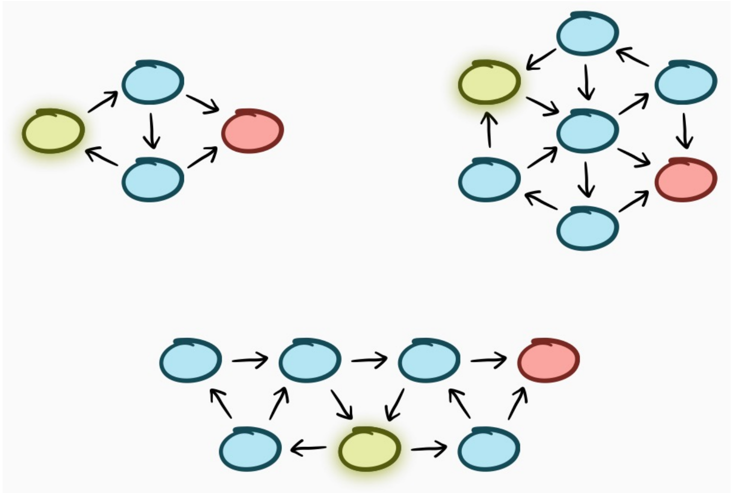
Features in Pandora's box

Observable multi-stage feedback

Features in Markov chain selection

New design principle: Gittins index

Optimal in related sequential decision problems



Why Gittins index?

Varying evaluation costs

Features in Pandora's box

This talk's focus

Smart stopping time

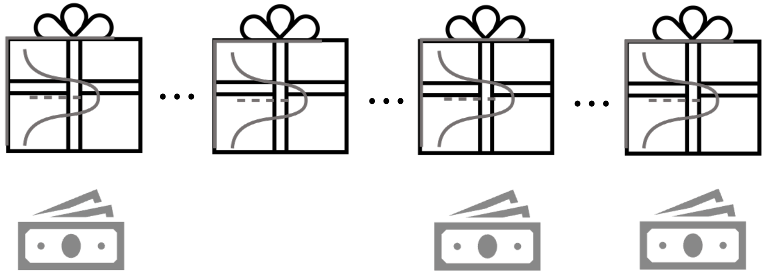
Features in Pandora's box

Observable multi-stage feedback

Features in Markov chain selection

New design principle: Gittins index

Optimal in related sequential decision problems



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

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

Coauthors

Varying evaluation costs
[NeurIPS’24]

Raul Astudillo

Smart stopping time
[Under review]

Linda Cai

Peter Frazier

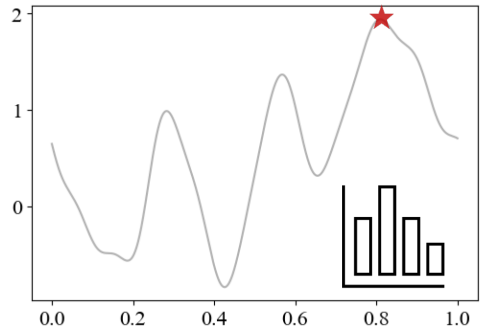
Alexander Terenin

Ziv Scully

Observable multi-stage feedback
[Ongoing work]

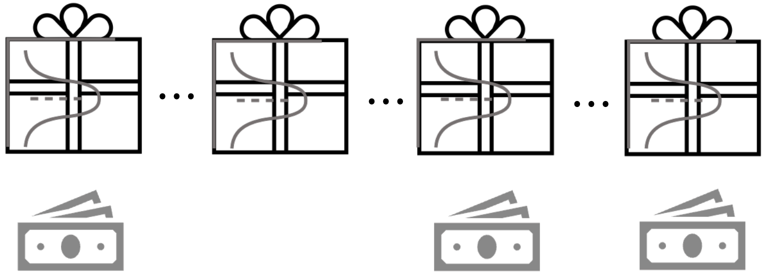
Outline

Studied Problem



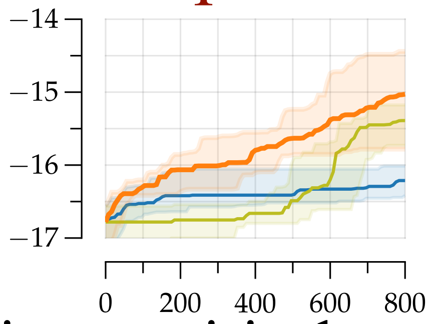
Cost-aware Bayesian optimization

Key idea



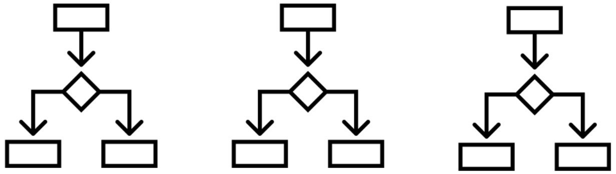
Link to simplified problem
and Gittins index theory

Impact



Competitive empirical performance

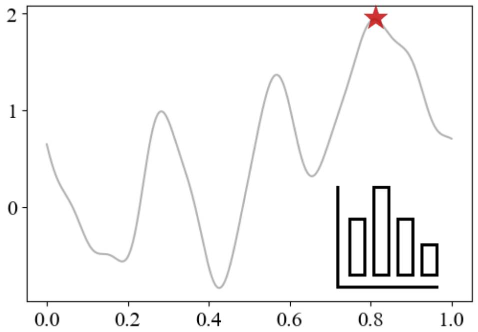
Future direction



“Exotic” Bayesian optimization

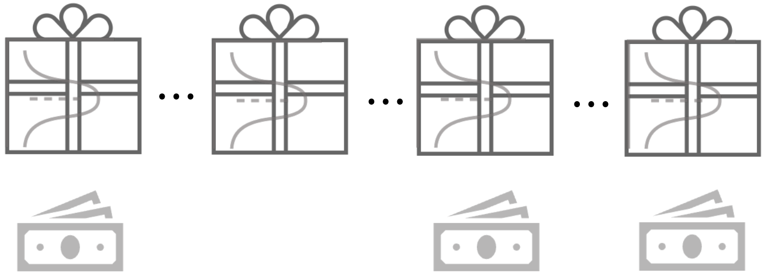
Outline

Studied Problem



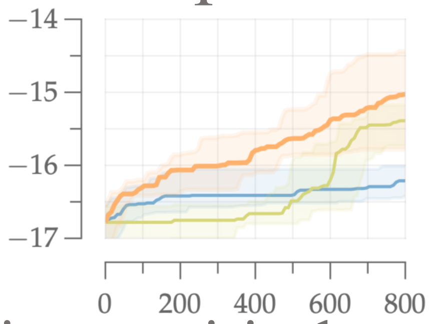
Cost-aware Bayesian optimization

Key idea



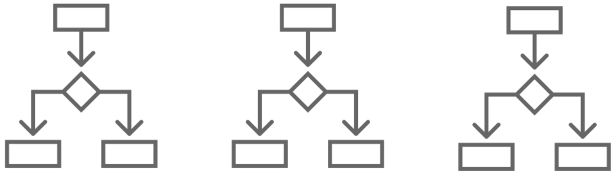
Link to simplified problem and Gittins index theory

Impact



Competitive empirical performance

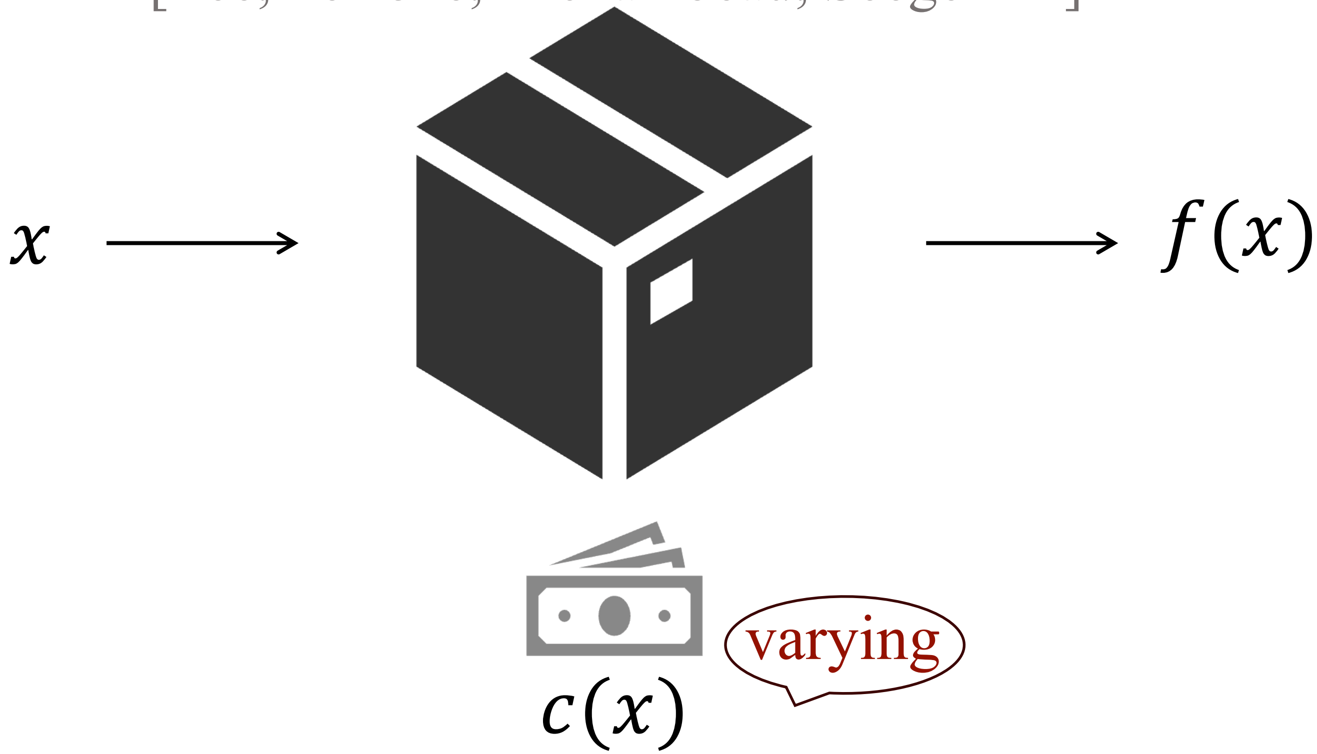
Future direction



"Exotic" Bayesian optimization

Cost-aware Bayesian Optimization

[Lee, Perrone, Archambeau, Seeger'21]



