

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)

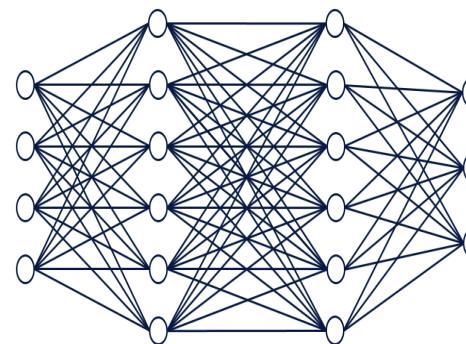
Joint work with Linda Cai (UC Berkeley), Theodore Brown (UCL), Raul Astudillo (MBZUAI), Peter Frazier, Alexander Terenin, and Ziv Scully (Cornell)

INFORMS Applied Probability Society Conference 2025

World of Hyperparameter Optimization

Hyperparameter tuning:

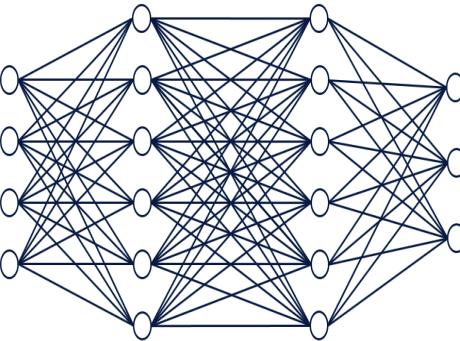
Training hyperparameters



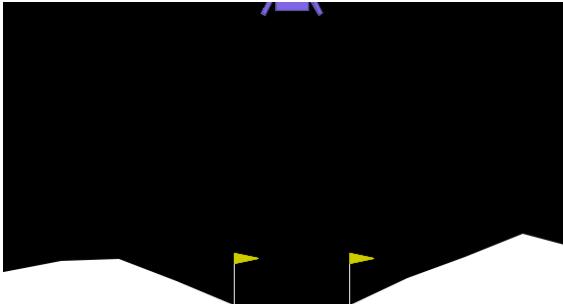
Accuracy

World of Hyperparameter Optimization

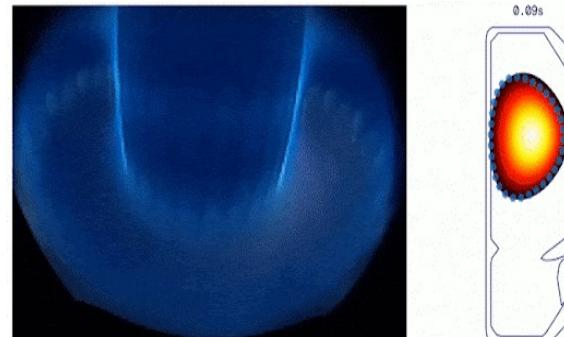
Hyperparameter tuning:

Training hyperparameters →  Accuracy

Control optimization:

Control variables →  Reward

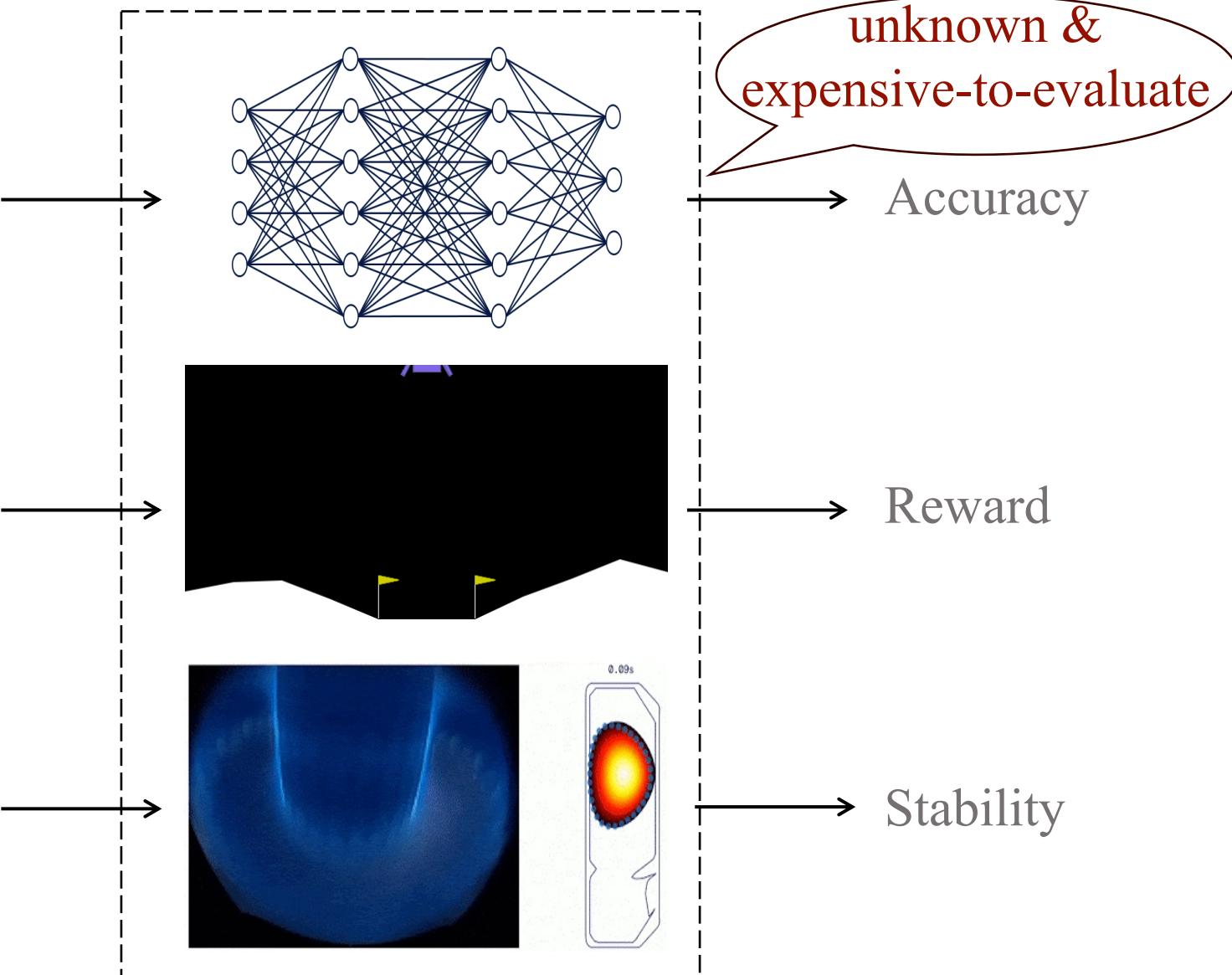
Plasma physics:

Fusion reactor design →  Stability

World of Hyperparameter Optimization

Hyperparameter tuning:

Training hyperparameters



Black-Box Optimization

Black-box optimization:

Input hyperparameters x →



unknown &
expensive-to-evaluate

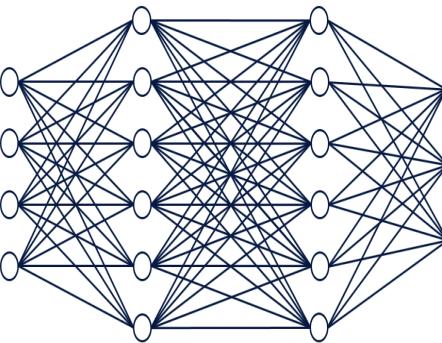
→ Performance metric $f(x)$

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

Naïve (Non-Adaptive) Approach: Grid Search

Hyperparameter tuning:

Training hyperparameters



unknown &
expensive-to-evaluate

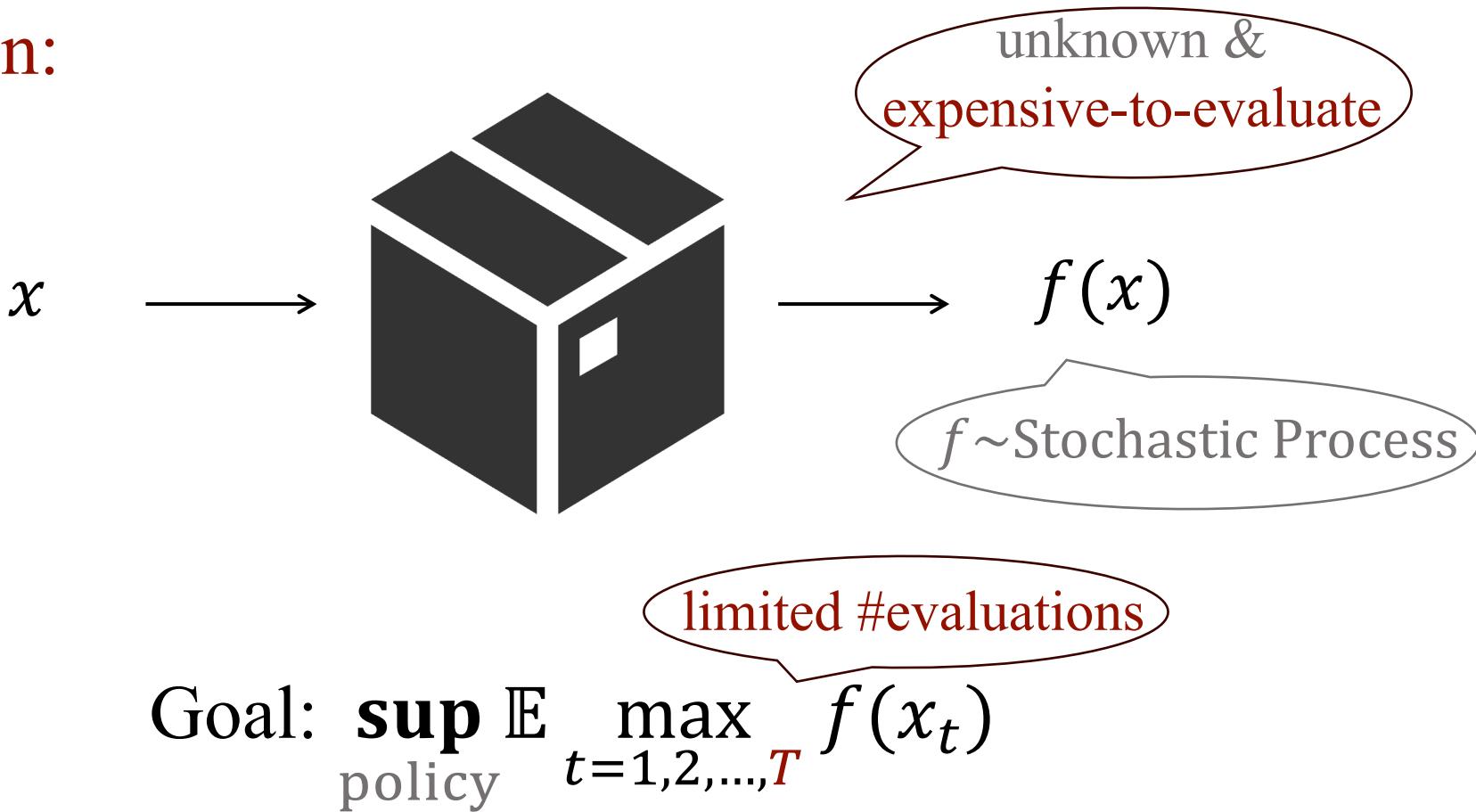
Accuracy

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!

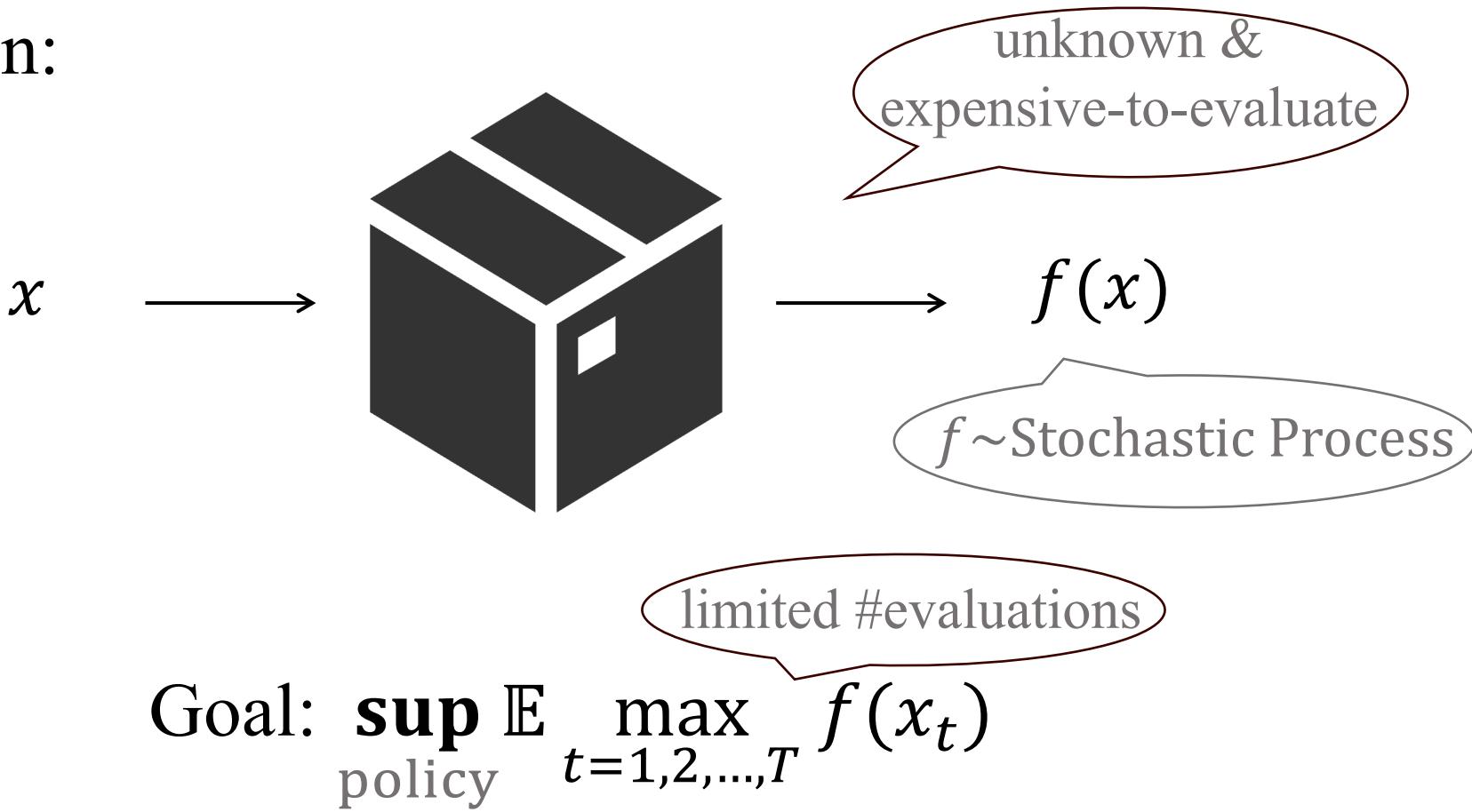
Adaptive Approach: Bayesian Optimization

Black-box function:



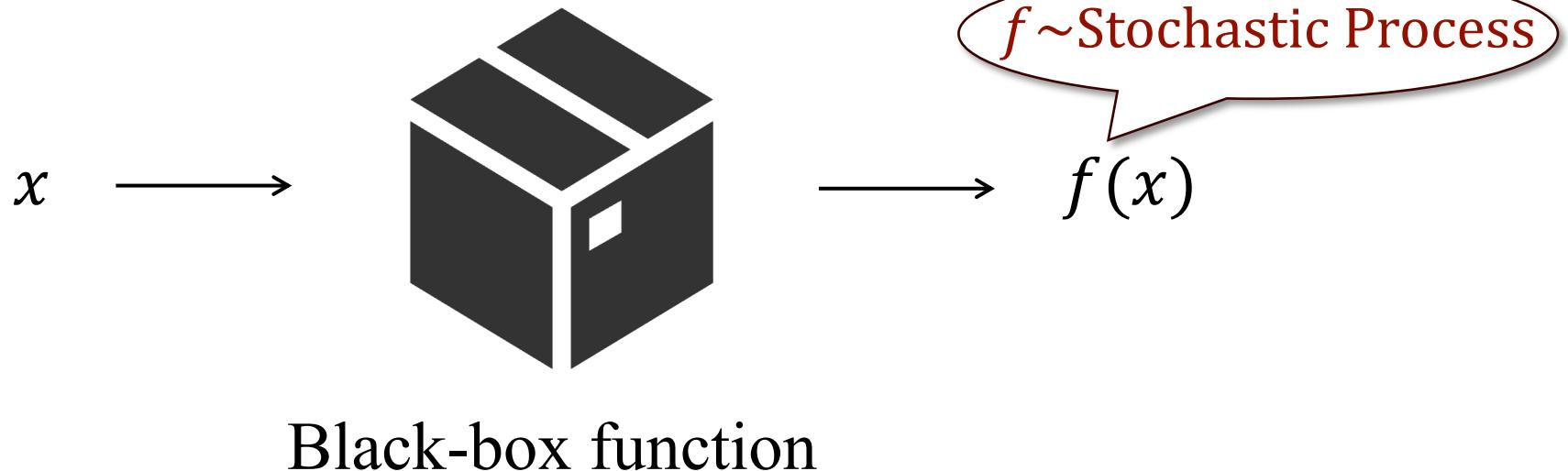
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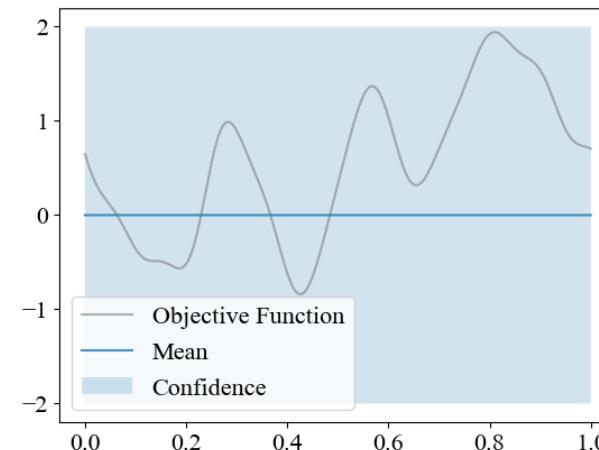
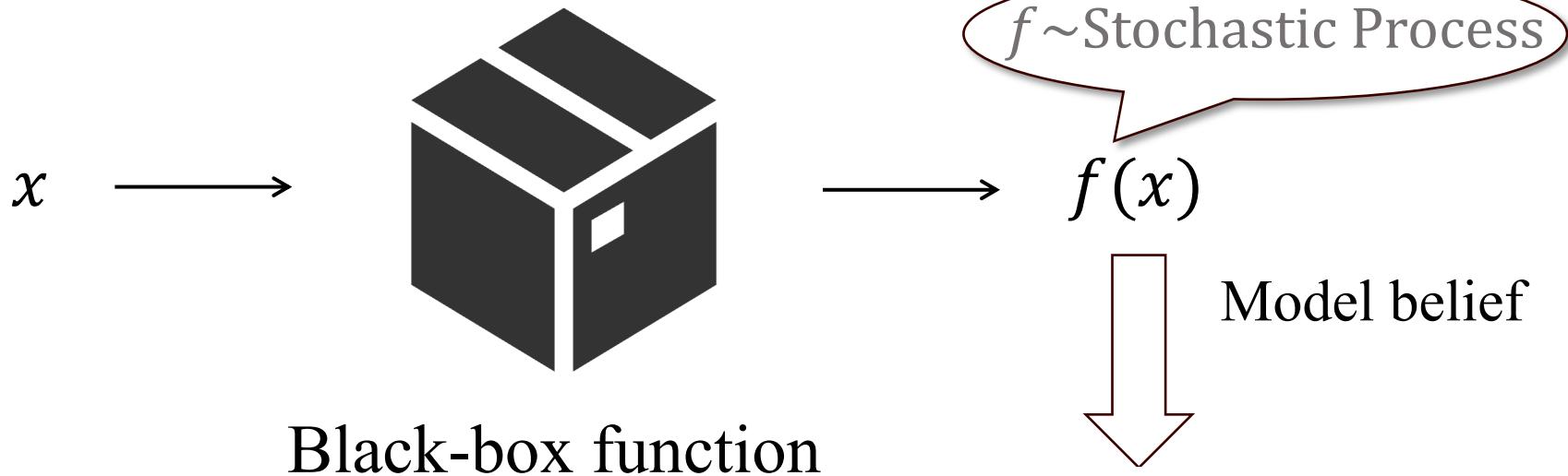
Key idea: maintain probabilistic belief about f

Bayesian Optimization



Bayesian Optimization

Time 0



Probabilistic model
(e.g., Gaussian process)

Bayesian Optimization

Time t

x_1, \dots, x_t

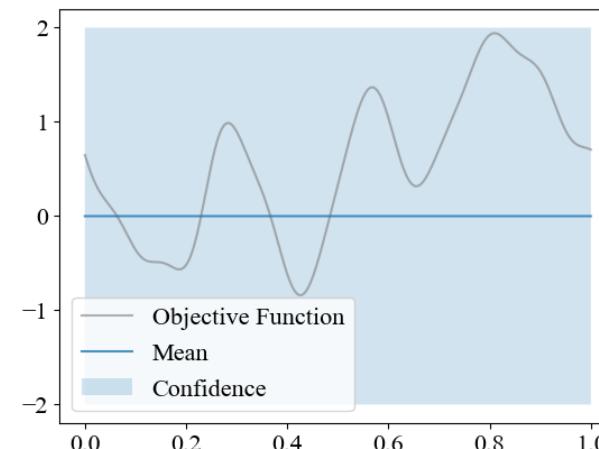


Black-box function

$f \sim \text{Stochastic Process}$

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

Model belief



Probabilistic model
(e.g., Gaussian process)

Bayesian Optimization

Time t

x_1, \dots, x_t \longrightarrow

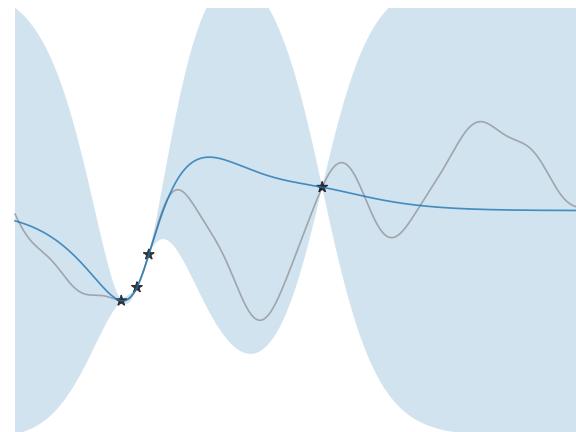


Black-box function

$f \sim \text{Stochastic Process}$

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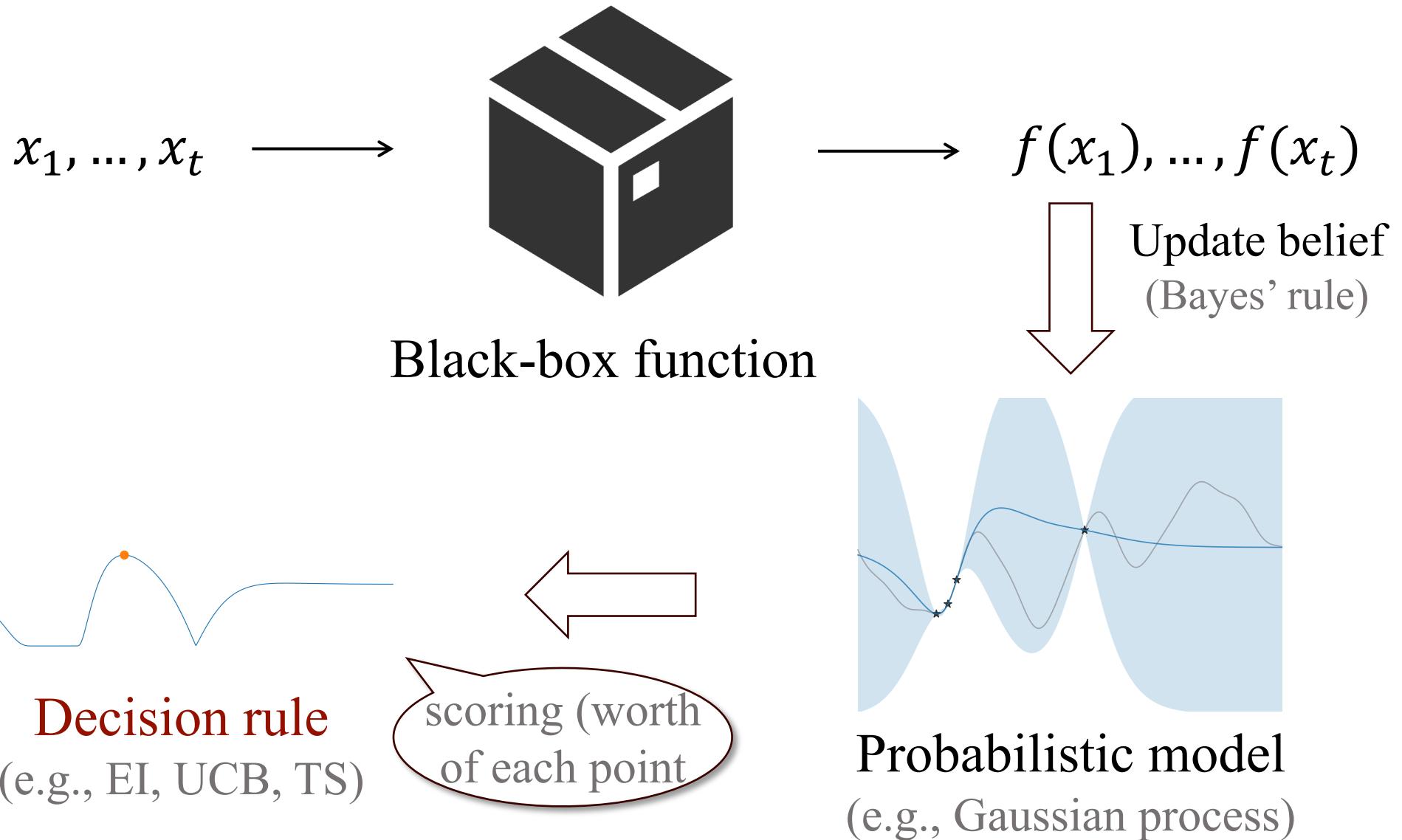
Update belief
(Bayes' rule)



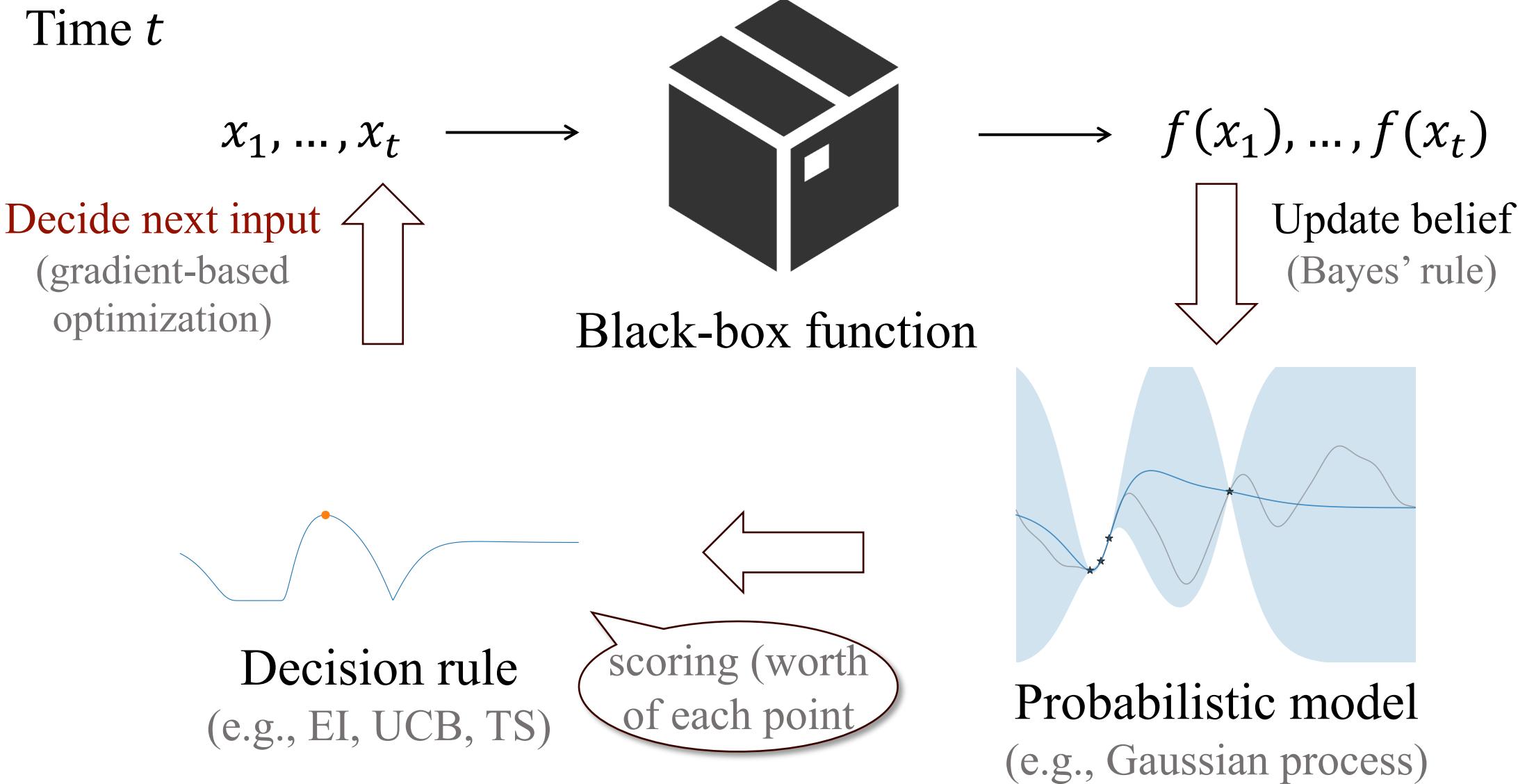
Probabilistic model
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Bayesian Optimization

