NeurIPS'24 & INFORMS Data Mining Paper Competition Finalist

Cost-Aware Bayesian Optimization with Adaptive Stopping via Gittins Indices

Qian Xie 谢倩 (Cornell ORIE)

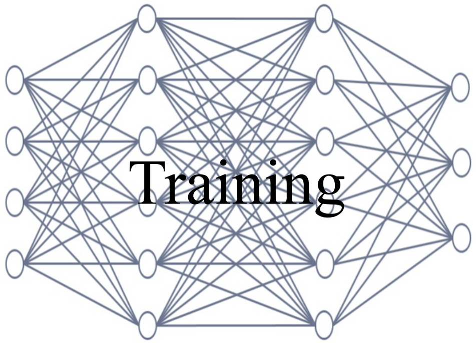
Joint work with Linda Cai (UC Berkeley), Theodore Brown (UCL), Raul Astudillo (MBZUAI), Peter Frazier, Alexander Terenin, and Ziv Scully (Cornell)

INFORMS Annual Meeting 2025 Job Market Showcase

Motivation: World of Optimization under Uncertainty

ML model training:

Training hyperparameters
(e.g., learning rate, # layers)



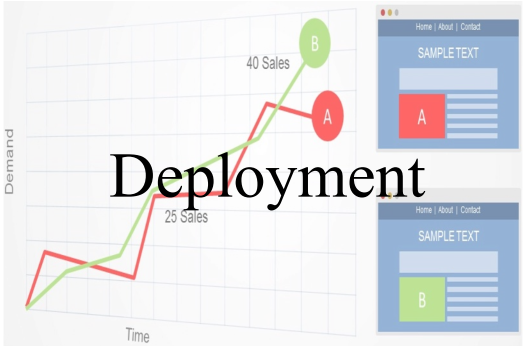
Accuracy

Motivation: World of Optimization under Uncertainty

ML model training:

Training hyperparameters (e.g., learning rate, # layers) ⟶  Training ⟶ Accuracy

Adaptive experimentation:

Decision/design variables (e.g., layout, pricing level) ⟶ 

Deployment ⟶ Revenue

Motivation: World of Optimization under Uncertainty

Black-box optimization:

Input x →  → Performance metric $f(x)$

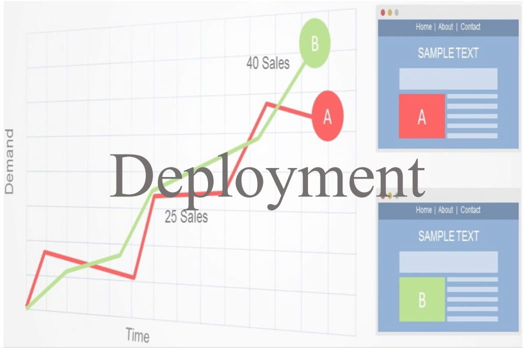
non-analytical & no gradient info

ML model training:

Training hyperparameters (e.g., learning rate, # layers) → 

→ Accuracy

Adaptive experimentation:

Decision/design variables (e.g., layout, pricing level) → 

→ Revenue

Motivation: World of Optimization under Uncertainty

Black-box optimization:

(gradient-based method not applicable)

non-analytical &
no gradient info

Input x $\longrightarrow$  $\longrightarrow$ Observed outcome $f(x)$

ML model training:

Training hyperparameters
(e.g., learning rate, # layers) $\longrightarrow$ 

$\longrightarrow$ Accuracy

Black-Box Optimization

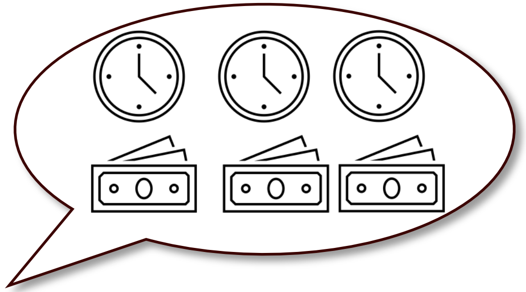
Black-box optimization:

(gradient-based method not applicable)