Cost-aware Bayesian Optimization

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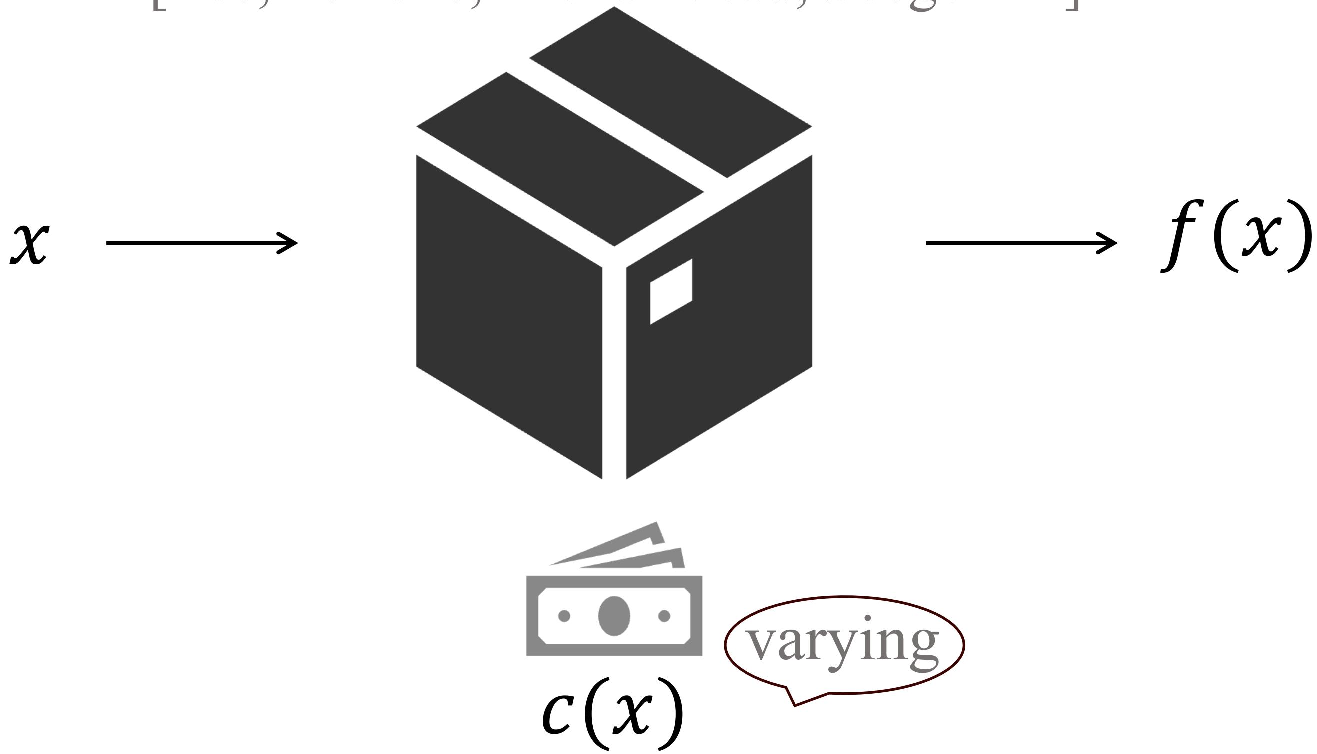
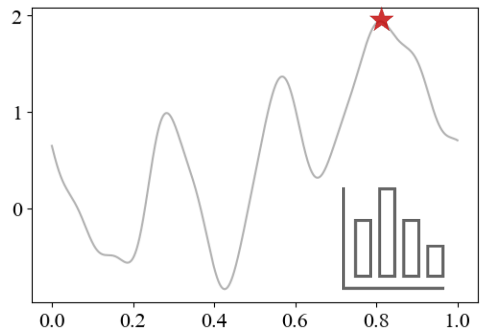


Goal: $\sup_{\text{policy}} \mathbb{E} \max_{t=1,2,\ldots,T} f(x_t)$

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

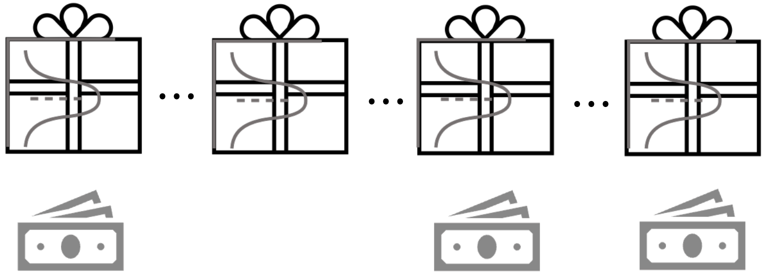
Outline

Studied Problem



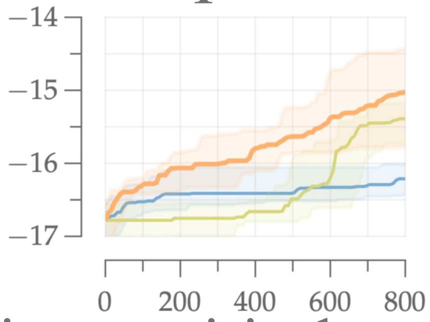
Cost-aware Bayesian optimization

Key idea



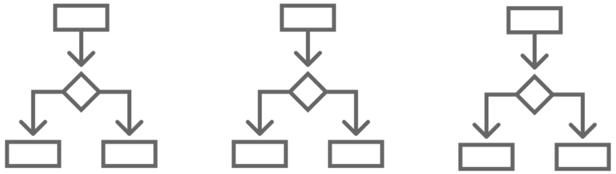
Link to simplified problem and Gittins index theory