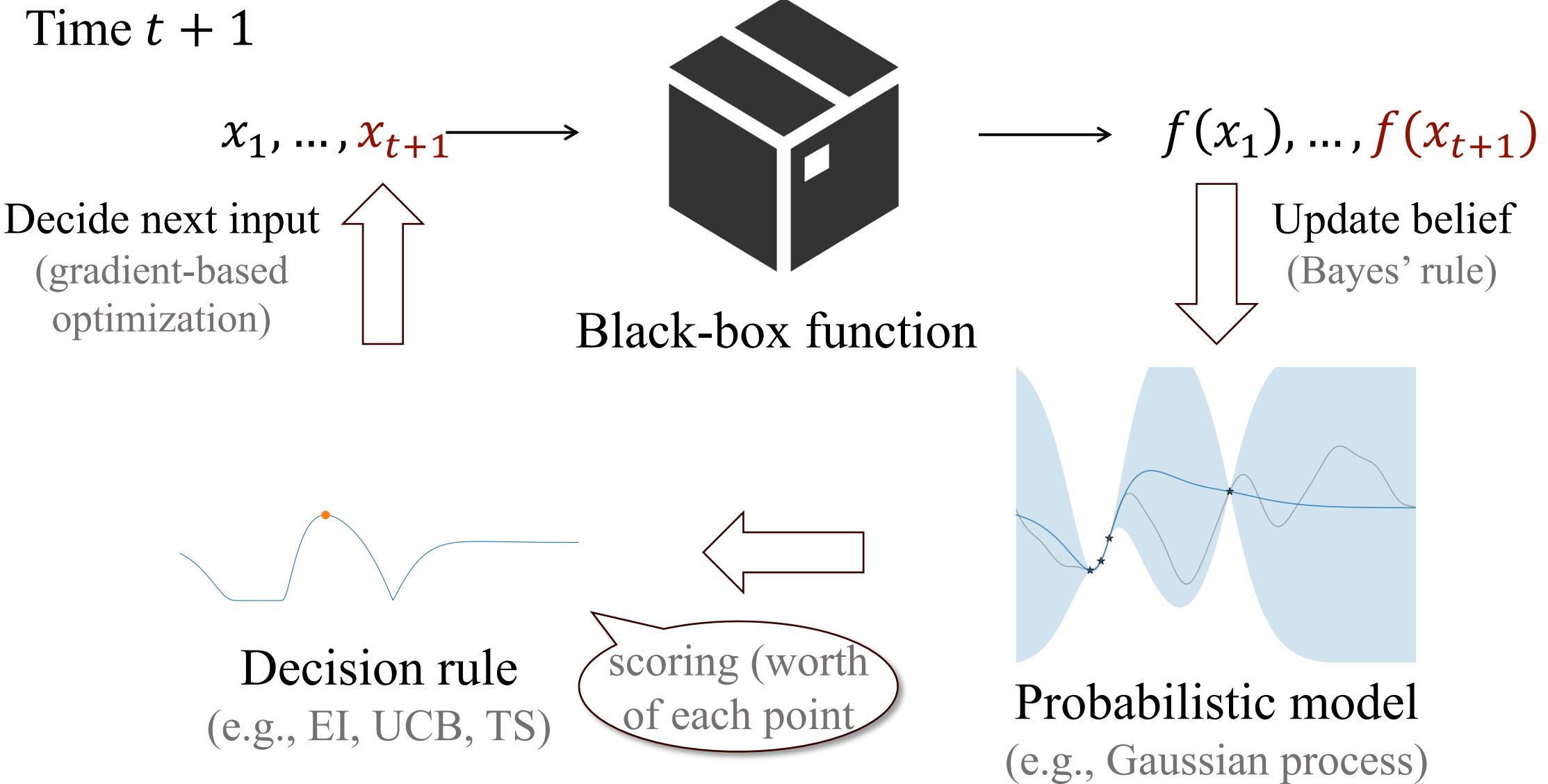
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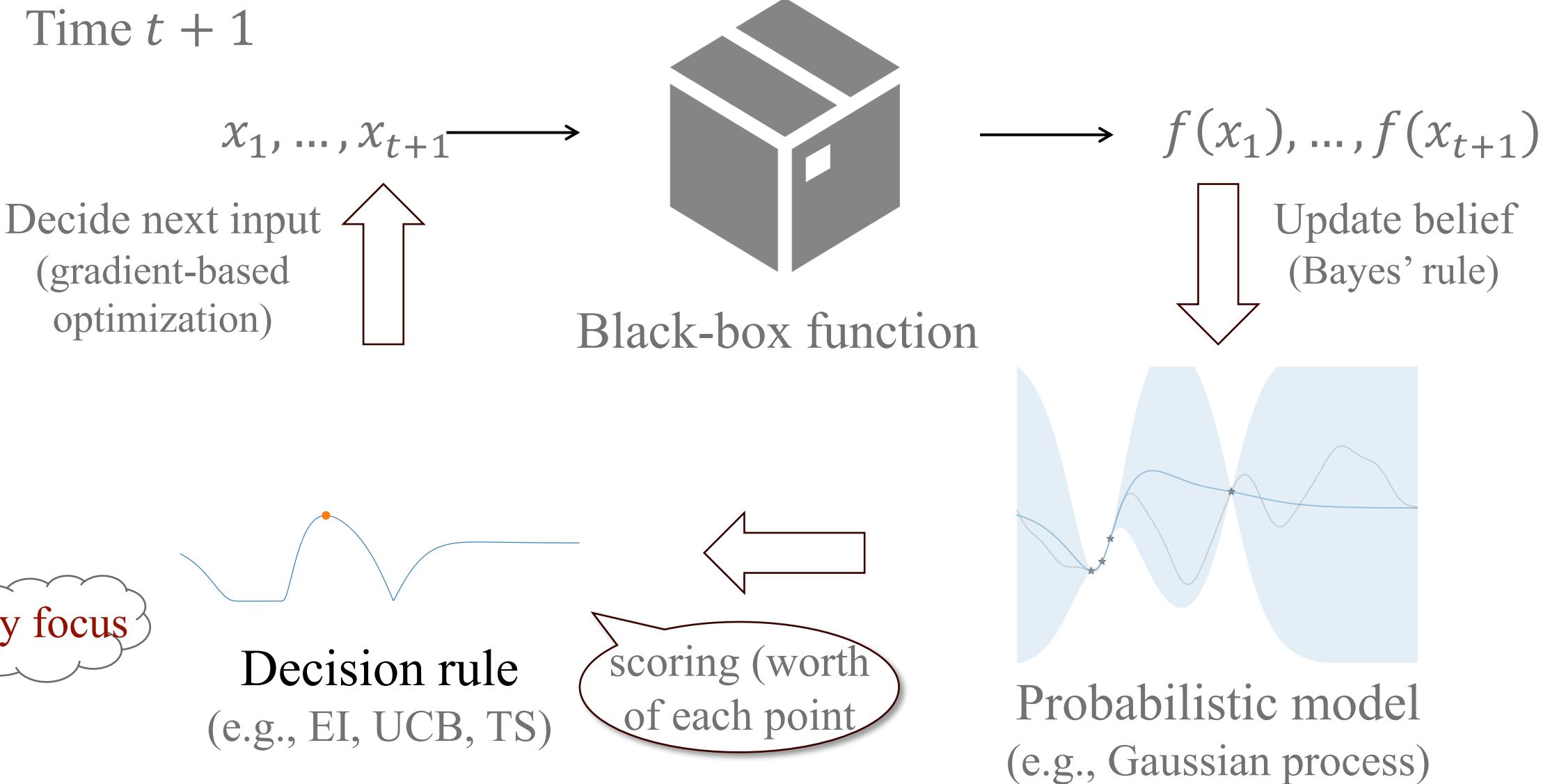
Bayesian Optimization



Bayesian Optimization



Bayesian Optimization



Popular Decision Rule: Expected Improvement

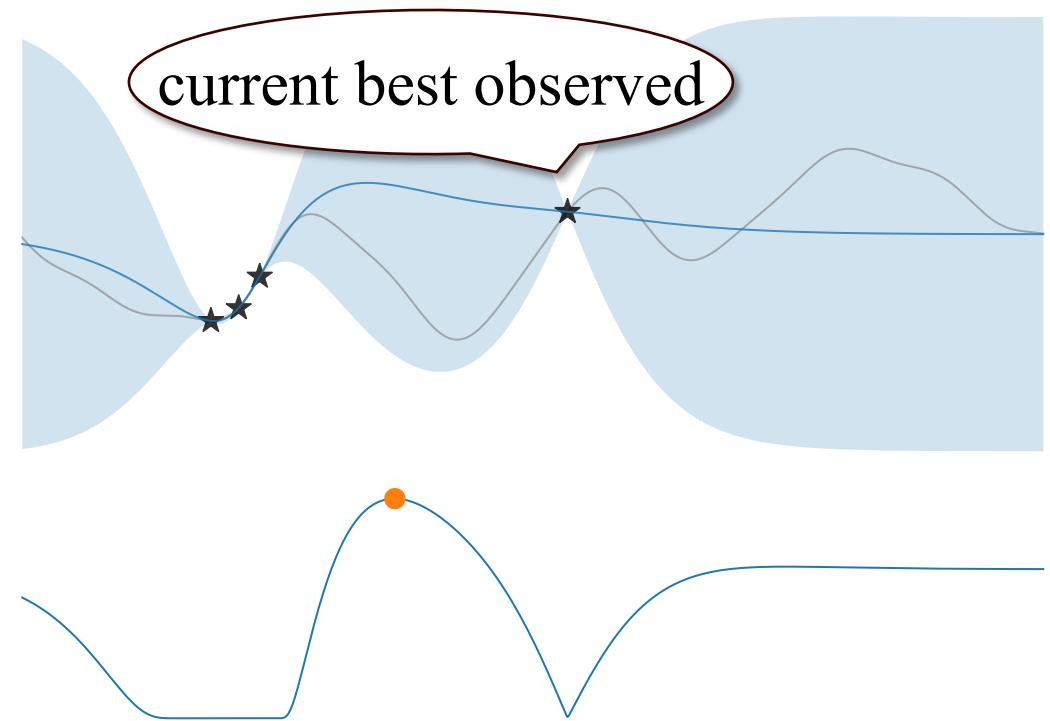
$$EI(x) = \mathbb{E}[\max(f(x) - y_{\text{best}}, 0) \mid x_1, \dots, x_t]$$

current best observed
data
“improvement”

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

posterior distribution

One-step approximation to MDP



Expected improvement $EI(x)$

Popular Decision Rule: Expected Improvement

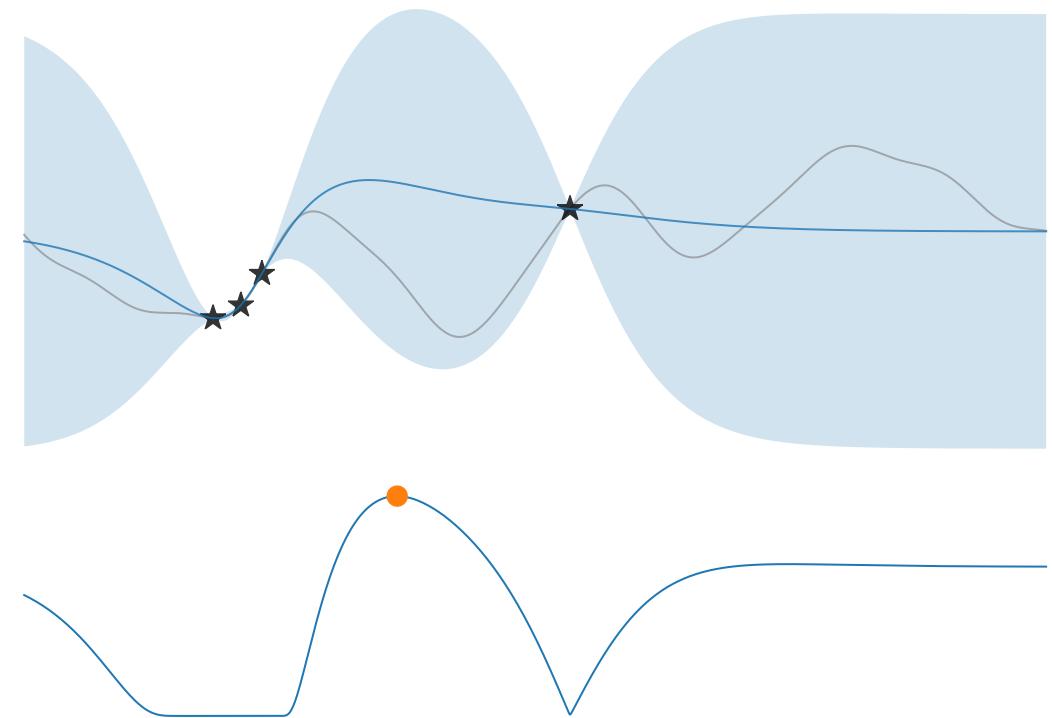
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One-step approximation to MDP

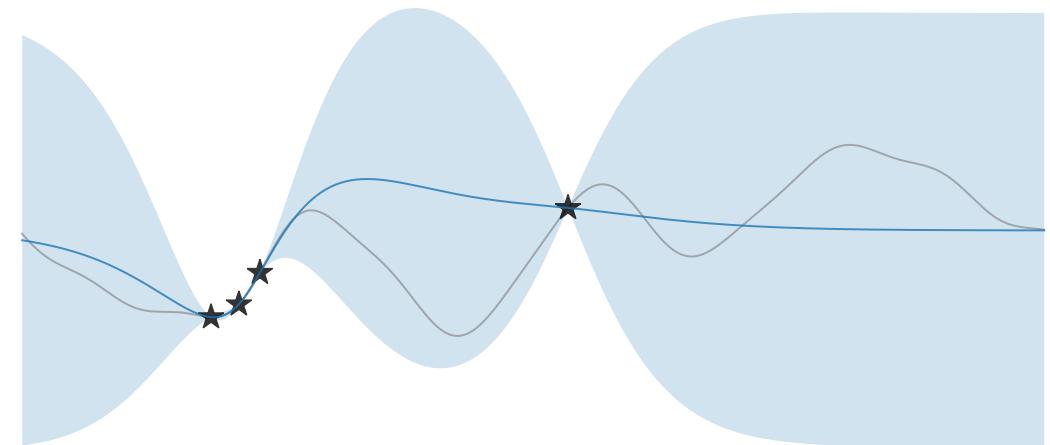


Expected improvement $EI(x)$

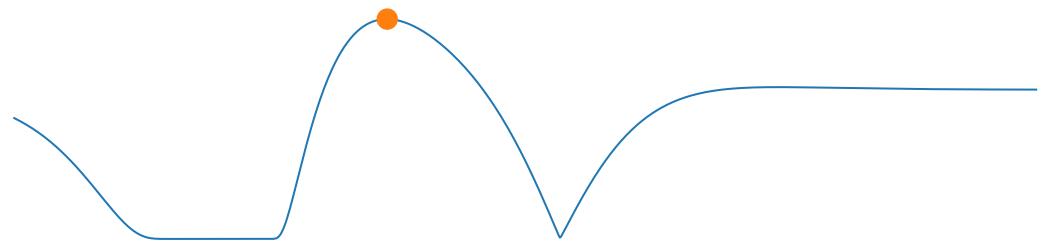
Improvement-based
design principle

Existing Design Principles

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



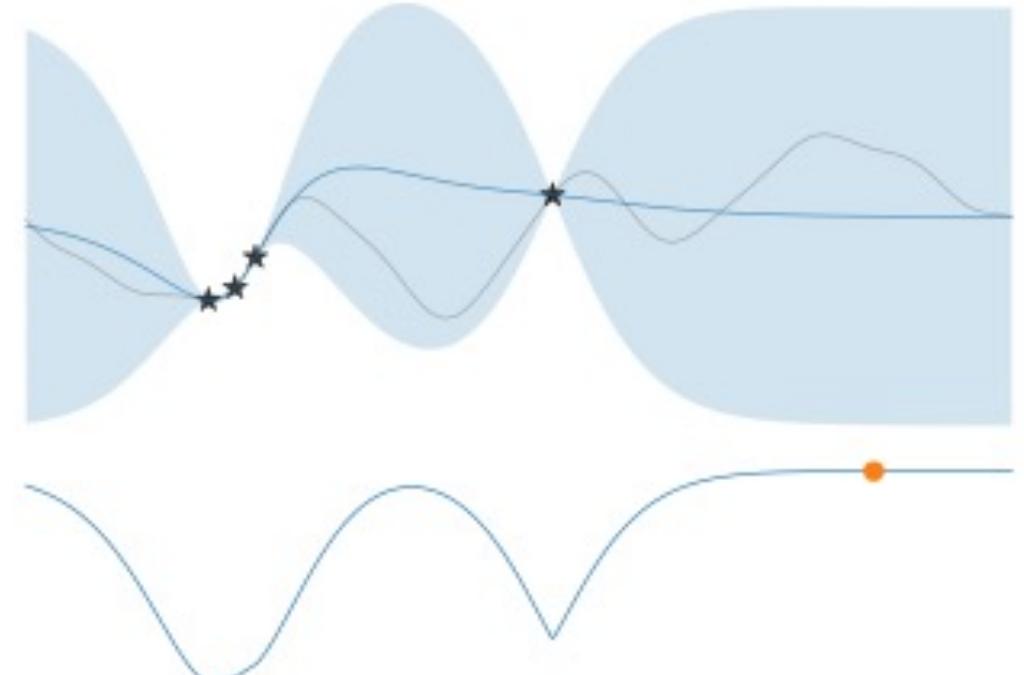
Expected improvement $EI(x)$



Improvement-based
design principle

New Design Principle: Gittins Index

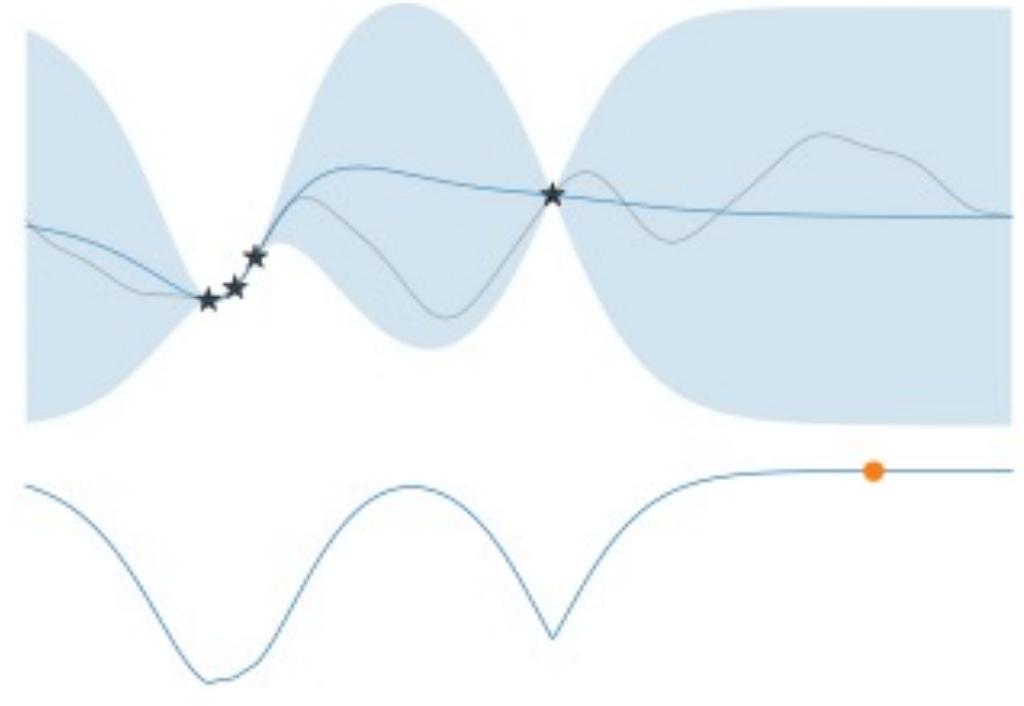
- Improvement-based (e.g., EI)
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- **Gittins Index**



Gittins index $GI(x)$

New Design Principle: Gittins Index

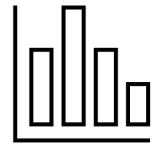
- Improvement-based (e.g., EI)
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- Confidence bounds (UCB/LCB)
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- **Gittins Index**



Gittins index $GI(x)$

? Why another principle?