Input x $\longrightarrow$

expensive-to-evaluate

$\longrightarrow$ Observed outcome $f(x)$

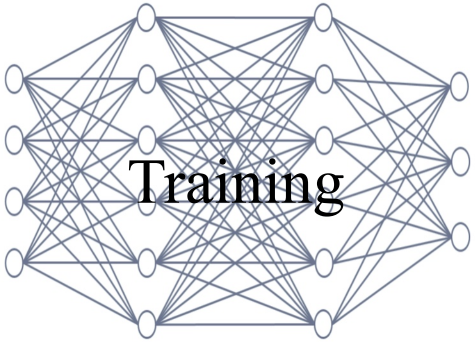


Training time

Compute credits

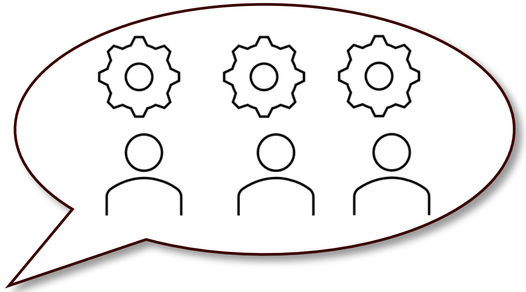
ML model training:

Training hyperparameters $\longrightarrow$
(e.g., learning rate, # layers)



Training

$\longrightarrow$ Accuracy

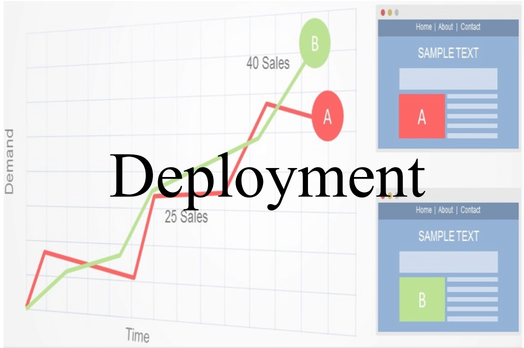


Operational cost

User experience

Adaptive experimentation:

Decision/design variables $\longrightarrow$
(e.g., layout, pricing level)



Deployment

$\longrightarrow$ Revenue

Black-Box Optimization

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

expensive-to-evaluate

High-level goal: Choose $x_1, \dots, x_T$ to maximize the expected best observed value

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

Data-Driven Black-Box Optimization

Input x $\longrightarrow$

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

expensive-to-evaluate

adaptively

High-level goal: Choose $x_1, \dots, x_T$ to maximize the expected best observed value

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

Fewer #evaluations

Data-Driven Black-Box Optimization

expensive-to-evaluate

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

adaptively

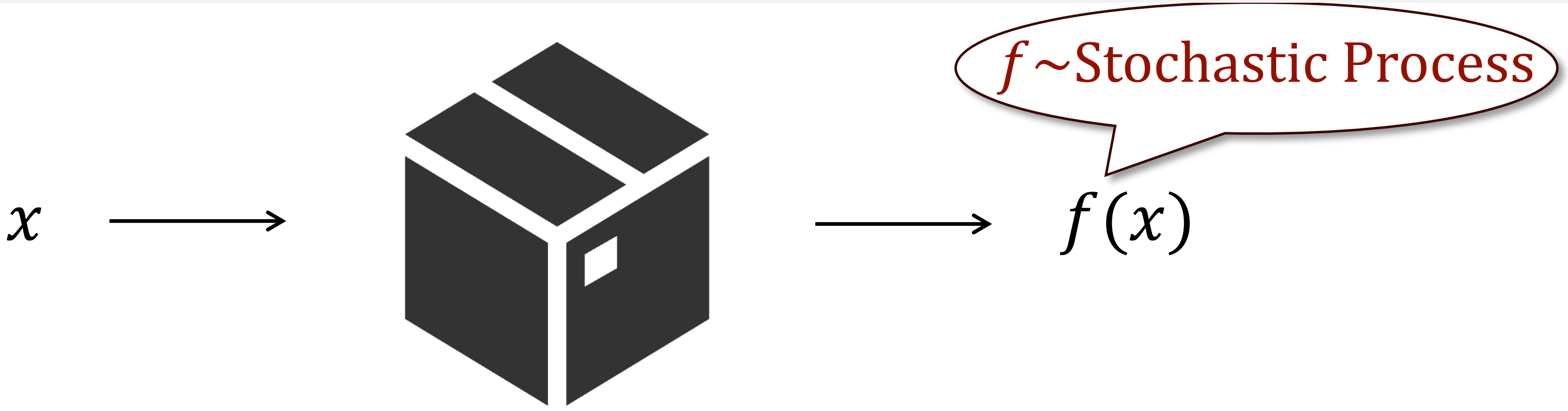
High-level goal: Choose $x_1, \ldots, x_T$ to maximize the expected best observed value