Impact



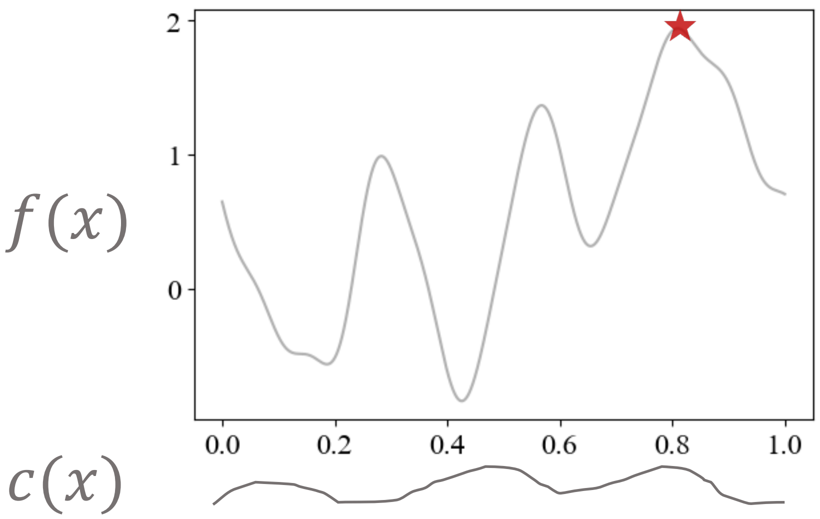
Competitive empirical performance

Future direction

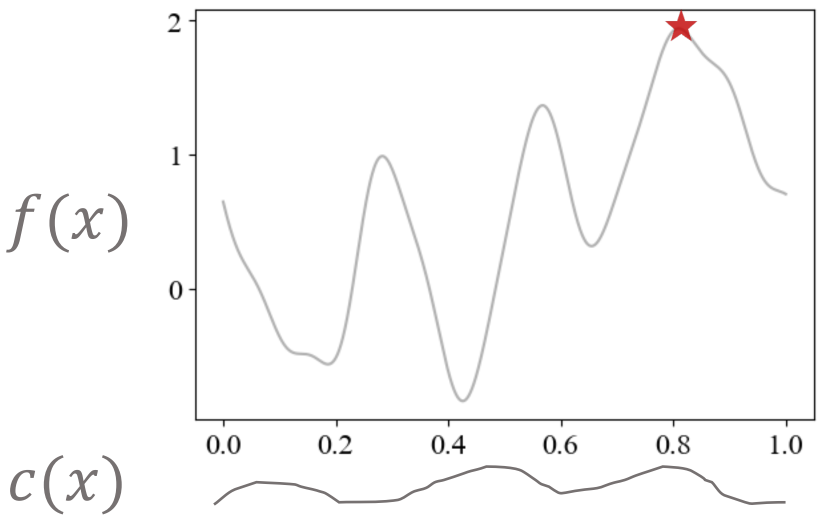


"Exotic" Bayesian optimization

Cost-aware Bayesian Optimization



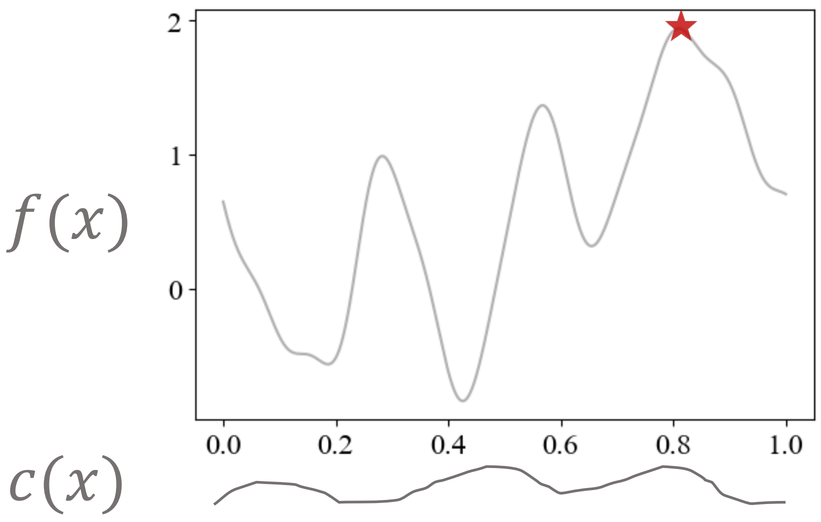
Cost-aware Bayesian Optimization



Continuous

Correlated

Cost-aware Bayesian Optimization



Continuous

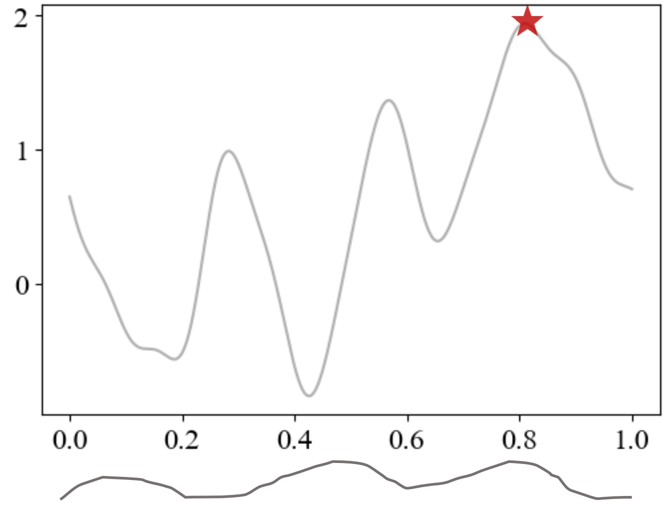
Correlated

Intractable MDP!

Cost-aware Bayesian Optimization   Pandora's Box

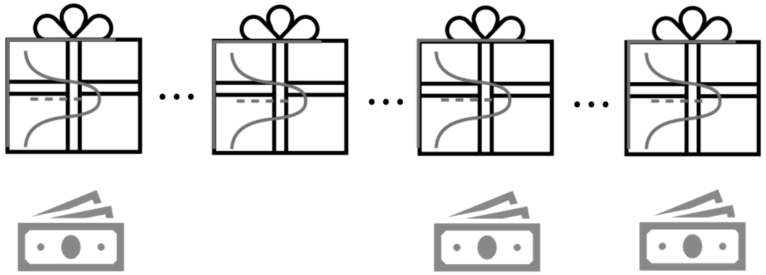
[Weitzman'79]

$f(x)$



$c(x)$

$\Longrightarrow$



$f(x)$

$c(x)$

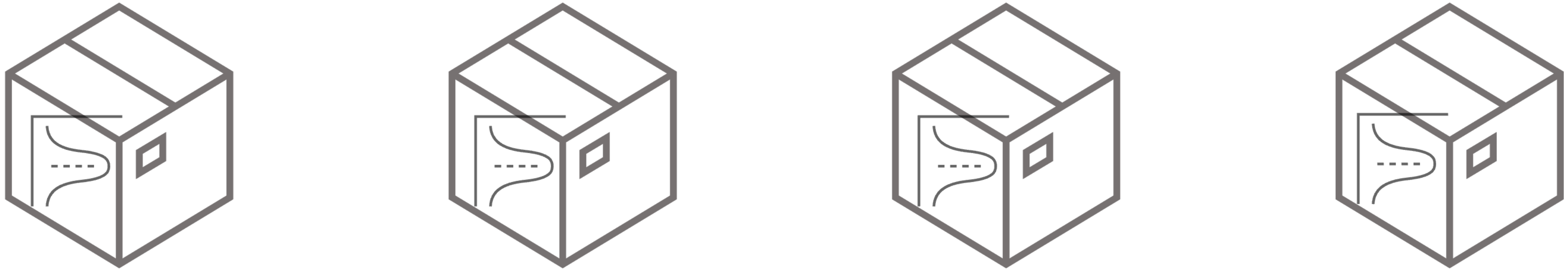
Continuous $\Longrightarrow$ Discrete

Correlated $\Longrightarrow$ Independent

Intractable MDP!