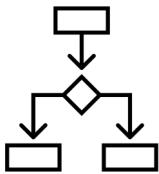
Under-explored Side Info and Flexibility



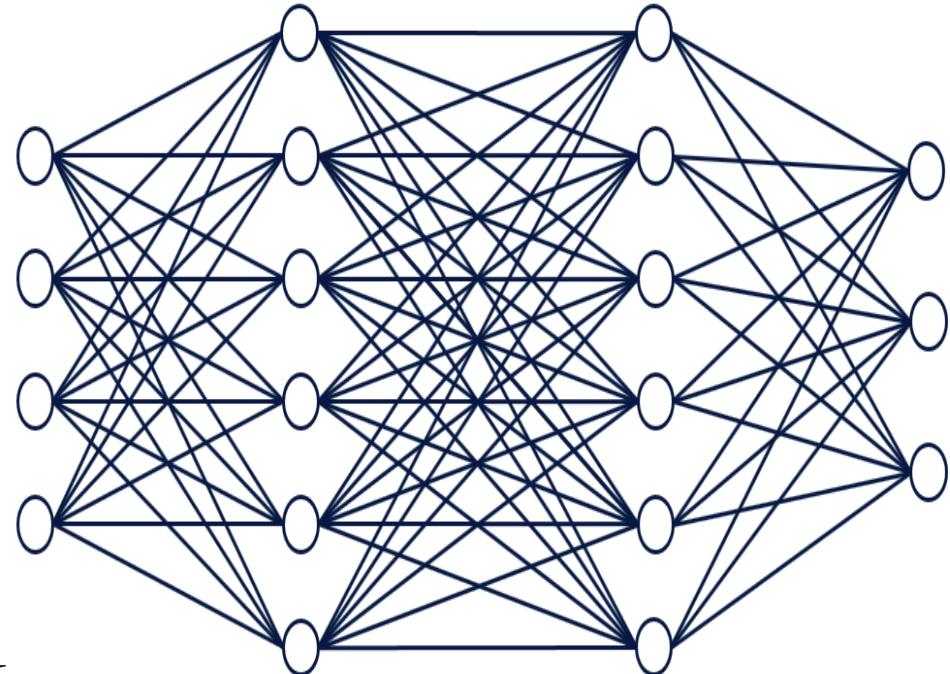
Varying evaluation costs



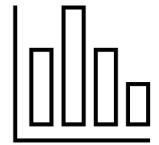
Smart stopping time



Observable multi-stage feedback



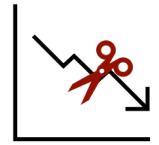
How does existing principle incorporate them?



Varying evaluation costs

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

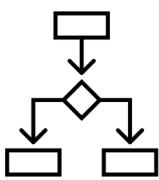
Why not subtraction?



Smart stopping time

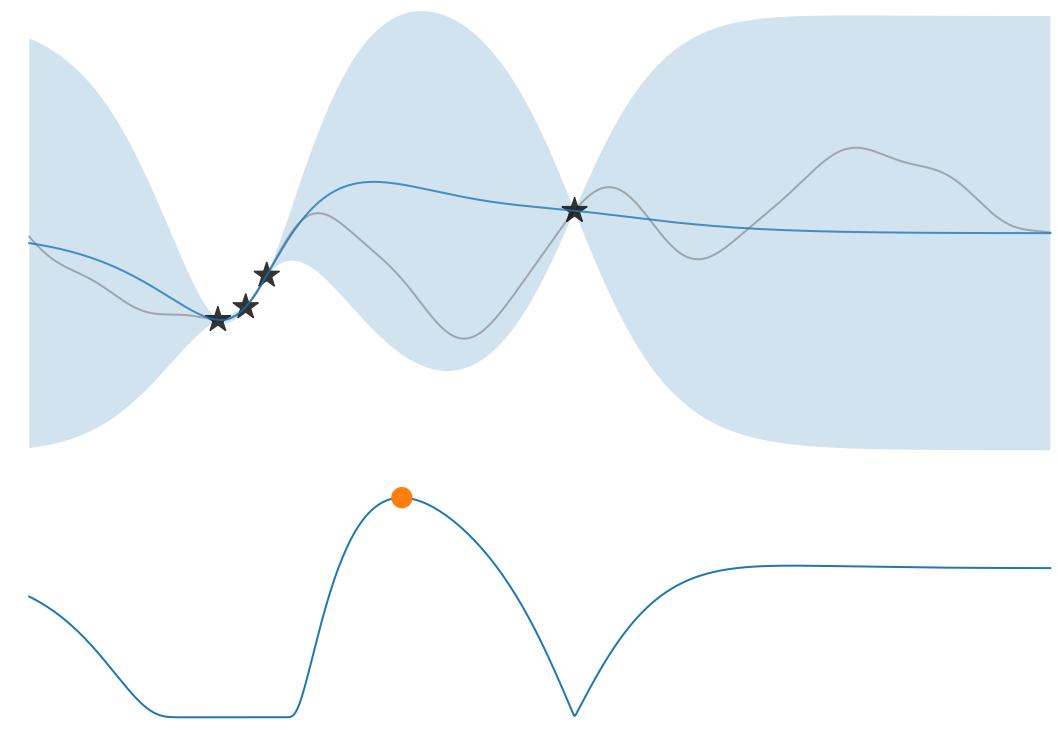
$$EI(x) \leq \theta$$

Which threshold?



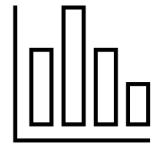
Observable multi-stage feedback

?



Expected improvement $EI(x)$

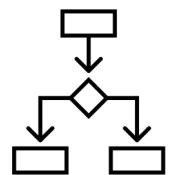
Under-explored Side Info and Flexibility



Varying evaluation costs



Smart stopping time

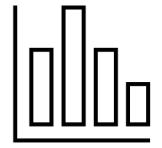


Observable multi-stage feedback



New design principle:
Gittins index

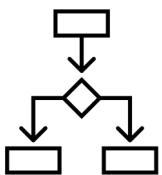
Why Gittins index?



Varying evaluation costs



Smart stopping time

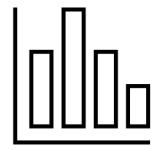


Observable multi-stage feedback

New design principle:
Gittins index

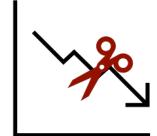
Optimal in related sequential
decision problems

Why Gittins index?



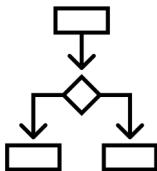
Varying evaluation costs

Features in **Pandora's box**



Smart stopping time

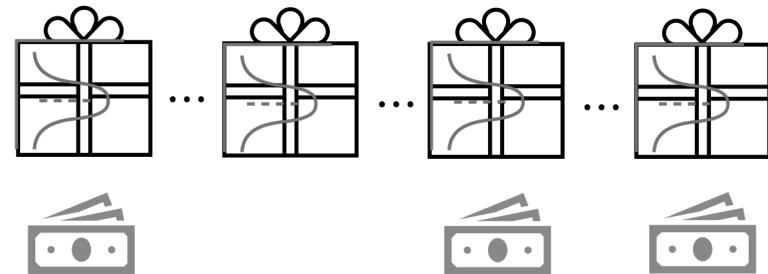
Features in **Pandora's box**



Observable multi-stage feedback

New design principle:
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Optimal in related sequential
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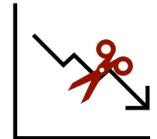


Why Gittins index?



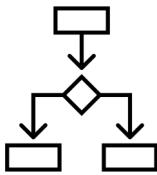
Varying evaluation costs

Features in Pandora's box



Smart stopping time

Features in Pandora's box

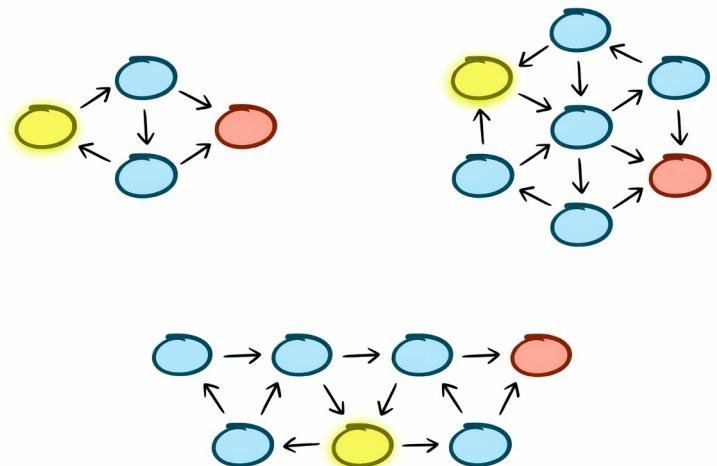


Observable multi-stage feedback

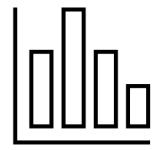
Features in Markov chain selection

New design principle:
Gittins index

Optimal in related sequential
decision problems

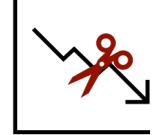


Why Gittins index?



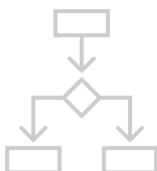
Varying evaluation costs

Features in Pandora's box



Smart stopping time

Features in Pandora's box



Observable multi-stage feedback

Features in Markov chain selection

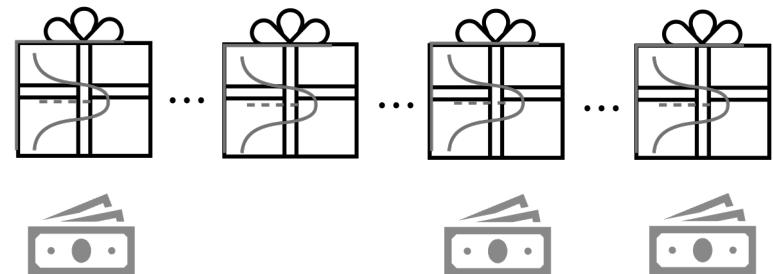


"Cost-aware Bayesian Optimization via the
Pandora's Box Gittins Index." NeurIPS'24.



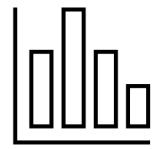
New design principle:
Gittins index

Optimal in related sequential
decision problems



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

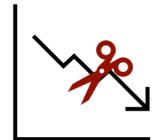
Coauthors



Varying evaluation costs
[NeurIPS'24]



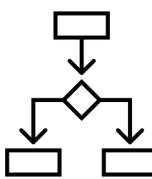
Raul Astudillo



Smart stopping time
[Under review]



Linda Cai



Observable multi-stage feedback
[Ongoing work]

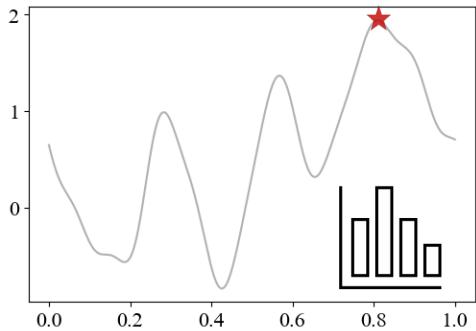


Peter Frazier Alexander Terenin Ziv Scully



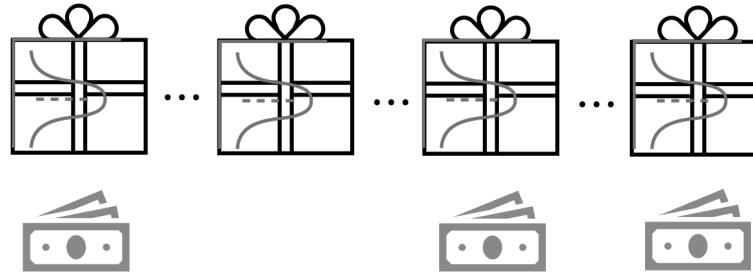
Outline

Studied Problem



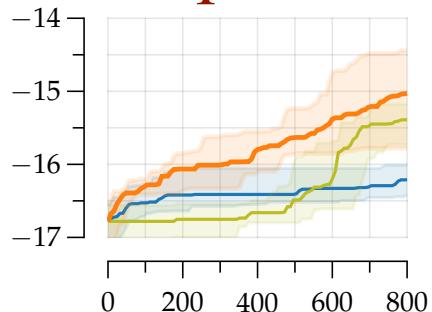
Cost-aware Bayesian optimization

Key idea



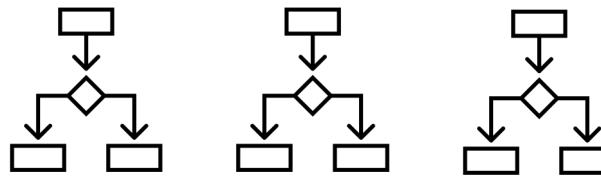
Link to simplified problem
and Gittins index theory