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

Fewer #evaluations

Efficient framework: Bayesian optimization

Bayesian Optimization



Black-box function

Bayesian Optimization

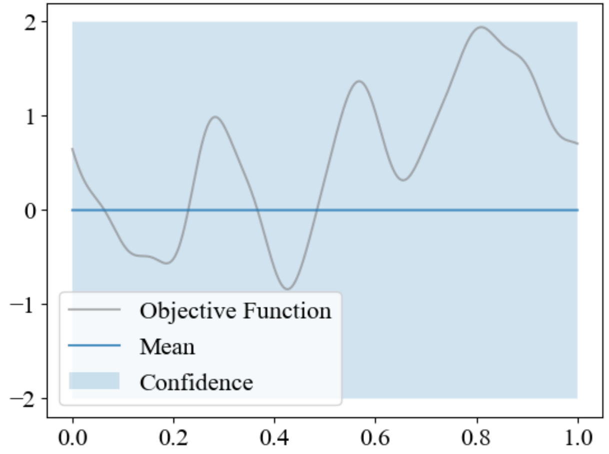
Time 0

x →  → $f(x)$

Black-box function

$f \sim$Stochastic Process

Model belief



Probabilistic model

(e.g., Gaussian process)

Bayesian Optimization

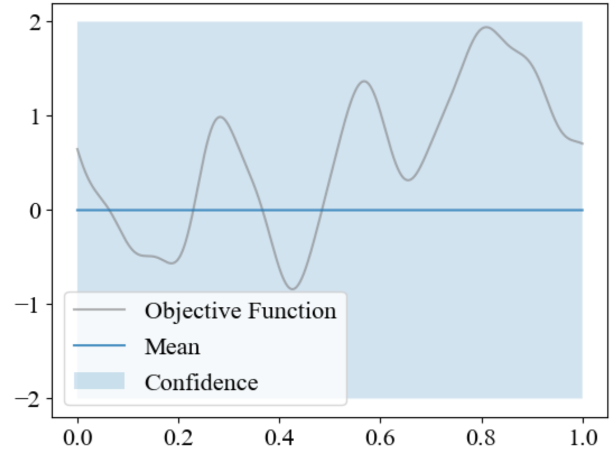
Time t

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

$f \sim$Stochastic Process

Black-box function

Model belief



Probabilistic model
(e.g., Gaussian process)

Bayesian Optimization

Time t

$x_1, \dots, x_t \longrightarrow$

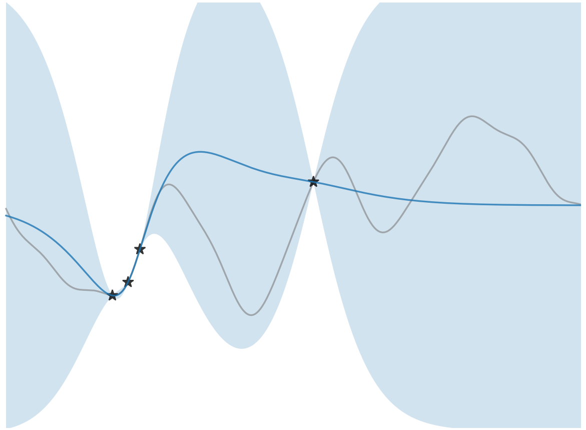
Black-box function

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

$f \sim$Stochastic Process

Update belief

(Bayes' rule)



Probabilistic model

(e.g., Gaussian process)

Bayesian Optimization

Time t

$x_1, \ldots, x_t \longrightarrow$

Black-box function

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

Update belief

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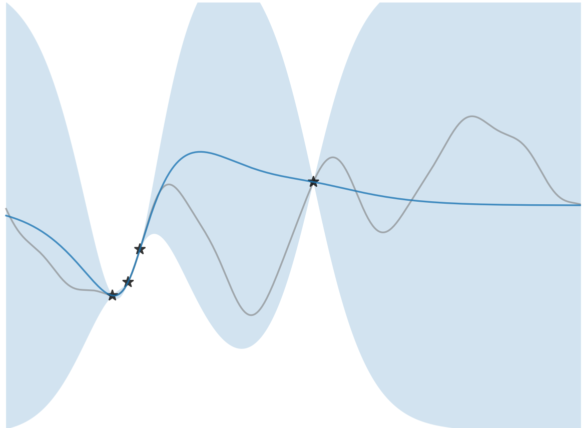
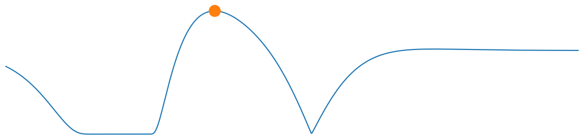