Pandora’s Box

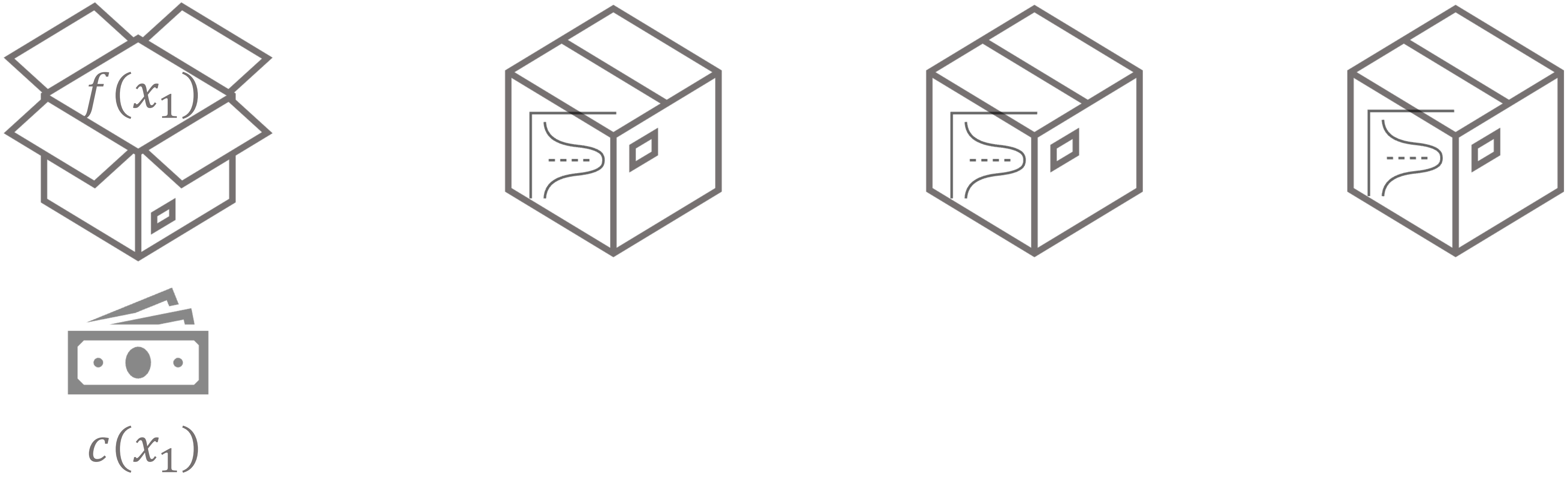
$t = 0$



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

Pandora's Box

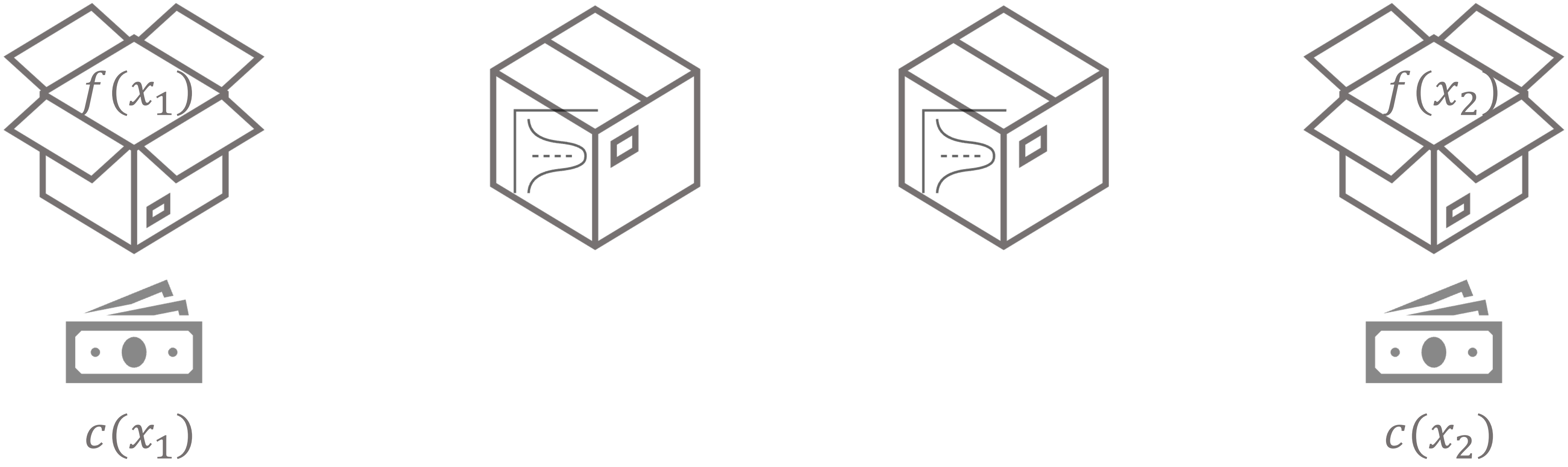
$t = 1$



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

Pandora's Box

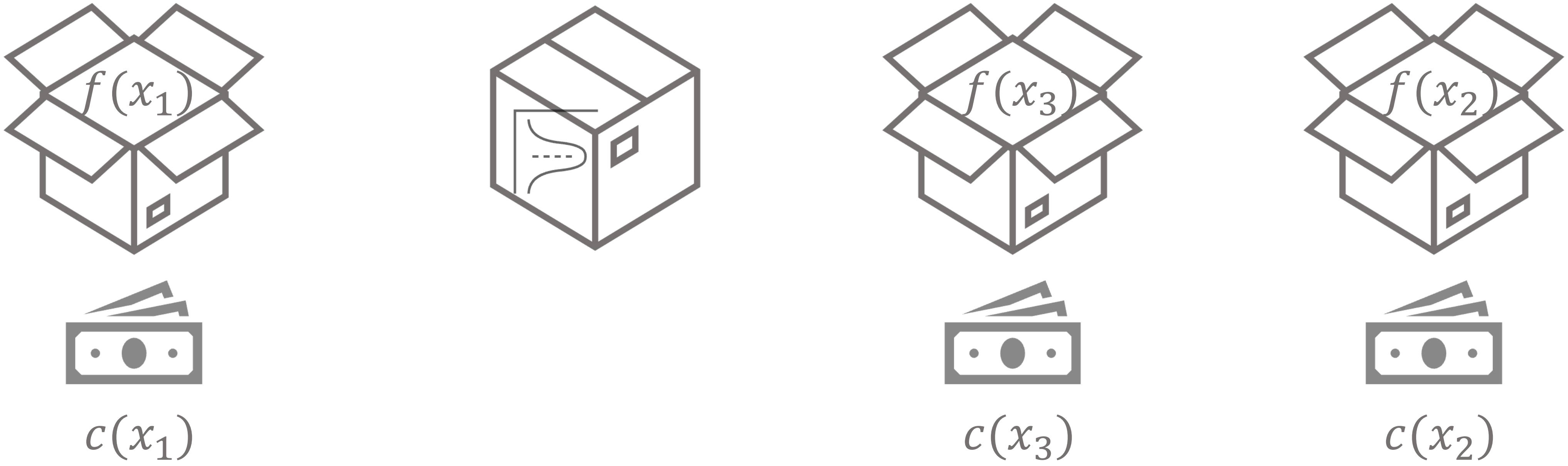
$t = 2$



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

Pandora's Box

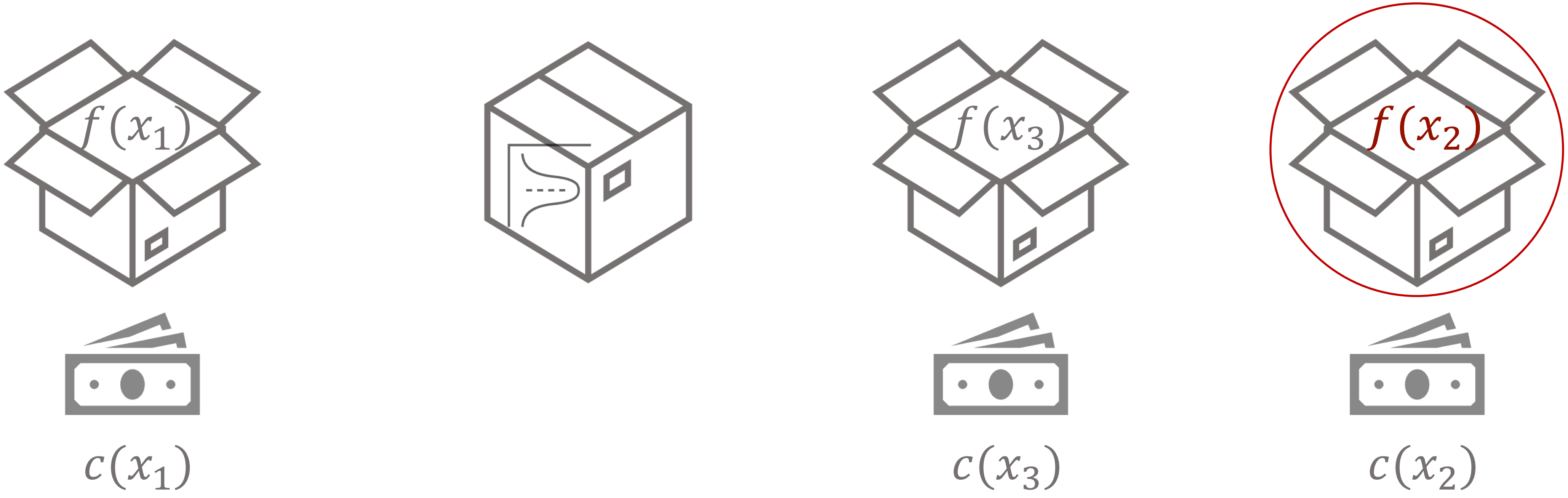
$t = 3$



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

Pandora's Box

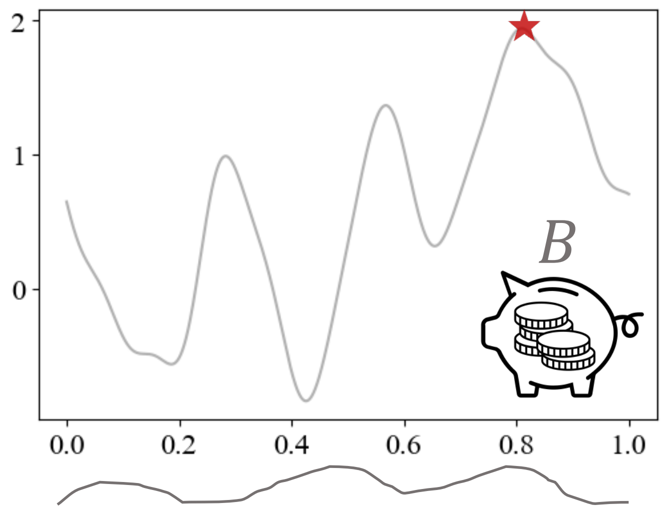
$t = T$, stop



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

Cost-aware Bayesian Optimization

$f(x)$



$c(x)$

Continuous

Correlated

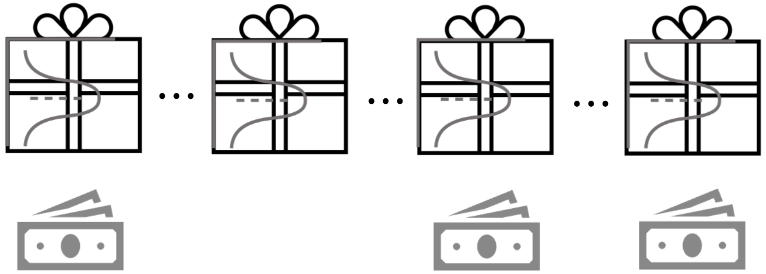
Budget-constrained

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

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

Pandora's Box

[Weitzman'79]



$f(x)$

$c(x)$

Discrete

Independent

Cost-per-sample

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

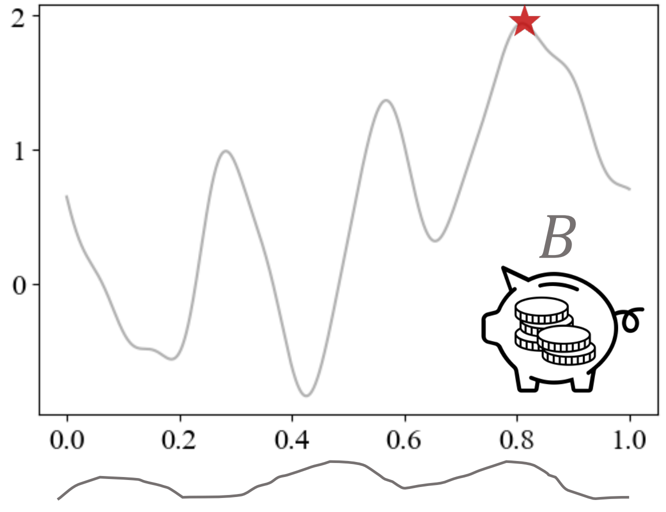
Cost-aware Bayesian Optimization

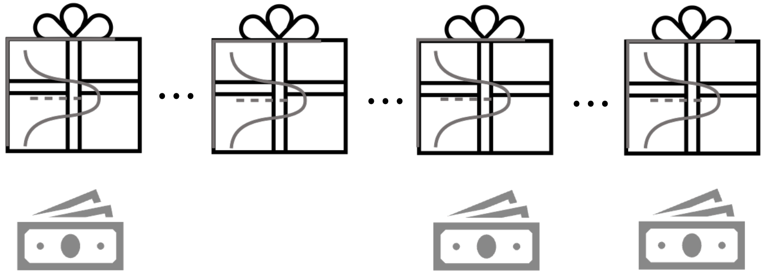
Pandora's Box

[Weitzman'79]

$f(x)$

$c(x)$





$f(x)$

$c(x)$

Continuous

Discrete

Correlated

Independent

Expected-budget-constrained

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

Cost-per-sample

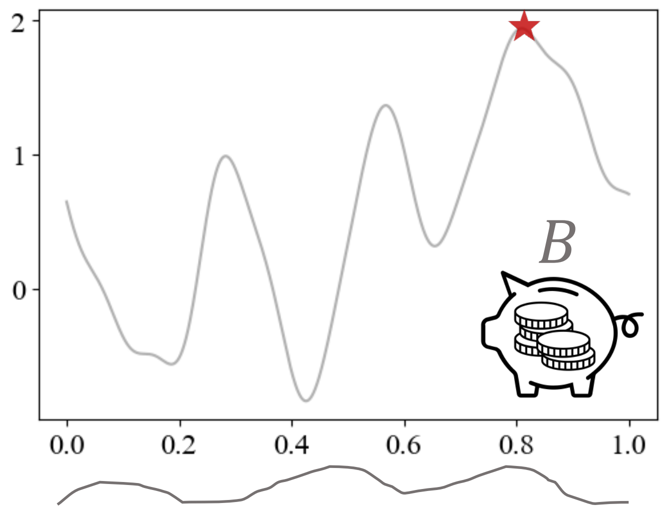
$$\sup_{\text{policy}} \mathbb{E}\left(\max_{t=1,2,\dots,T} f(x_t) - \sum_{t=1}^{T} c(x_t) \right)$$