Impact



Competitive empirical performance

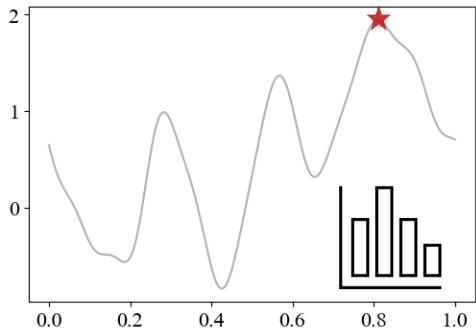
Future direction



“Exotic” Bayesian optimization

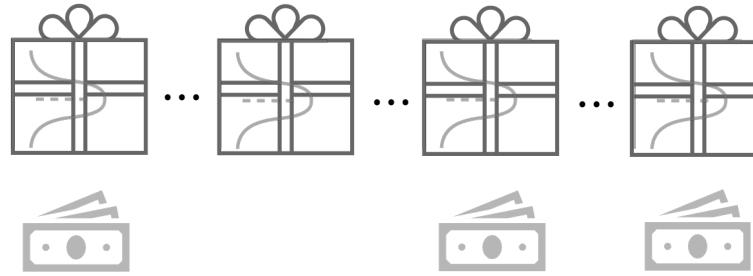
Outline

Studied Problem



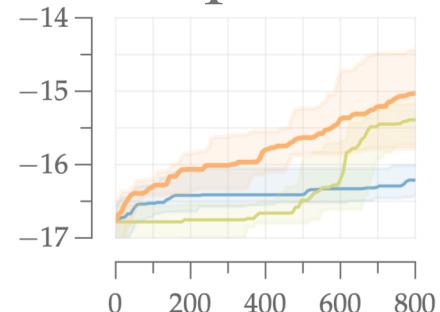
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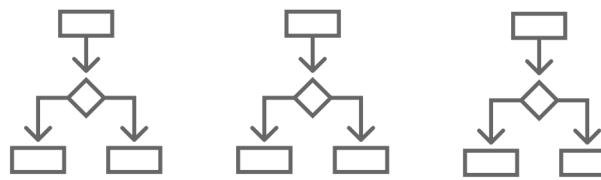
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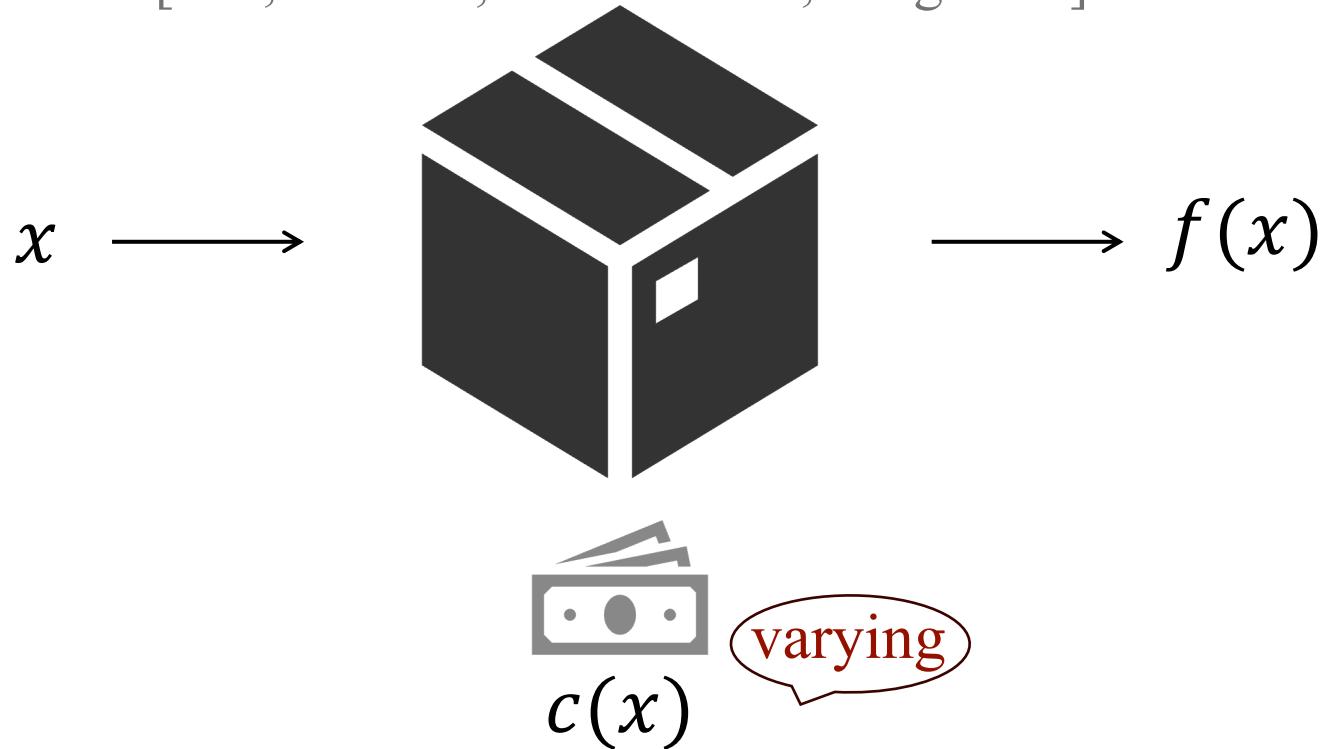
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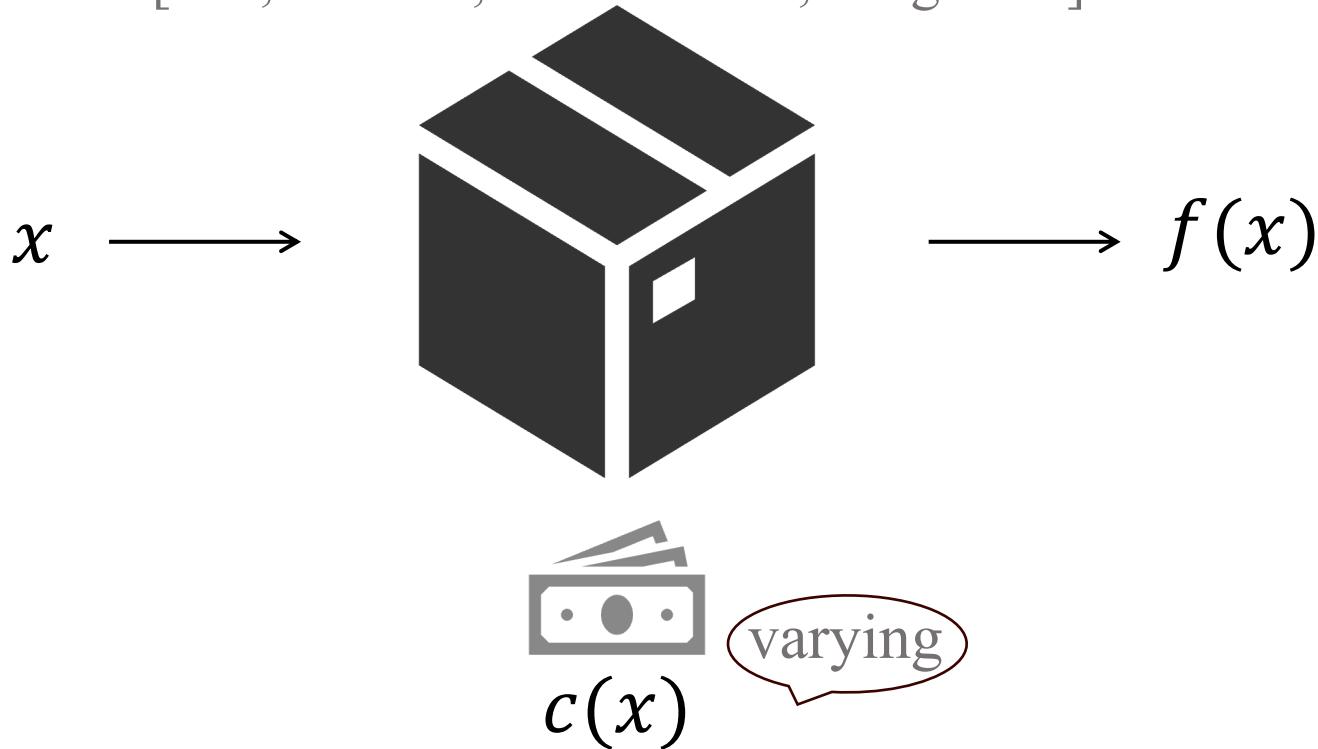
Cost-aware Bayesian Optimization

[Lee, Perrone, Archambeau, Seeger'21]



Cost-aware Bayesian Optimization

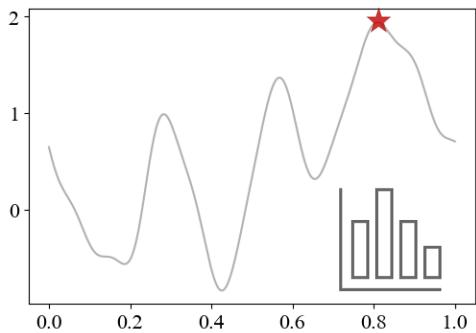
[Lee, Perrone, Archambeau, Seeger'21]



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

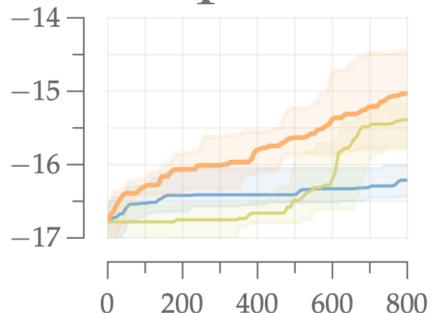
Outline

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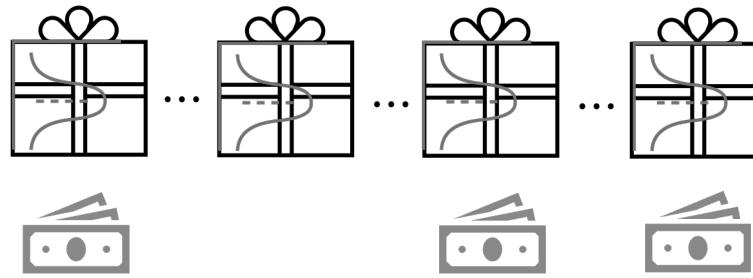
Cost-aware Bayesian optimization

Impact



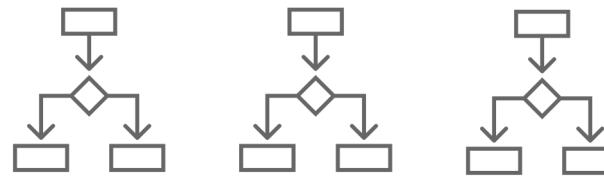
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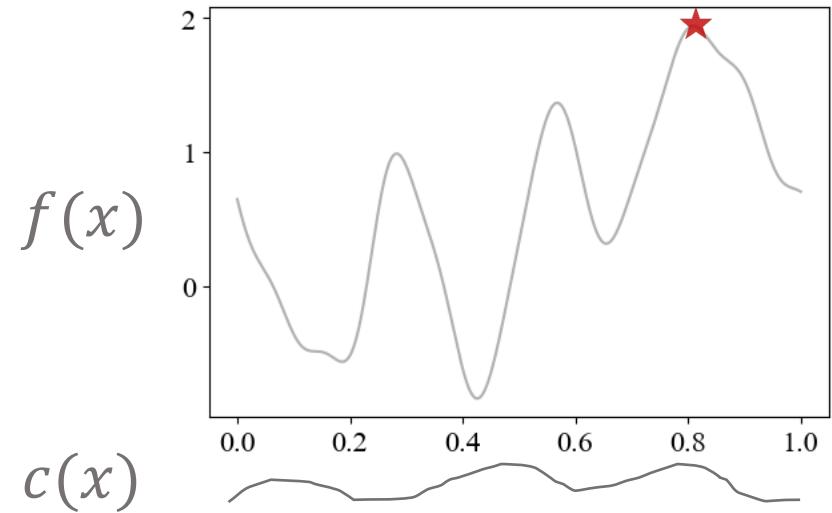
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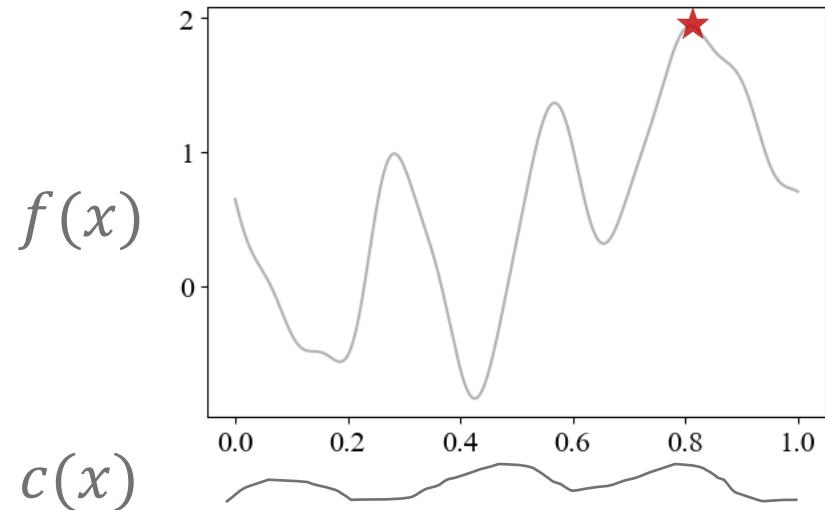


“Exotic” Bayesian optimization

Cost-aware Bayesian Optimization



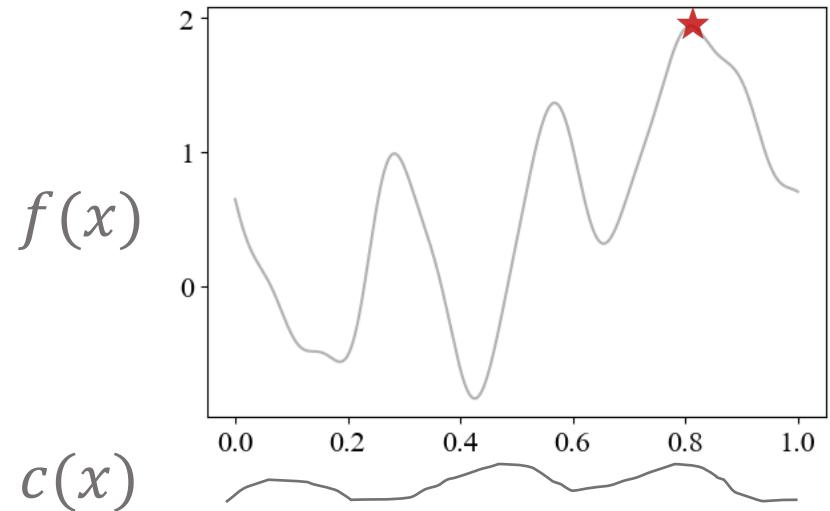
Cost-aware Bayesian Optimization



Continuous

Correlated

Cost-aware Bayesian Optimization

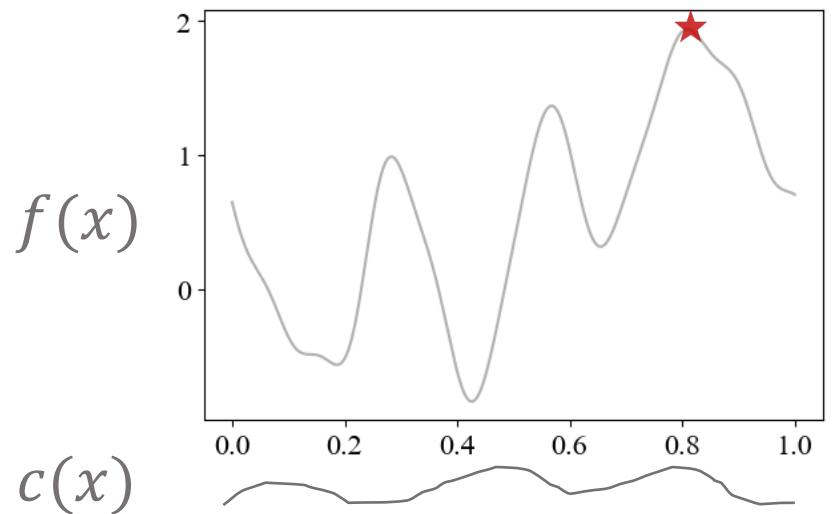


Continuous

Correlated

Intractable MDP!

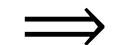
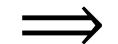
Cost-aware Bayesian Optimization



$c(x)$

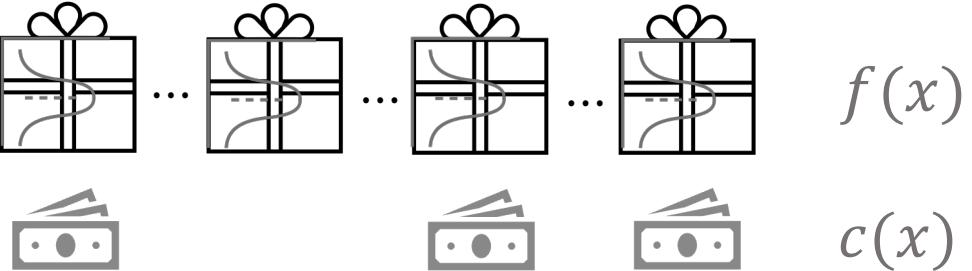
Continuous

Correlated



Pandora's Box

[Weitzman'79]



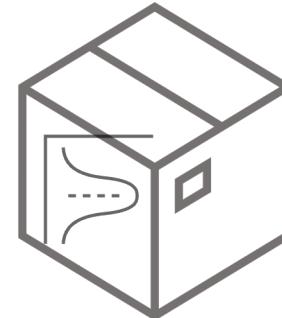
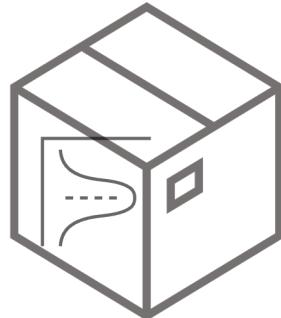
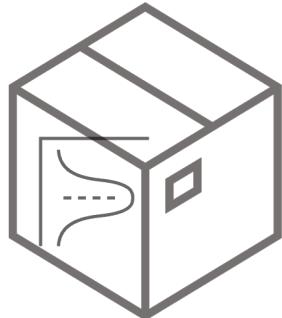
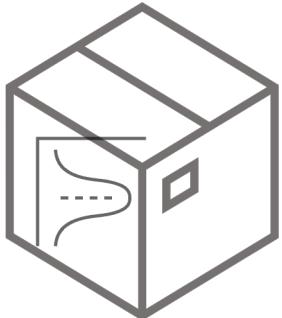
$f(x)$

$c(x)$

Intractable MDP!