Probabilistic model

(e.g., Gaussian process)

scoring (worth of each point



Decision rule

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

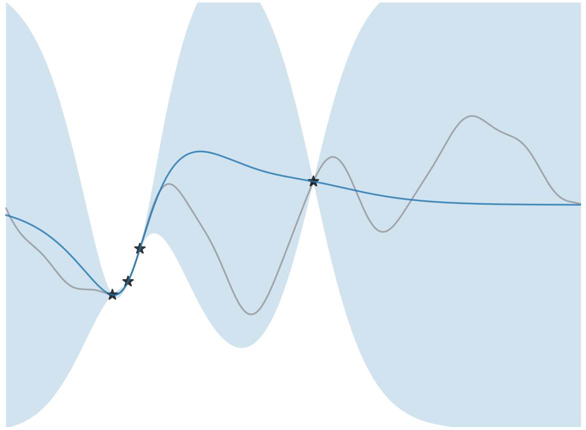
Bayesian Optimization

Time t

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

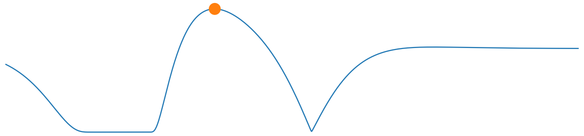
Black-box function

Update belief
(Bayes' rule)



Probabilistic model
(e.g., Gaussian process)

scoring (worth of each point



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

Decide next input
(gradient-based optimization)

Bayesian Optimization

Time $t + 1$

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

Black-box function

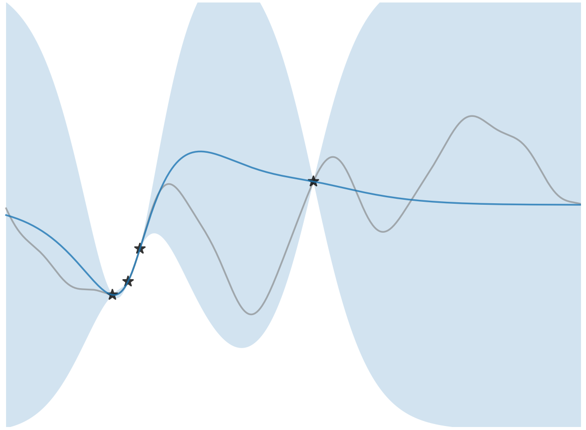
$f(x_1), \dots, f(x_{t+1})$

Decide next input

(gradient-based optimization)

Update belief

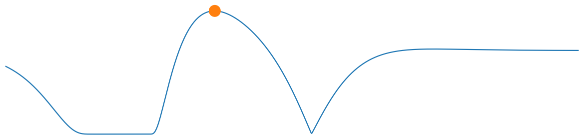
(Bayes' rule)



Probabilistic model

(e.g., Gaussian process)

scoring (worth of each point



Decision rule

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

Bayesian Optimization

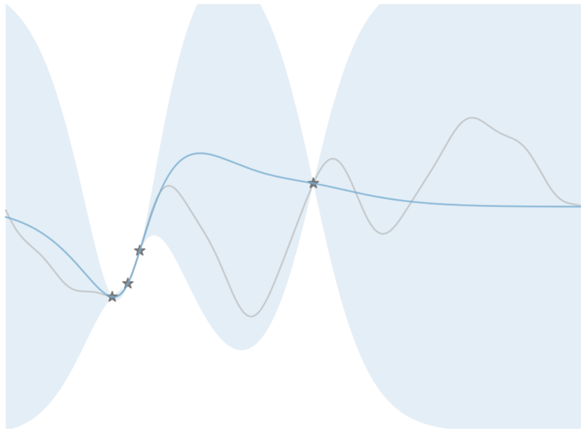
Time $t + 1$

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

Black-box function

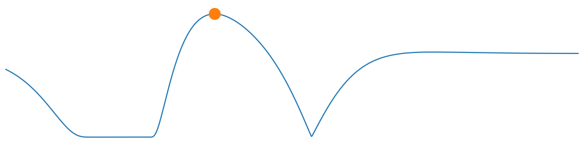
Decide next input
(gradient-based
optimization)