Cost-aware Bayesian Optimization

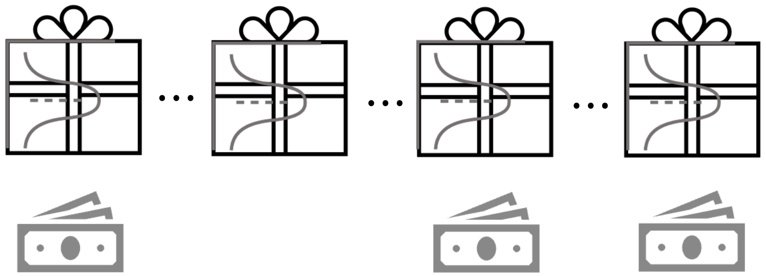
Pandora's Box

[Weitzman'79]

$f(x)$



$c(x)$



$f(x)$

$c(x)$

Continuous

Discrete

Correlated

Independent

Ebc & Cps

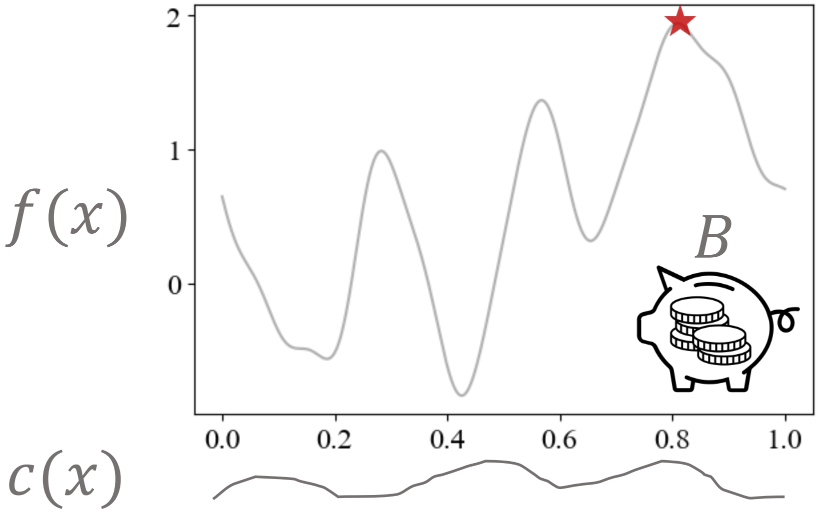
$$\sup_{\text{policy}} \mathbb{E} \max_{t=1,2,\ldots,T} f(x_t)$$

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

Cost-per-sample

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

Cost-aware Bayesian Optimization



Continuous

Correlated

Ebc & Cps

Intractable MDP!

Pandora's Box

[Weitzman'79]

Discrete

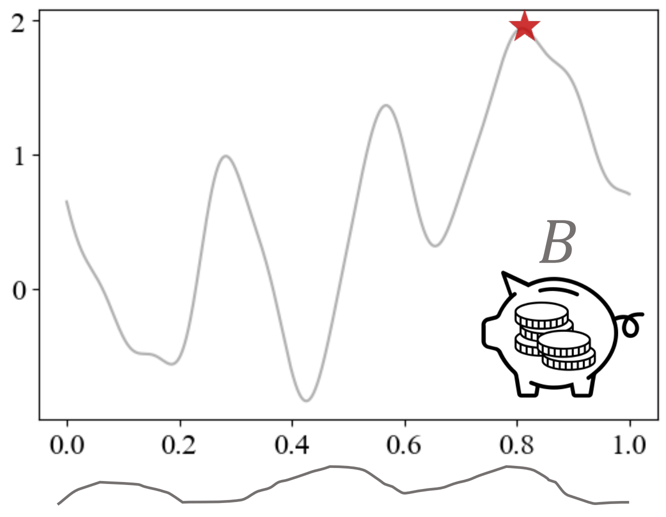
Independent

Cost-per-sample

Optimal policy: Gittins index

Cost-aware Bayesian Optimization

$f(x)$



$c(x)$

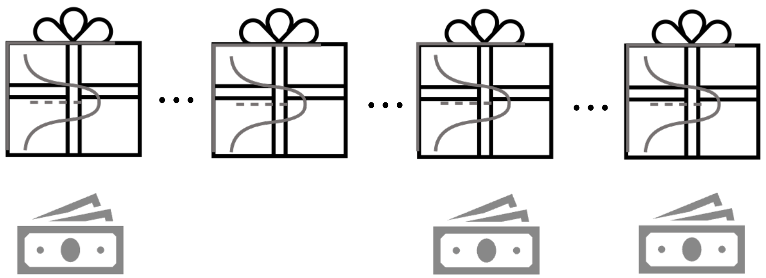
Continuous

Correlated

Ebc & Cps

Pandora's Box

[Weitzman'79]



$f(x)$

$c(x)$

Discrete

Independent

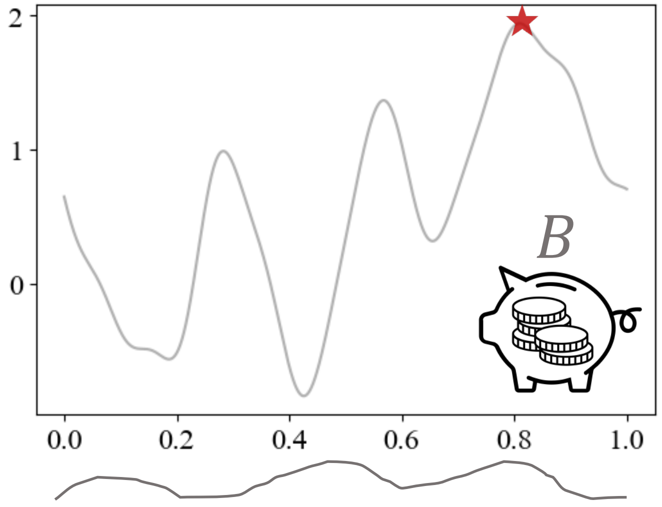
Cost-per-sample

How to translate?

$\Longleftarrow$ Optimal policy: Gittins index

Cost-aware Bayesian Optimization

$f(x)$



$c(x)$

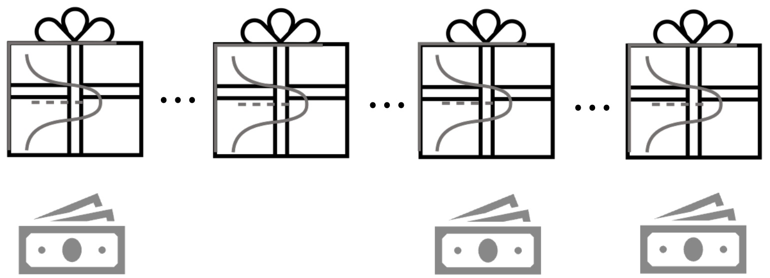
Continuous

Correlated

Ebc & Cps

Pandora's Box

[Weitzman'79]



Discrete

Independent

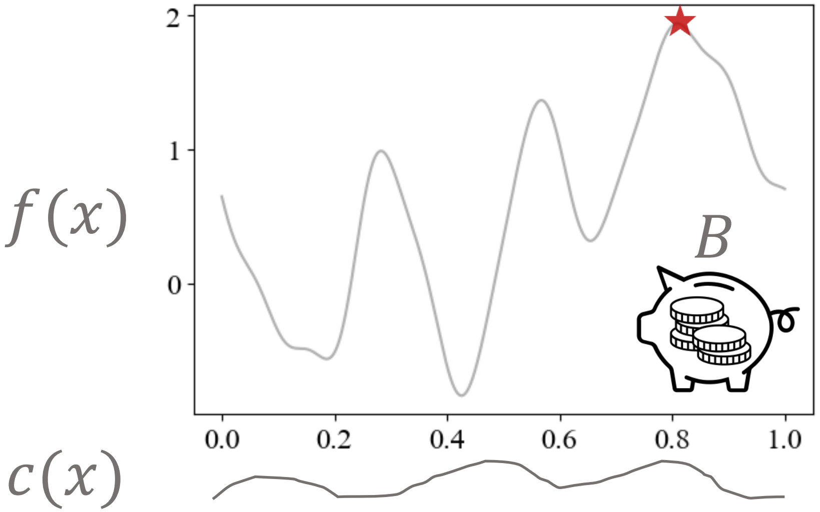
Cost-per-sample

incorporate posterior

Acquisition function $\Longleftarrow$ Optimal policy: Gittins index

+ stopping rule

Cost-aware Bayesian Optimization



Continuous

Correlated

Pandora's Box

[Weitzman'79]