Pandora's Box

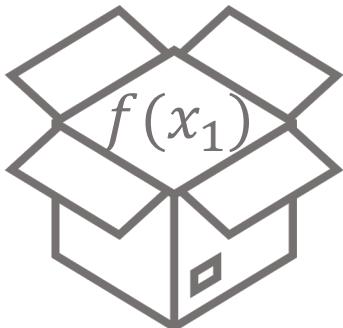
$t = 0$



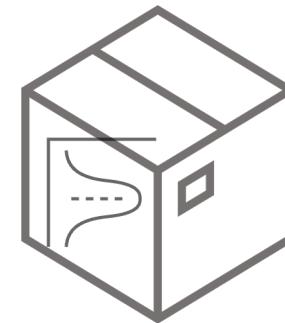
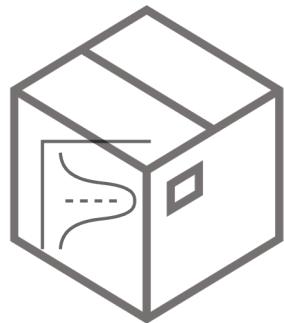
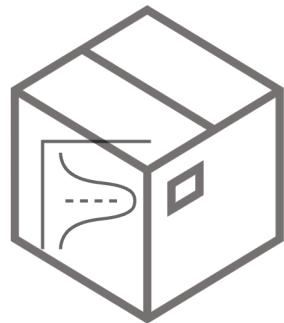
$$\sup_{\text{policy}} \mathbb{E} \left(\max_{t=1,2,\dots,T} f(x_t) - \sum_{t=1}^T c(x_t) \right)$$

Pandora's Box

$t = 1$



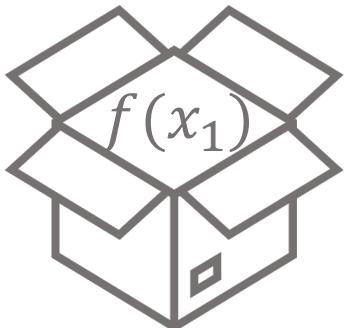
$c(x_1)$



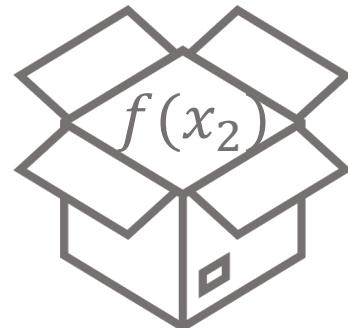
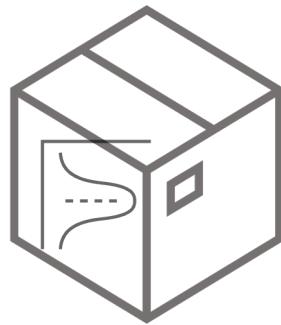
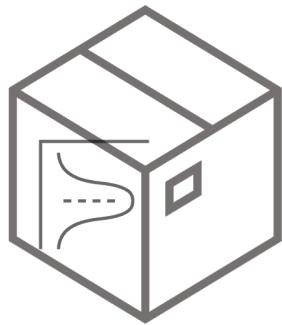
$$\sup_{\text{policy}} \mathbb{E} \left(\max_{t=1,2,\dots,T} f(x_t) - \sum_{t=1}^T c(x_t) \right)$$

Pandora's Box

$t = 2$



$c(x_1)$

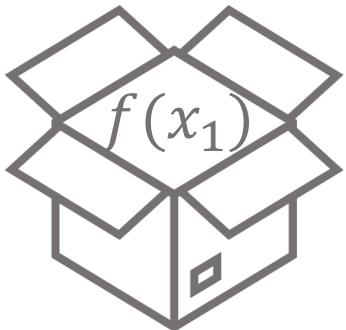


$c(x_2)$

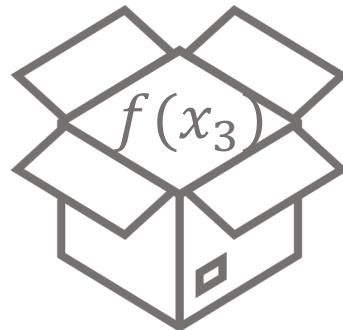
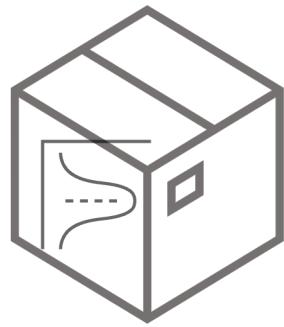
$$\sup_{\text{policy}} \mathbb{E} \left(\max_{t=1,2,\dots,T} f(x_t) - \sum_{t=1}^T c(x_t) \right)$$

Pandora's Box

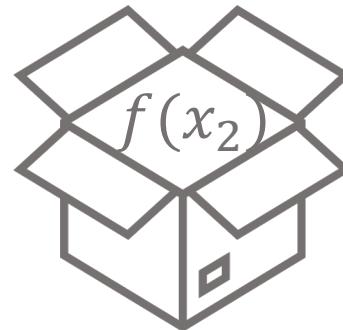
$t = 3$



$c(x_1)$



$c(x_3)$

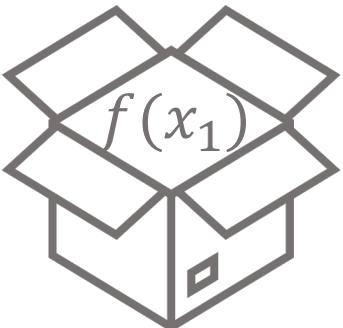


$c(x_2)$

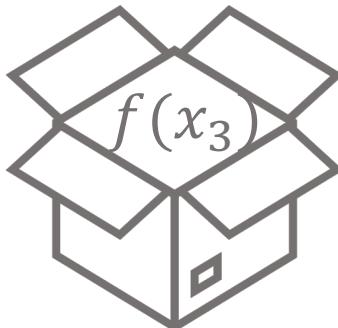
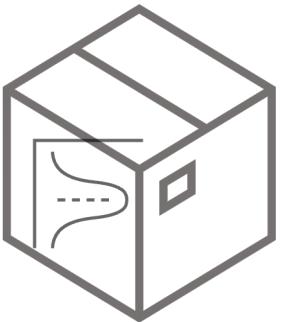
$$\sup_{\text{policy}} \mathbb{E} \left(\max_{t=1,2,\dots,T} f(x_t) - \sum_{t=1}^T c(x_t) \right)$$

Pandora's Box

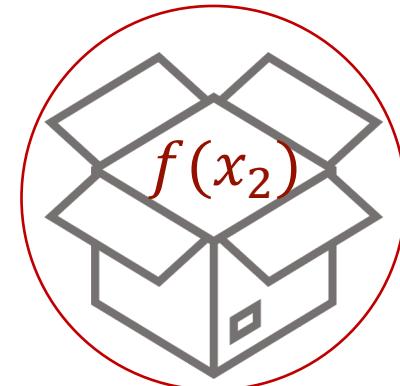
$t = T, \text{stop}$



$c(x_1)$



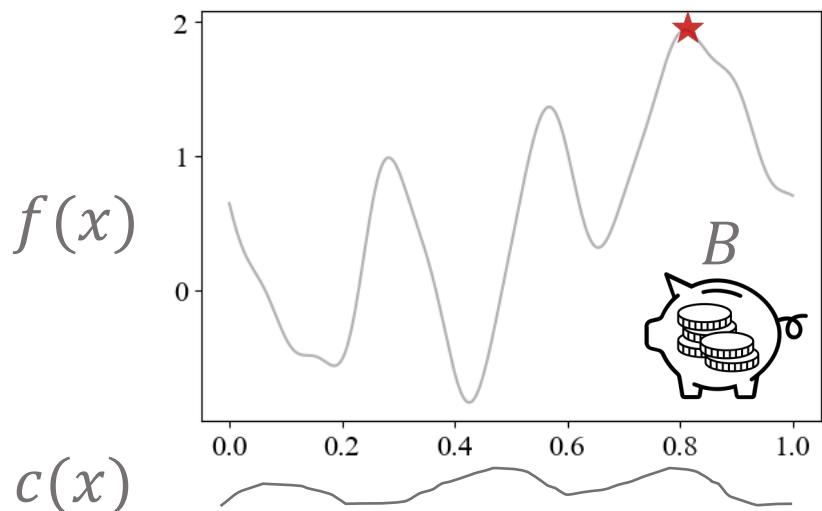
$c(x_3)$



$c(x_2)$

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

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]



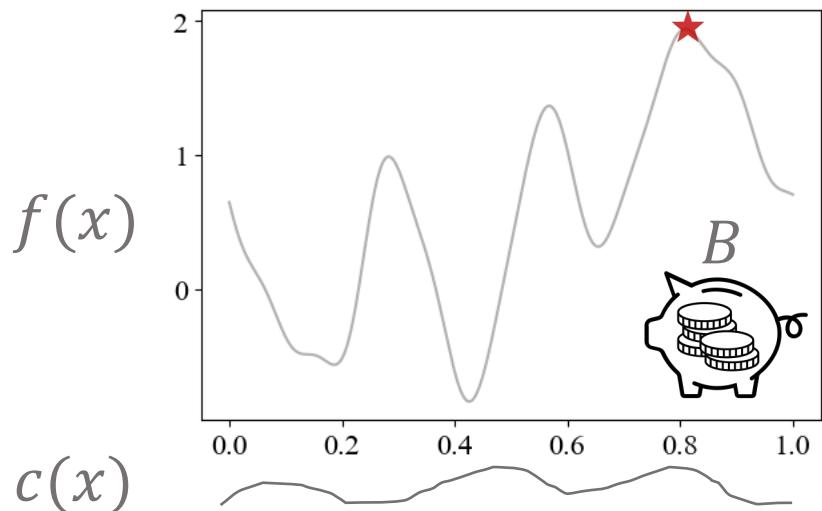
Discrete

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

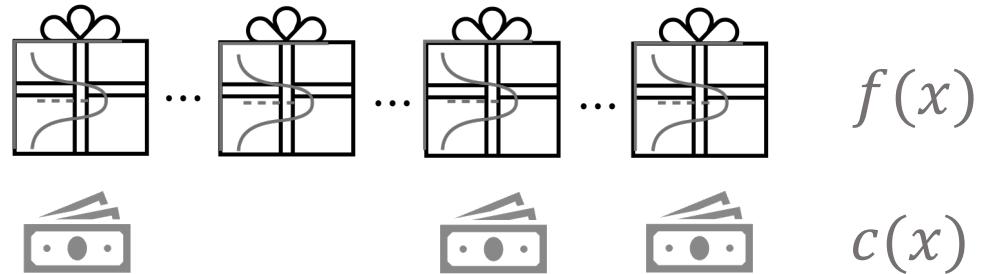
Correlated

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]



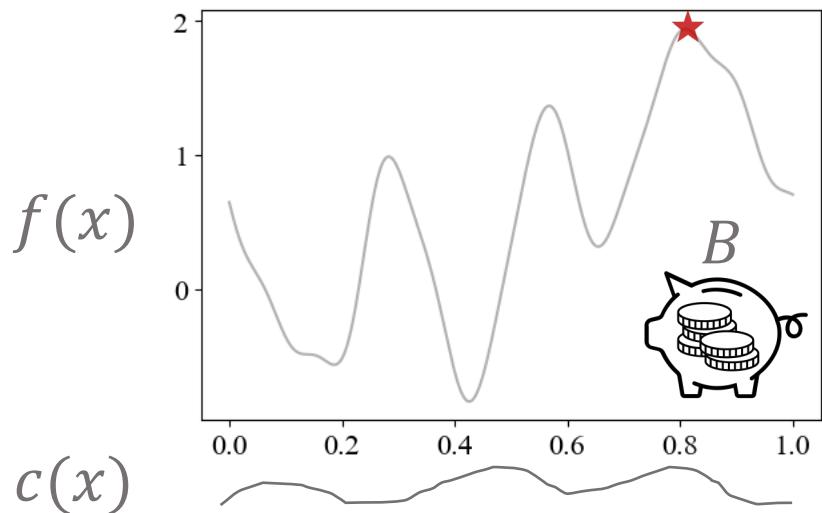
Discrete

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

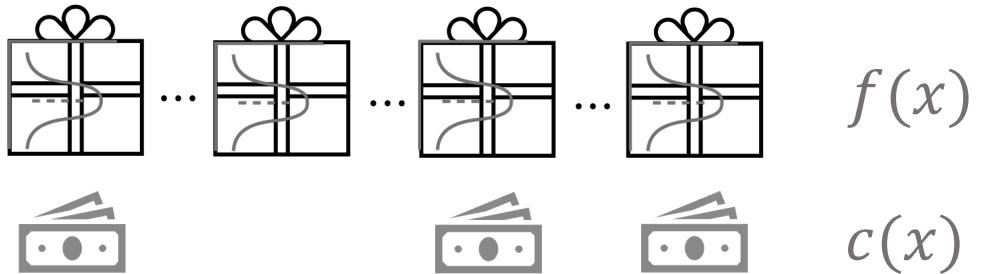
Correlated

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]



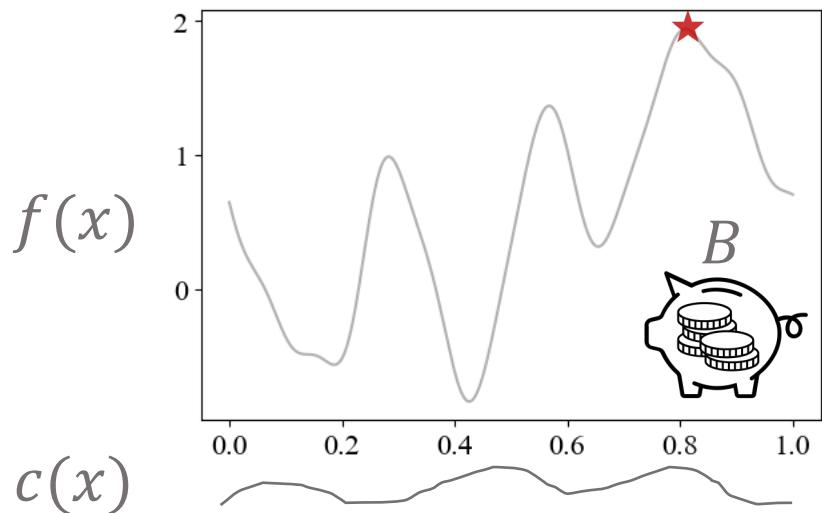
Discrete

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

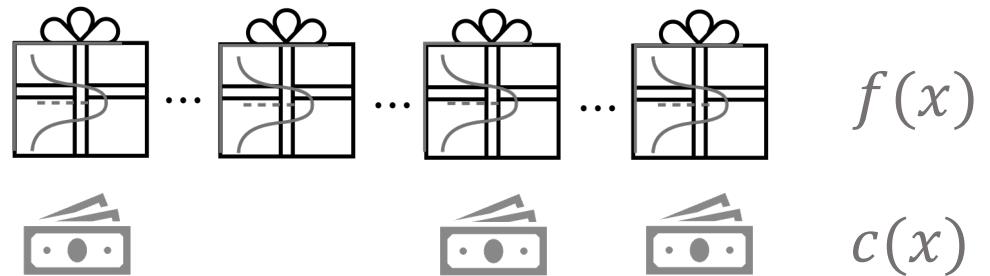
Correlated

Ebc & Cps

Intractable MDP!

Pandora's Box

[Weitzman'79]



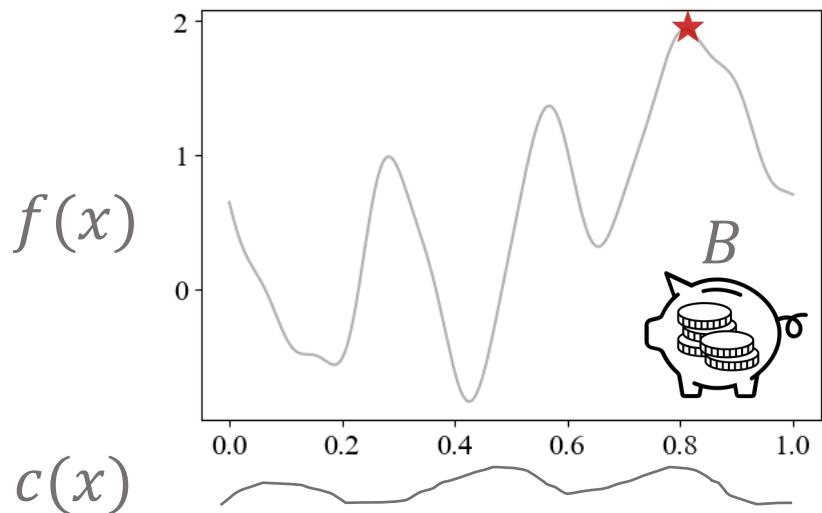
Discrete

Independent

Cost-per-sample

Optimal policy: Gittins index

Cost-aware Bayesian Optimization



Continuous

Correlated

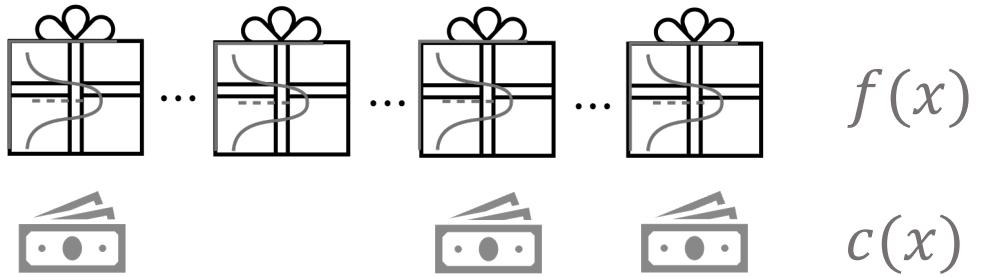
Ebc & Cps

How to translate?