Update belief
(Bayes' rule)



Probabilistic model
(e.g., Gaussian process)

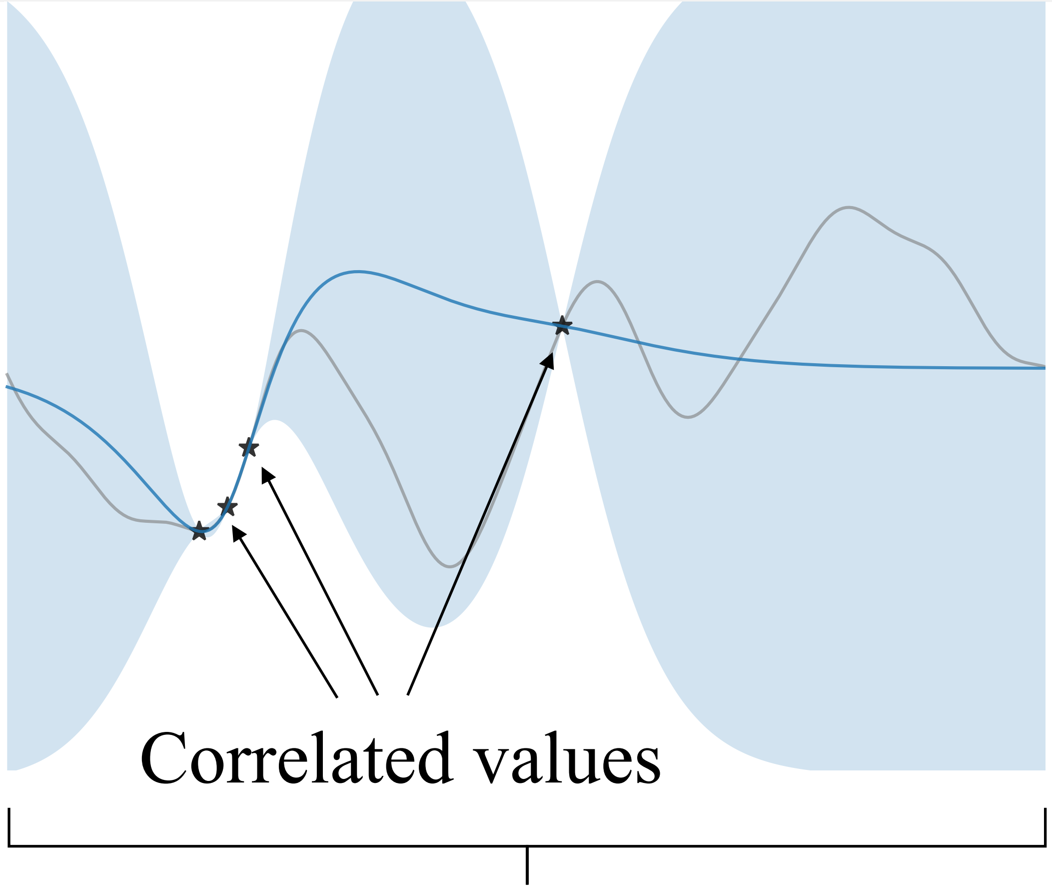
scoring (worth
of each point



My focus

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

Challenge in Decision Rule Design



Correlation & continuity $\Longrightarrow$ Intractable MDP $\Longrightarrow$ Optimal policy unknown