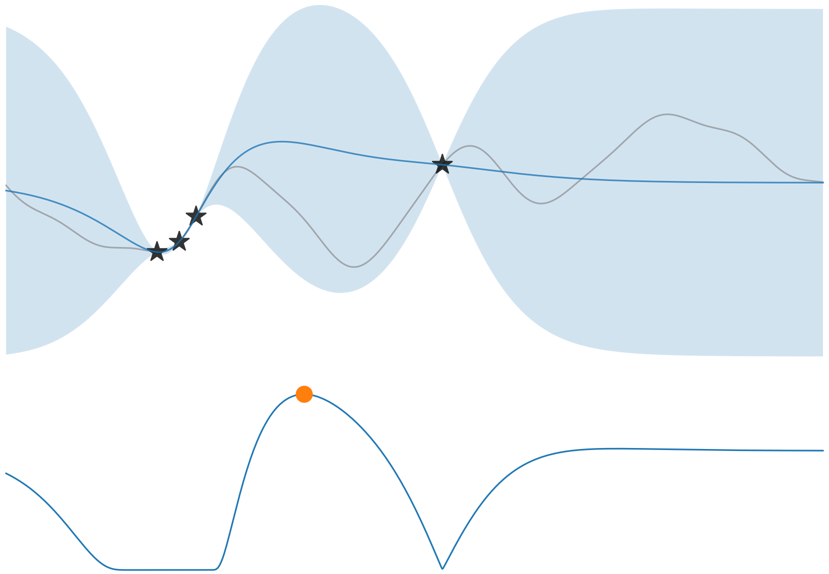
Discrete

Independent

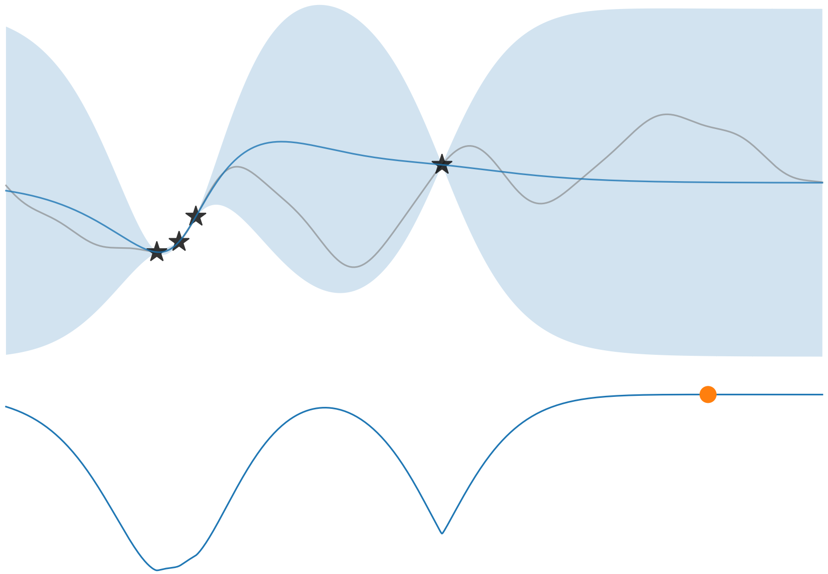
Acquisition function + stopping rule $\xLeftarrow{\text{incorporate posterior}}$ Optimal policy: Gittins index

How to compute?

Expected Improvement



Gittins Index



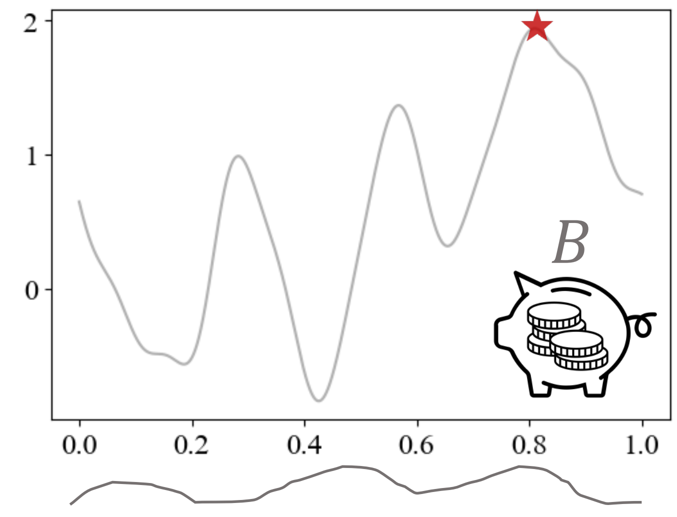
$\mathrm{EI}_{f|D}(x; g) := \mathbb{E}[\max(f(x) - g, 0) \mid D]$ $\mathrm{GI}_{f|D}(x) = g$ s.t. $\mathrm{EI}_{f|D}(x; g) = c(x)$

	Expected Improvement	Gittins Index
Selection rule:	$\max_x \mathrm{EI}_{f|D}(x; y_{\mathrm{best}})$	$\max_x \mathrm{GI}_{f|D}(x; c(x))$
Stopping rule:	$\mathrm{EI}_{f|D}(x; y_{\mathrm{best}}) \leq c$	$\mathrm{GI}_{f|D}(x; c(x)) \leq y_{\mathrm{best}}$

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

Cost-aware Bayesian Optimization

$f(x)$



$c(x)$

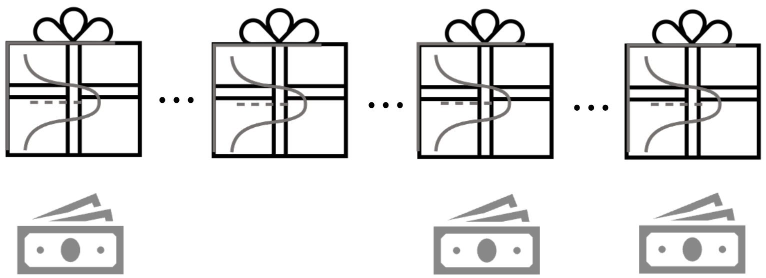
Continuous

Correlated

Ebc & Cps

Pandora's Box

[Weitzman'79]



$f(x)$

$c(x)$

Discrete

Independent

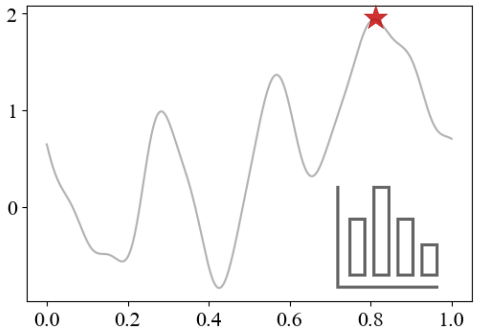
Cost-per-sample

Acquisition function + stopping rule $\overset{\text{incorporate posterior}}{\Longleftarrow}$ Gittins index is optimal

Empirically good?

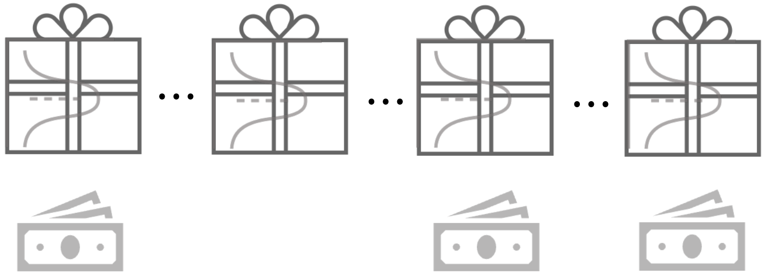
Outline

Studied Problem



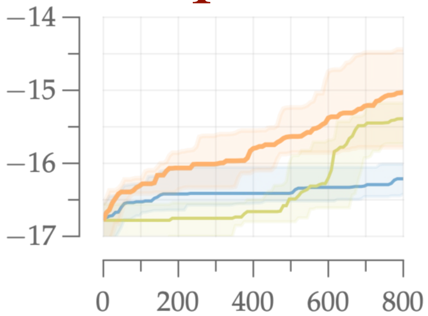
Cost-aware Bayesian optimization

Key idea



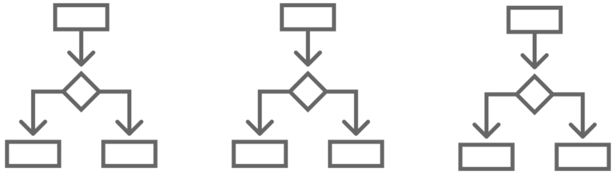
Link to Pandora's box and Gittins index theory

Impact



Competitive empirical performance

Future direction



"Exotic" Bayesian optimization

Experiment Setup: Objective Functions

Synthetic

Samples from prior

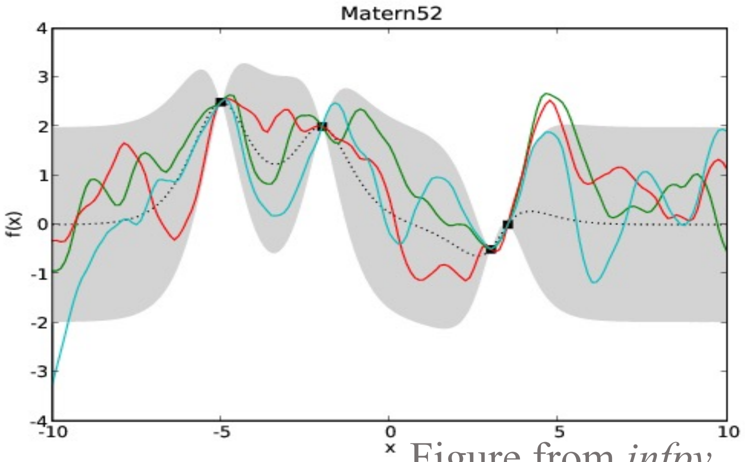


Figure from *infpy*

Ackley function

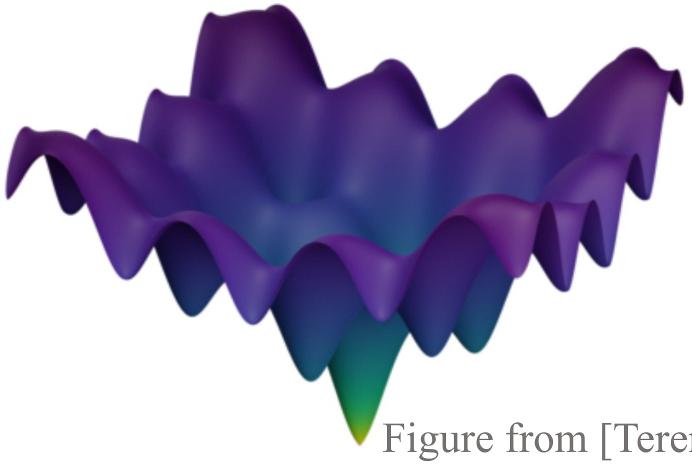


Figure from [Terenin'22]