Optimal policy: Gittins index

Pandora's Box

[Weitzman'79]

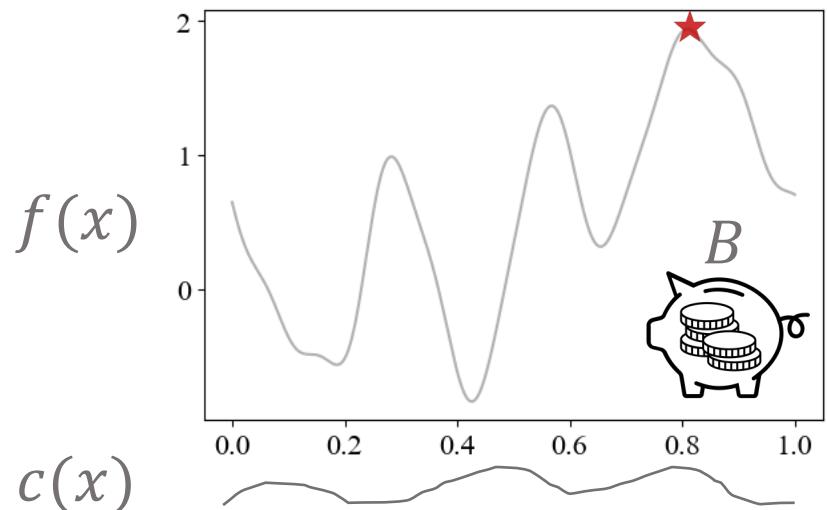


Discrete

Independent

Cost-per-sample

Cost-aware Bayesian Optimization



Continuous

Correlated

Ebc & Cps

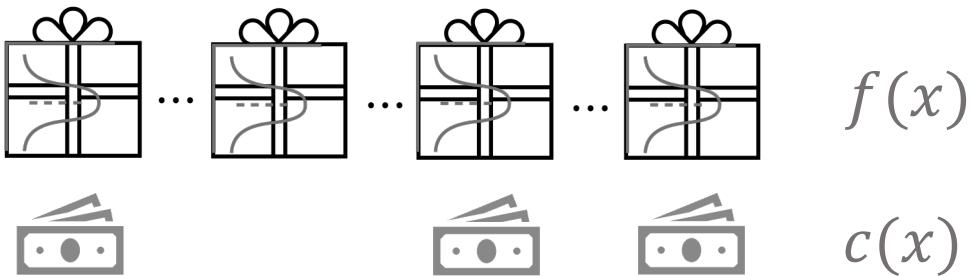
Acquisition function
+ stopping rule

incorporate posterior

Optimal policy: Gittins index

Pandora's Box

[Weitzman'79]

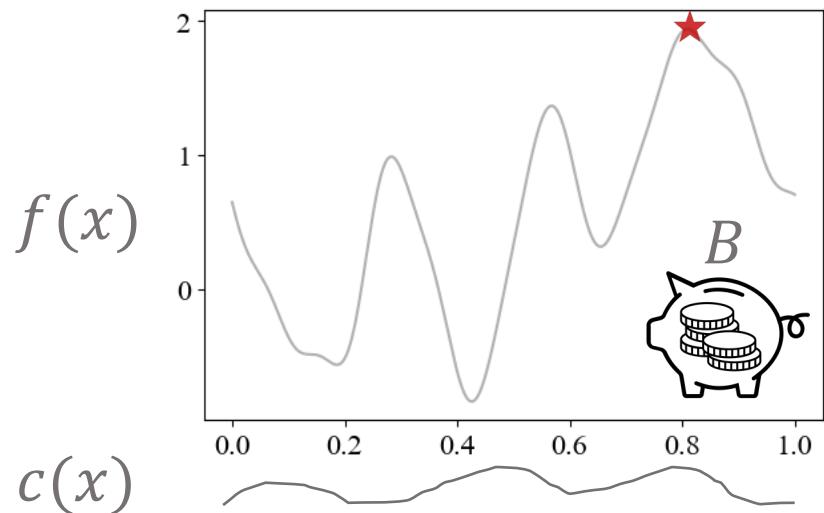


Discrete

Independent

Cost-per-sample

Cost-aware Bayesian Optimization



Continuous

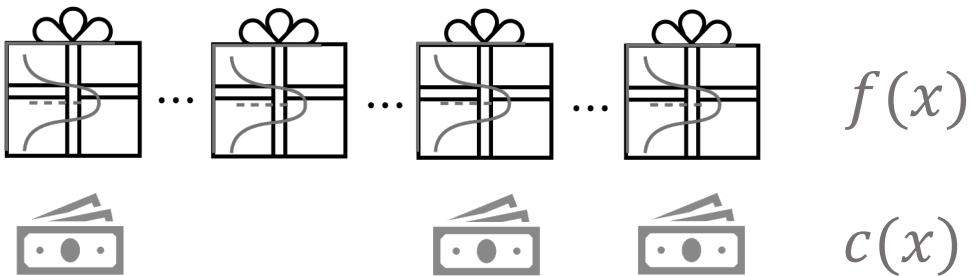
Correlated

How to compute?

Acquisition function
+ stopping rule \Leftarrow incorporate posterior
Optimal policy: Gittins index

Pandora's Box

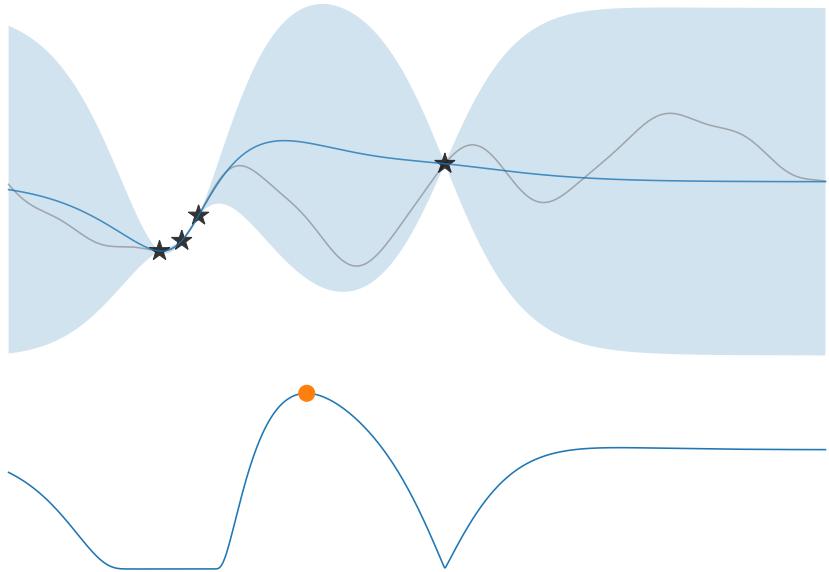
[Weitzman'79]



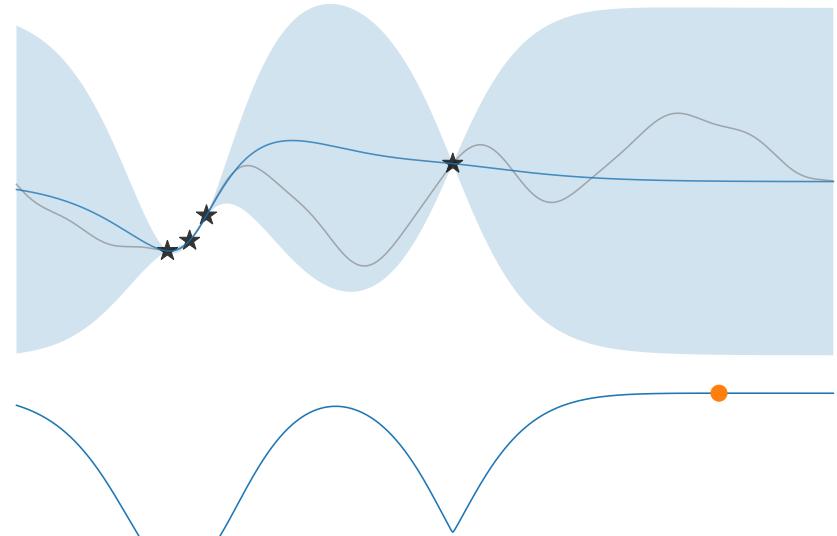
Discrete

Independent

Expected Improvement



Gittins Index



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

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

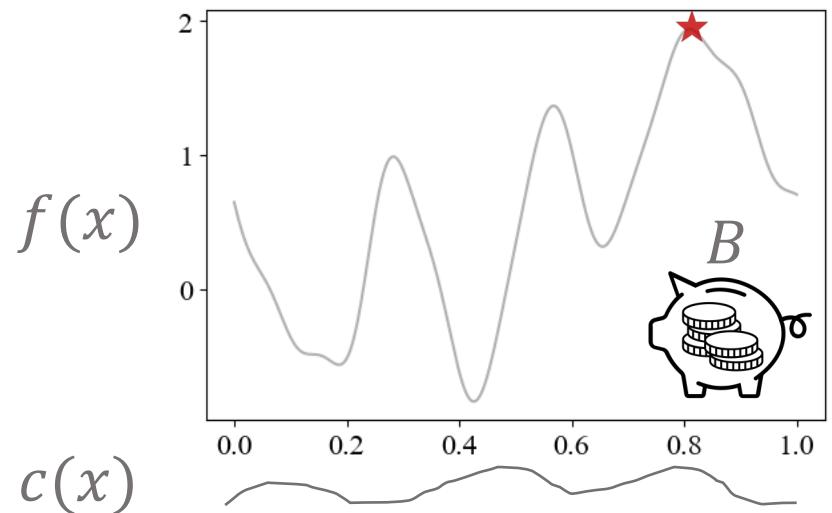
$\max_x \text{GI}_{f|D}(x; c(x))$

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 $\text{EI}_{f|D} + \text{bisection search!}$

Cost-aware Bayesian Optimization



Continuous

Correlated

Ebc & Cps

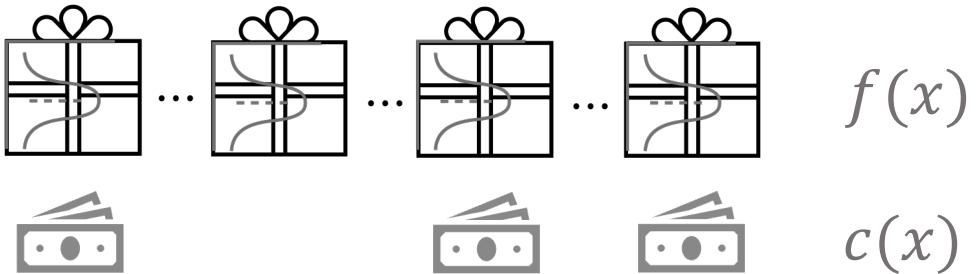
Acquisition function

+ stopping rule

Empirically good?

Pandora's Box

[Weitzman'79]



Discrete

Independent

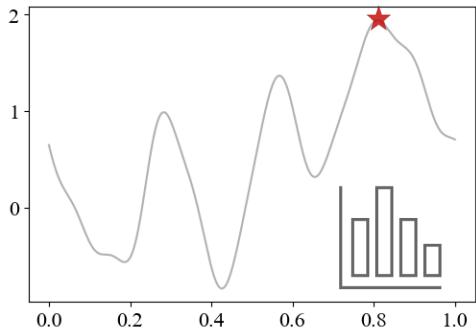
Cost-per-sample

incorporate posterior

Acquisition function \Leftarrow Gittins index is optimal

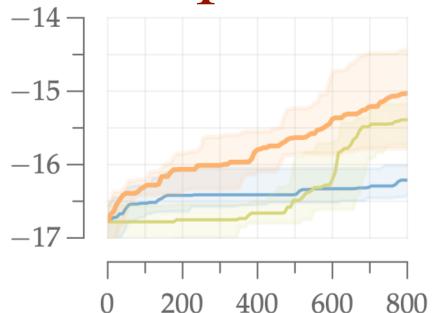
Outline

Studied Problem



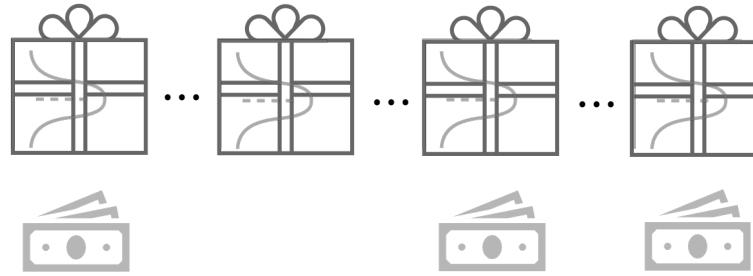
Cost-aware Bayesian optimization

Impact



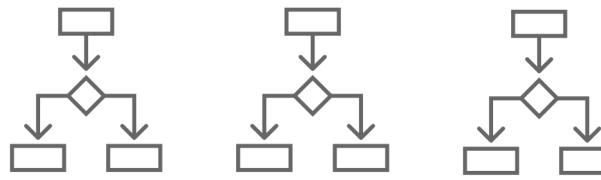
Competitive empirical performance

Key idea



Link to Pandora's box and
Gittins index theory

Future direction

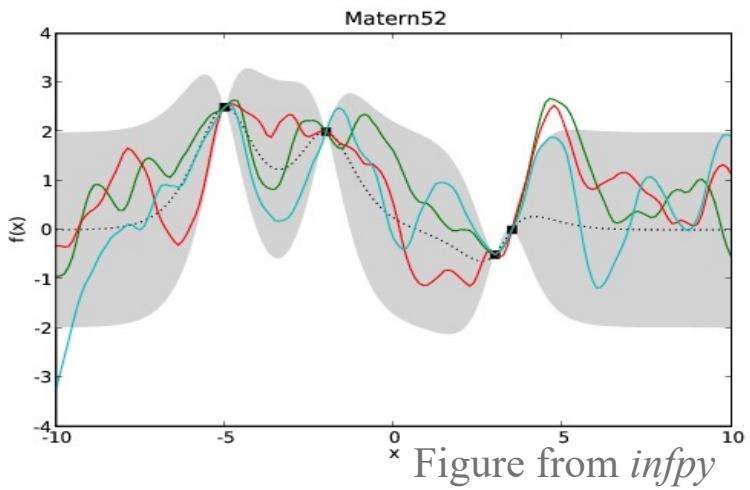


“Exotic” Bayesian optimization

Experiment Setup: Objective Functions

Synthetic

Samples from prior



Empirical

Pest Control



Figure from ChatGPT

Ackley function

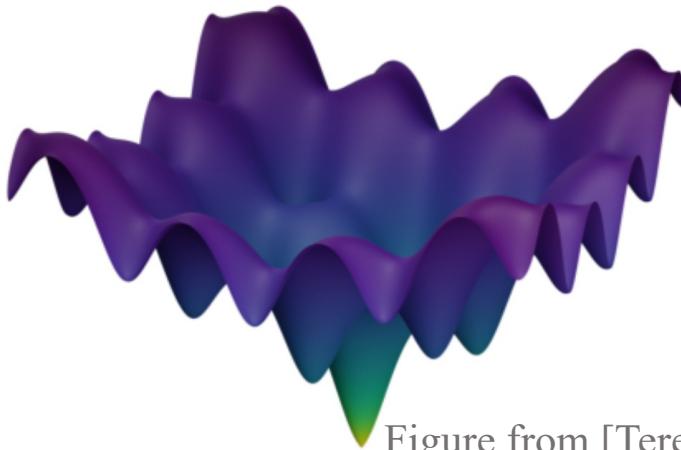


Figure from [Terenin'22]