Empirical

Pest Control

Figure from ChatGPT

Lunar Lander

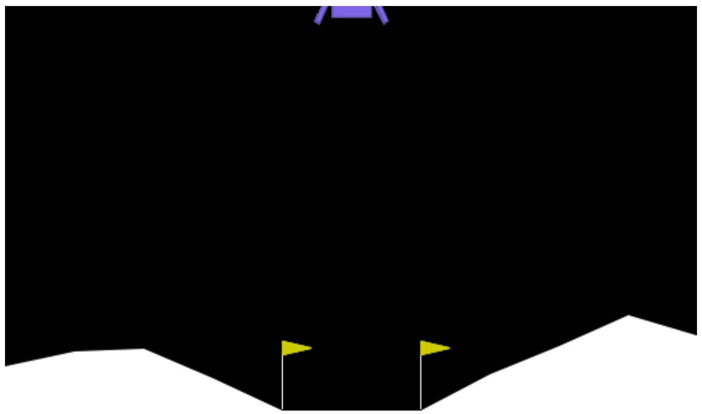
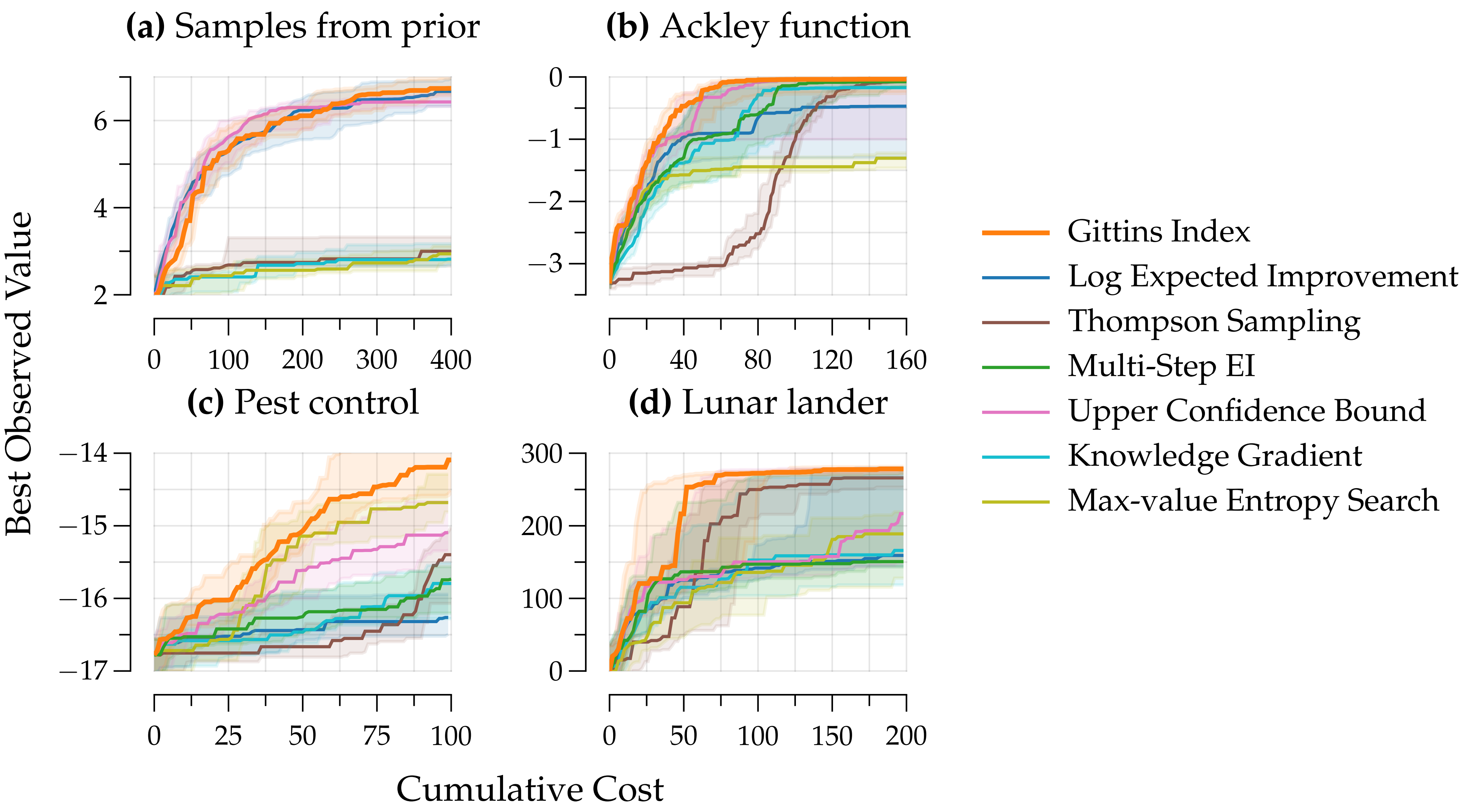
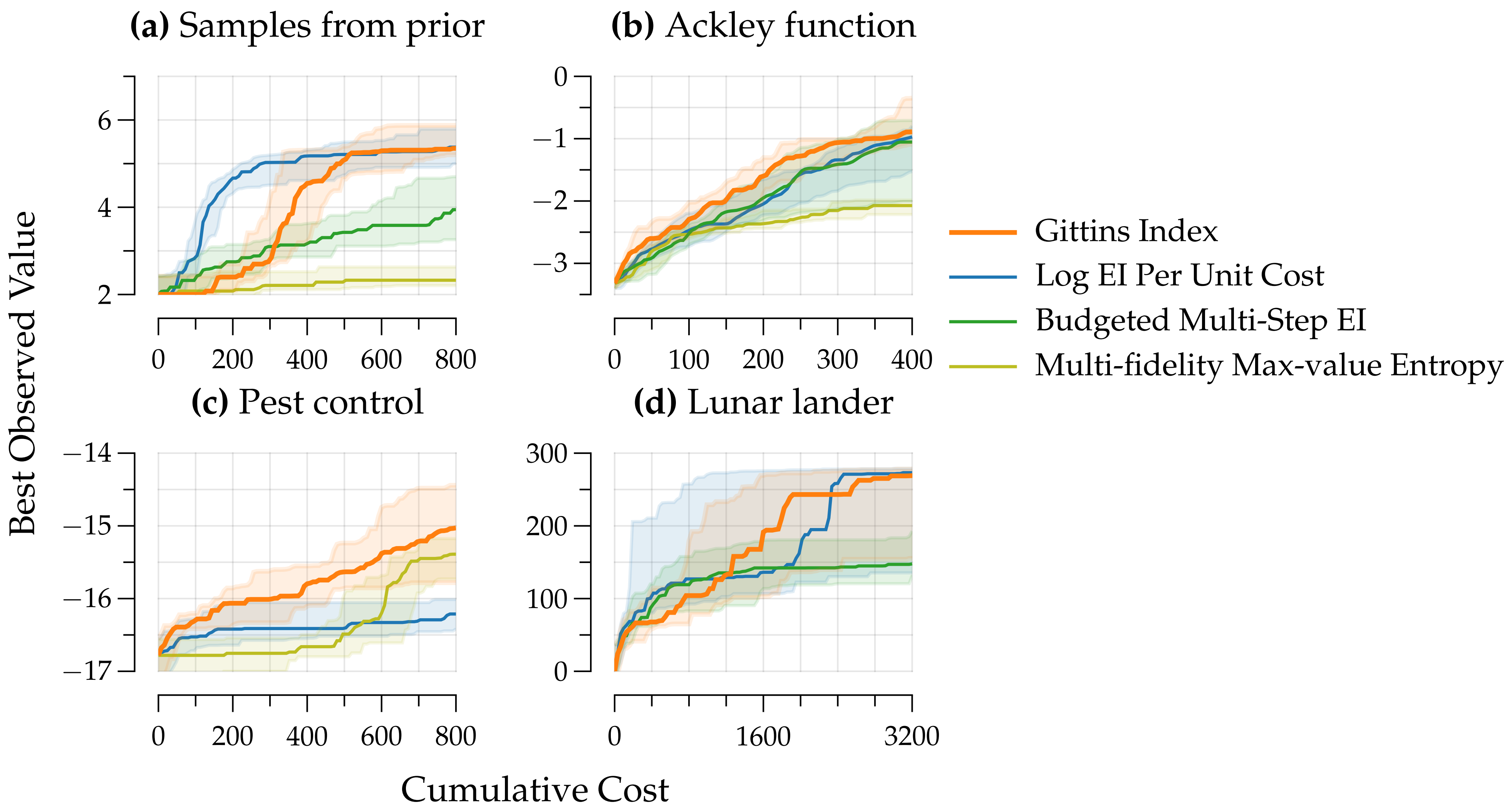


Figure from OpenAI Gym

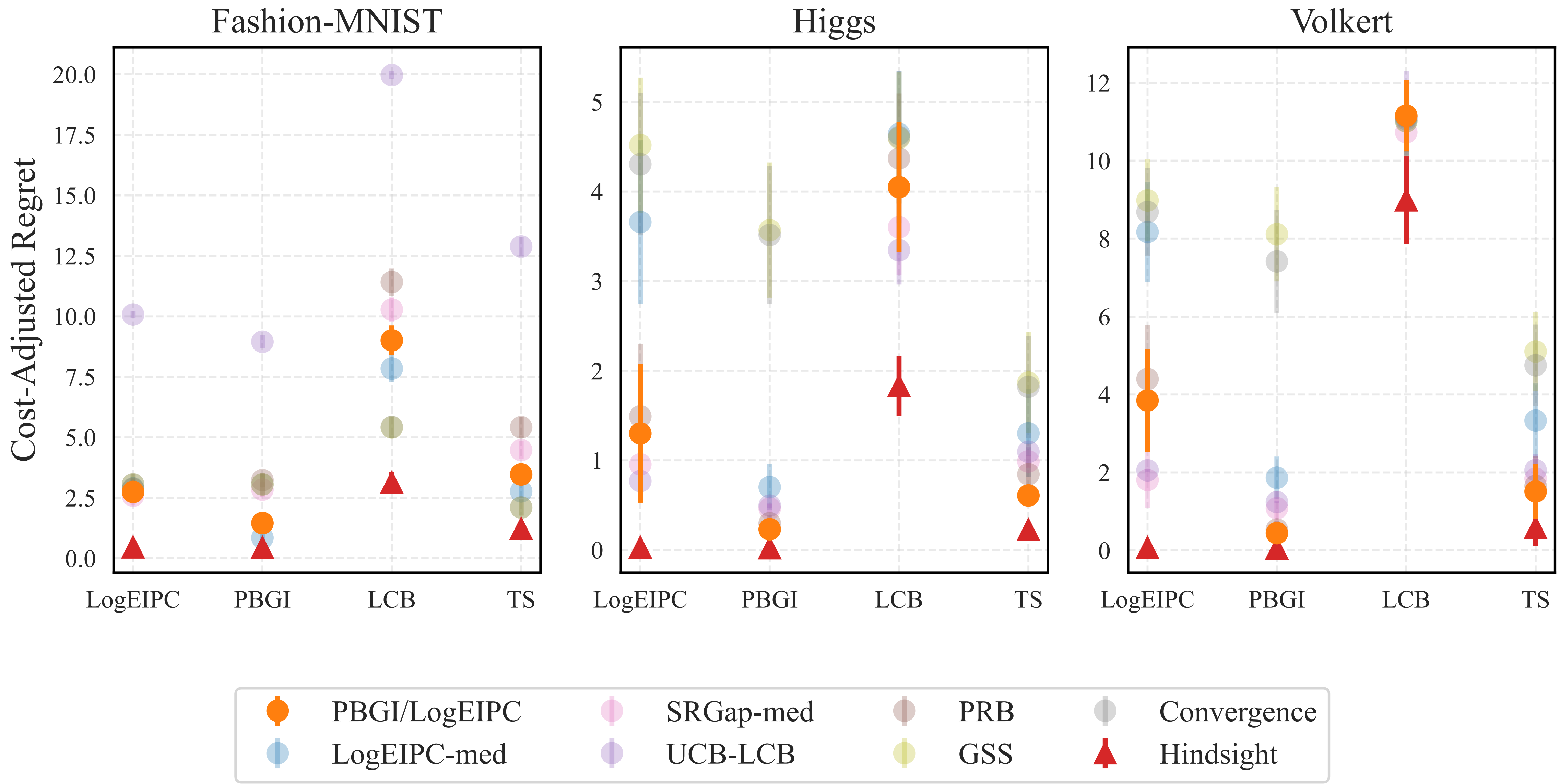
Uniform-cost: Gittins Index vs Baselines



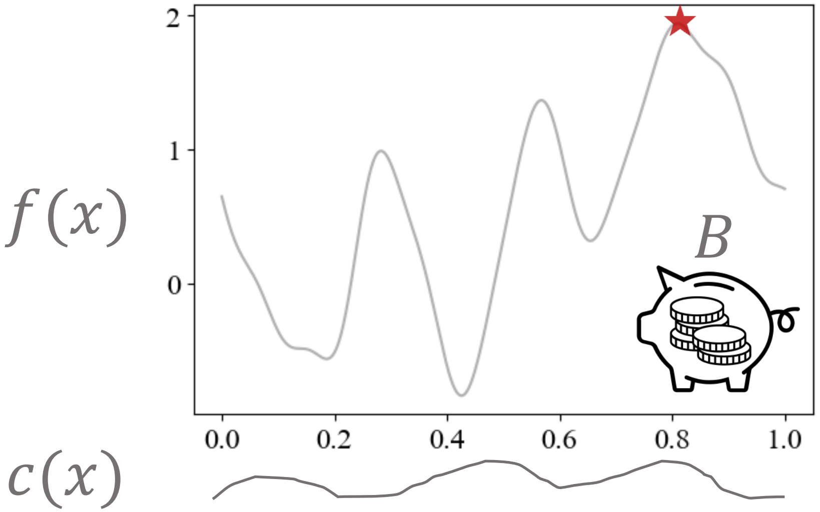
Varying-cost: Gittins Index vs Baselines



Stopping Rule: Gittins Index vs Baselines



Cost-aware Bayesian Optimization



Continuous

Correlated

Ebc & Cps

Pandora's Box

[Weitzman'79]

Discrete

Independent

Cost-per-sample

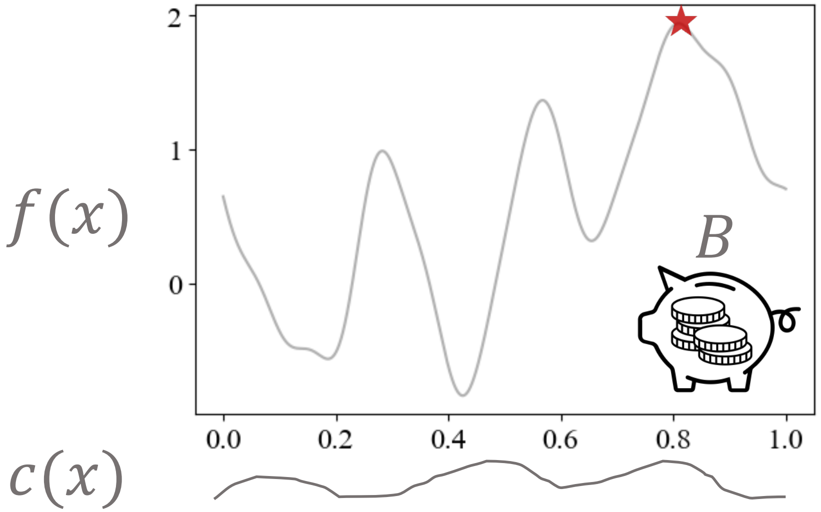
Acquisition function + stopping rule $\xLeftarrow{\text{incorporate posterior}}$ Gittins index is optimal

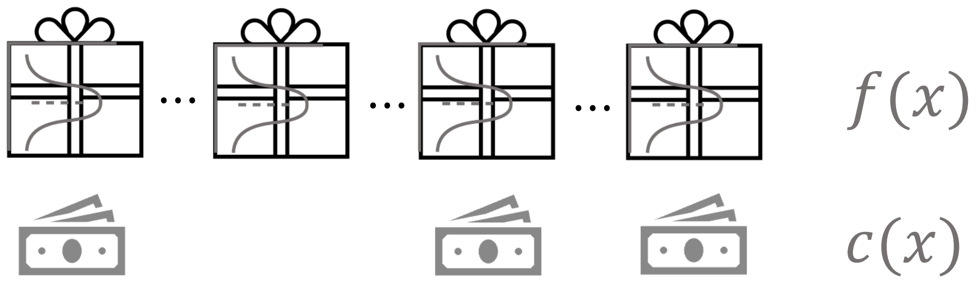
Theoretical guarantee?

Cost-aware Bayesian Optimization

Pandora's Box

[Weitzman'79]





Continuous | Discrete

Correlated | Independent

Ebc & Cps | Cost-per-sample

incorporate posterior

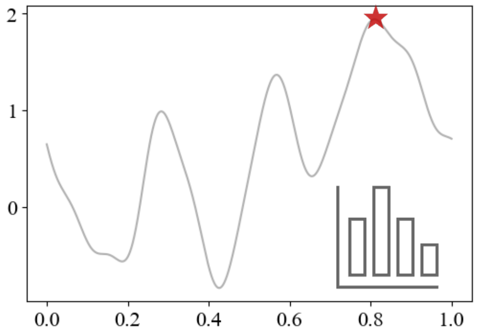
Acquisition function + stopping rule $\Longleftarrow$ Gittins index is optimal

Theoretical guarantee?

Yes! A bound on expected cost up to stopping

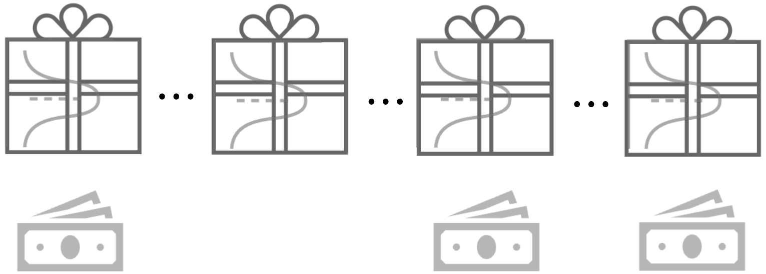
Gittins Index: A New Design Principle

Studied Problem



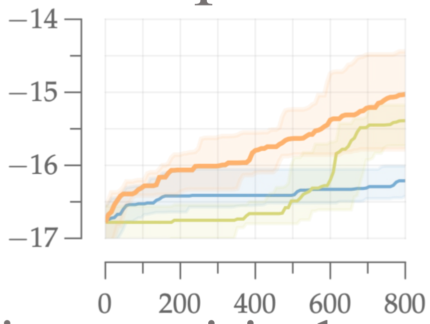
Cost-aware Bayesian optimization

Key idea



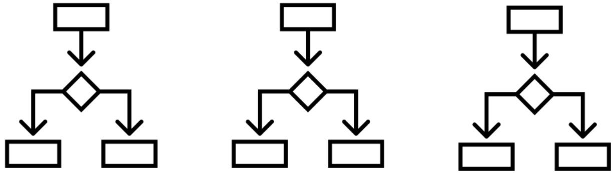
Link to Pandora's box and Gittins index theory

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."