Lunar Lander

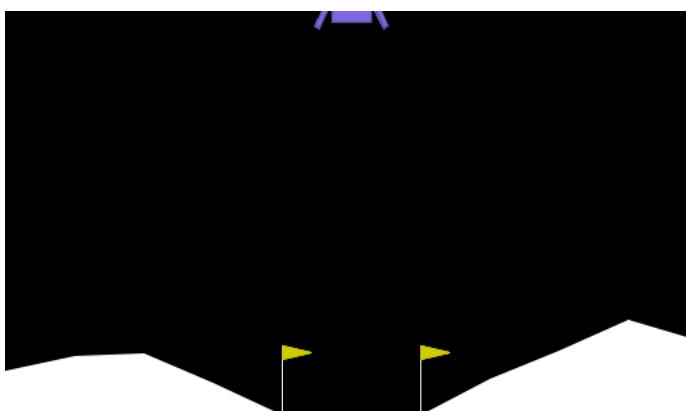
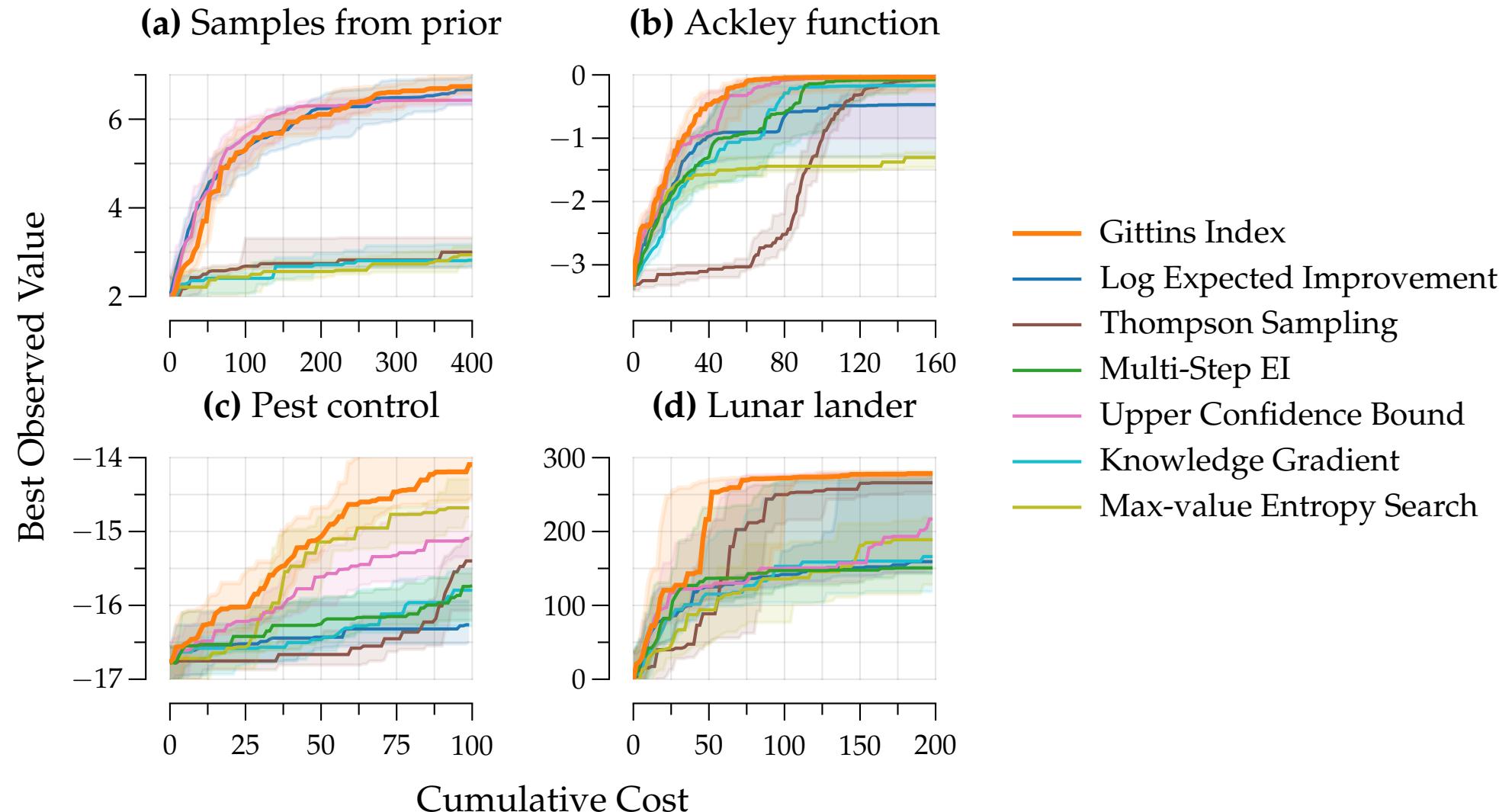
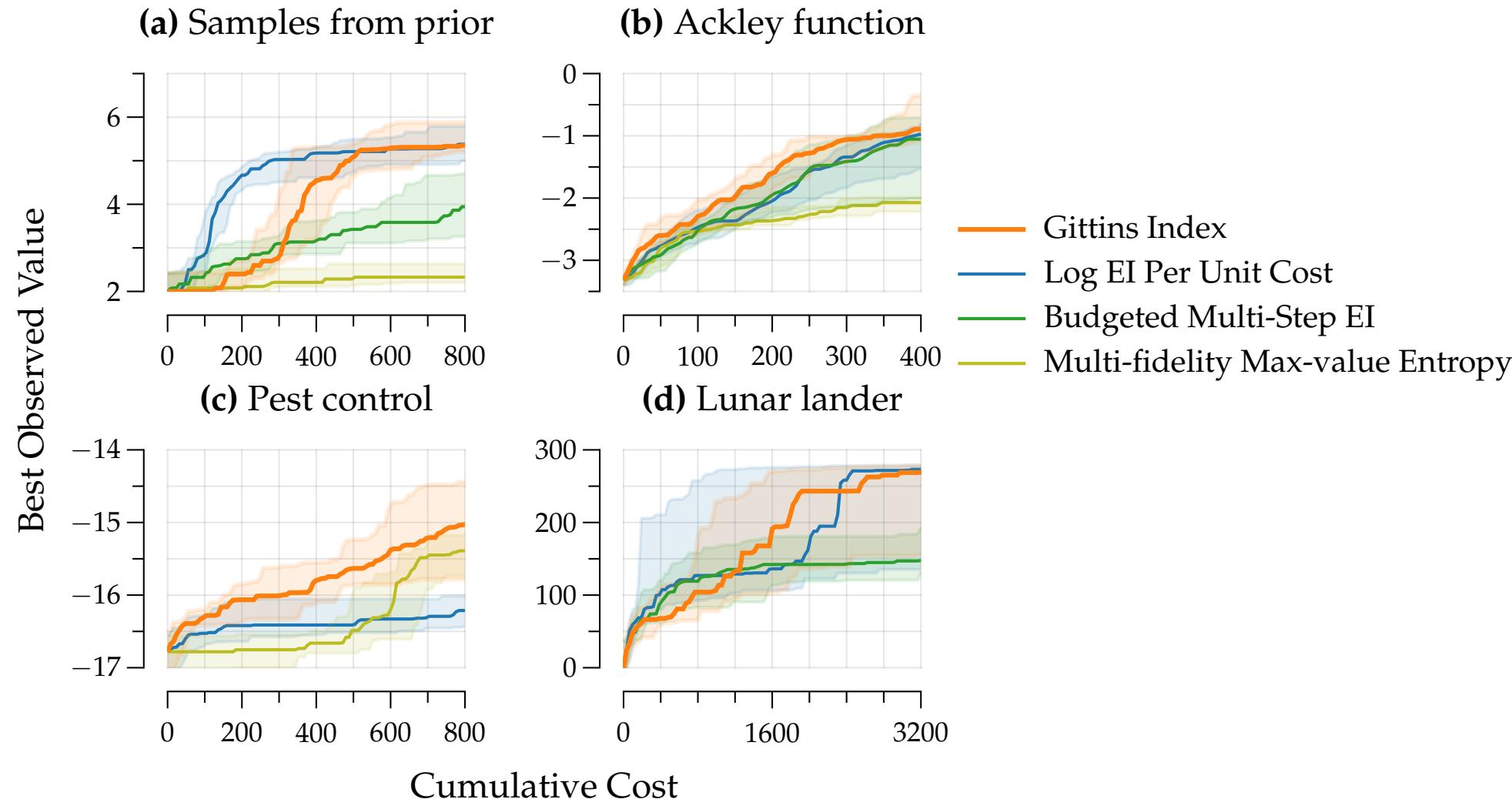


Figure from OpenAI Gym

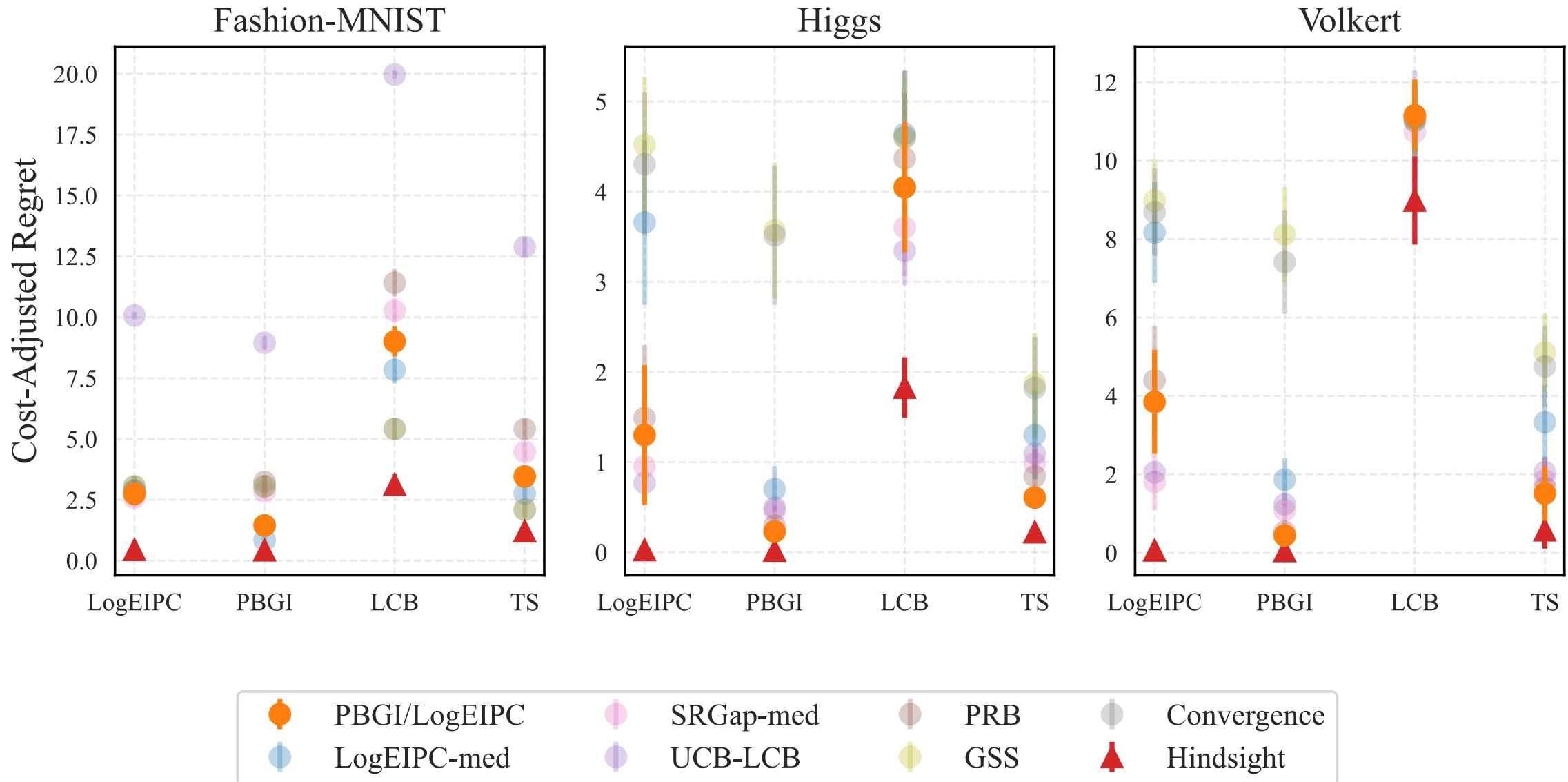
Uniform-cost: Gittins Index vs Baselines



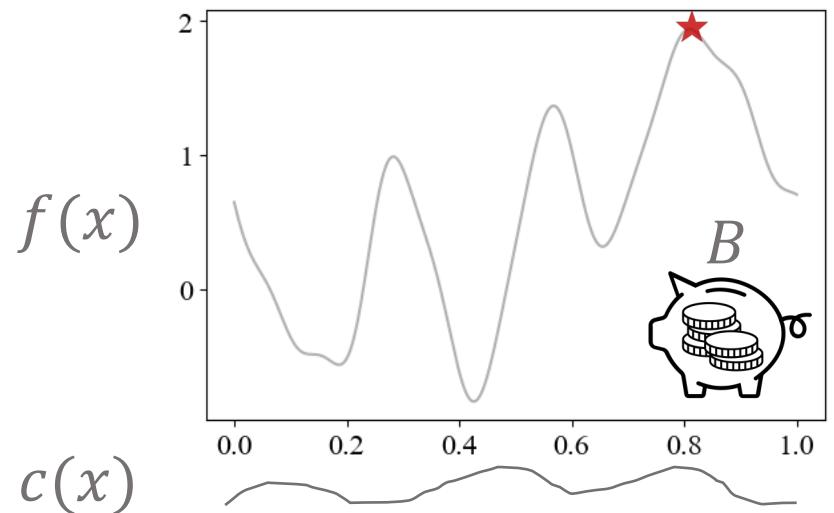
Varying-cost: Gittins Index vs Baselines



Stopping Rule: Gittins Index vs Baselines



Cost-aware Bayesian Optimization



Continuous

Correlated

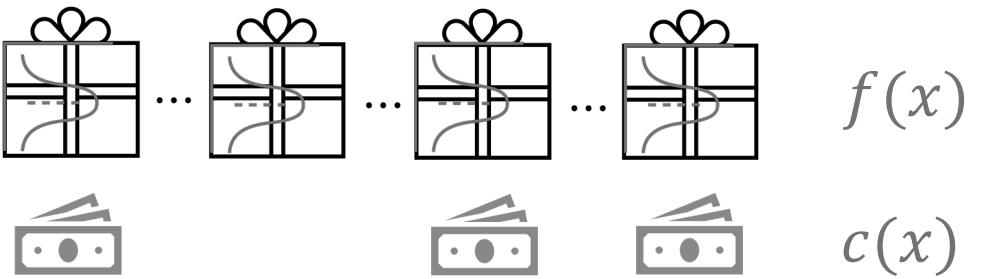
Ebc & Cps

Acquisition function
+ stopping rule

Theoretical guarantee?

Pandora's Box

[Weitzman'79]



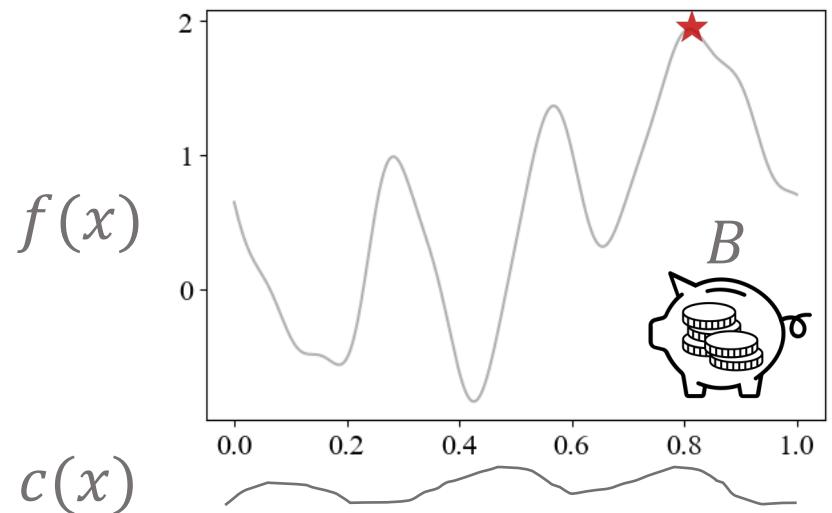
Discrete

Independent

Cost-per-sample

incorporate posterior
Acquisition function
+ stopping rule
 \Leftarrow Gittins index is optimal

Cost-aware Bayesian Optimization



Continuous

Correlated

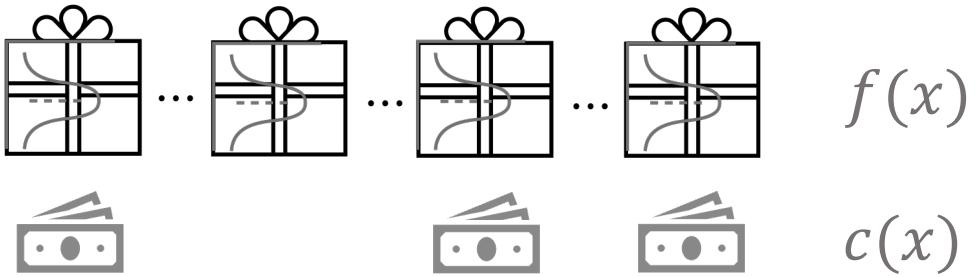
Ebc & Cps

Acquisition function
+ stopping rule

Theoretical guarantee?

Pandora's Box

[Weitzman'79]



Discrete

Independent

Cost-per-sample

incorporate posterior

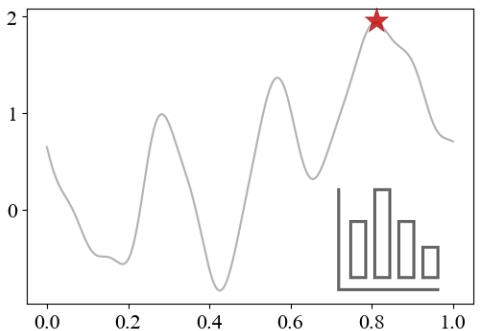
Acquisition function
+ stopping rule

iff Gittins index is optimal

Yes! A bound on expected cost up to stopping

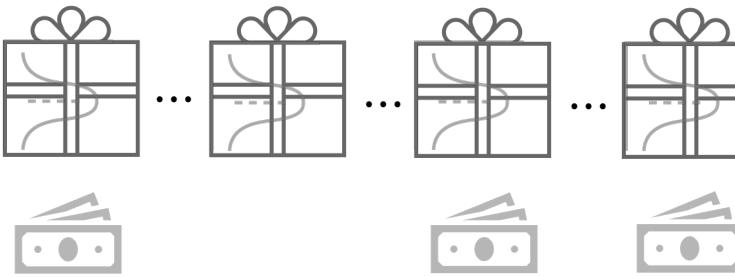
Gittins Index: A New Design Principle

Studied Problem



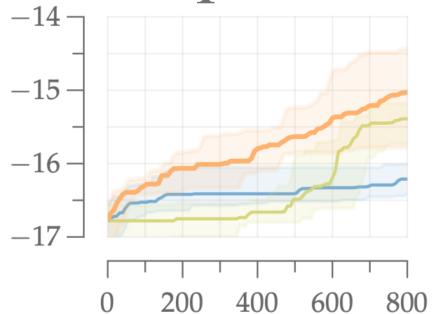
Cost-aware Bayesian optimization

Key idea



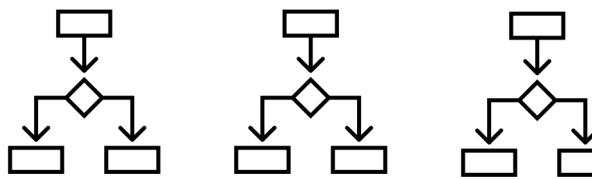
Link to Pandora's box and
Gittins index theory

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."