Popular Decision Rule: Expected Improvement

current best observed

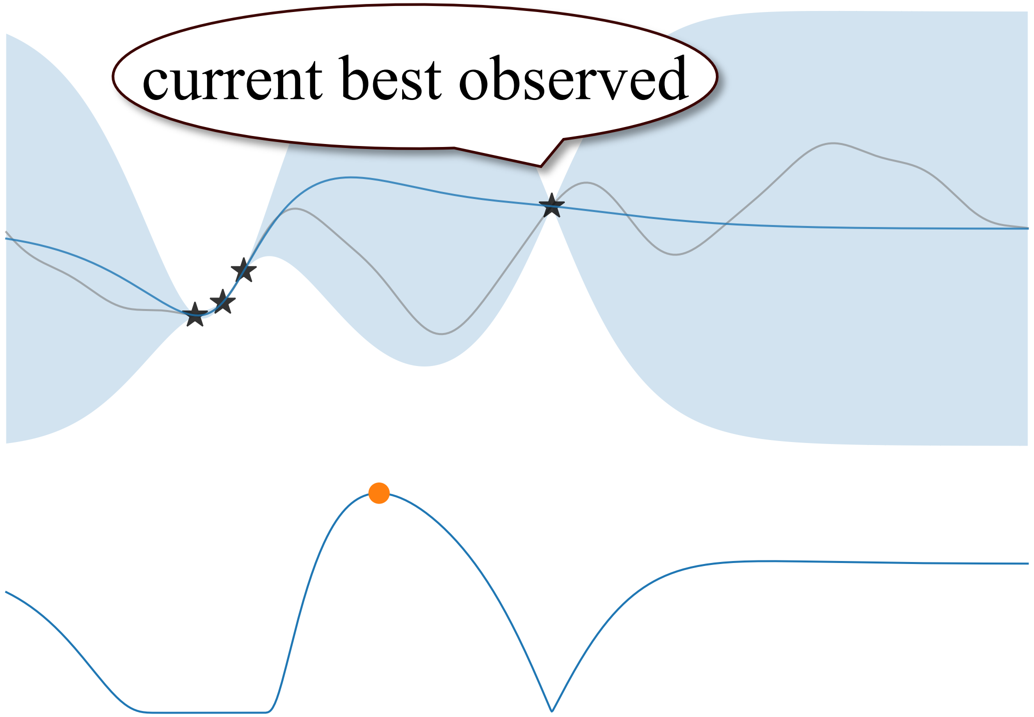
data

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

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

posterior distribution

One-step approximation to MDP



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

Popular Decision Rule: Expected Improvement

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

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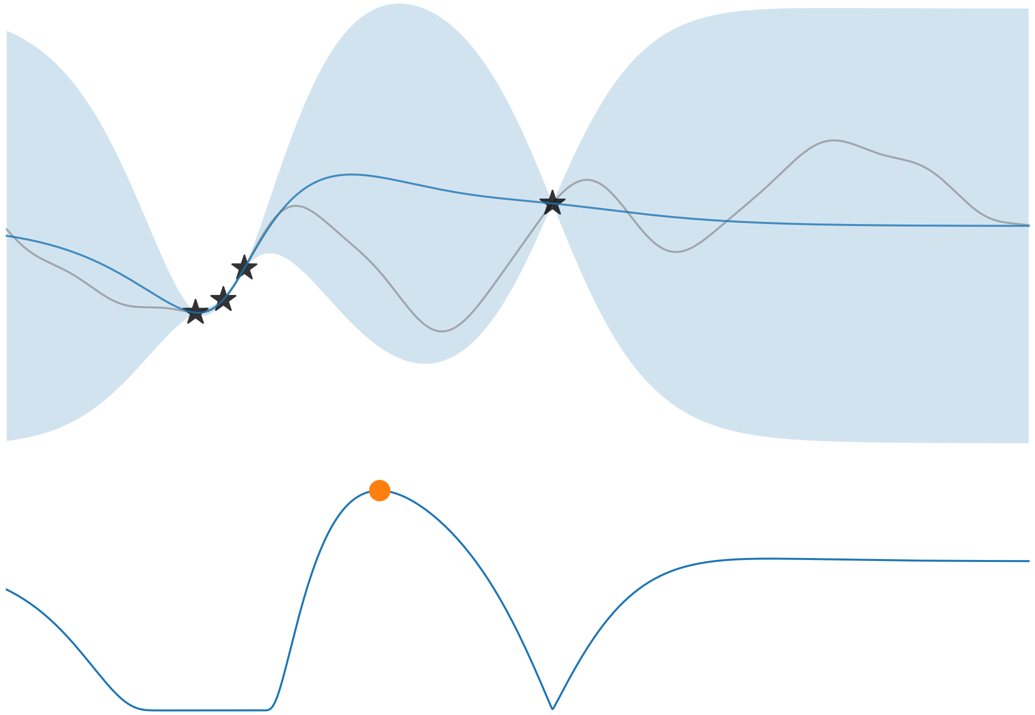
One-step approximation to MDP

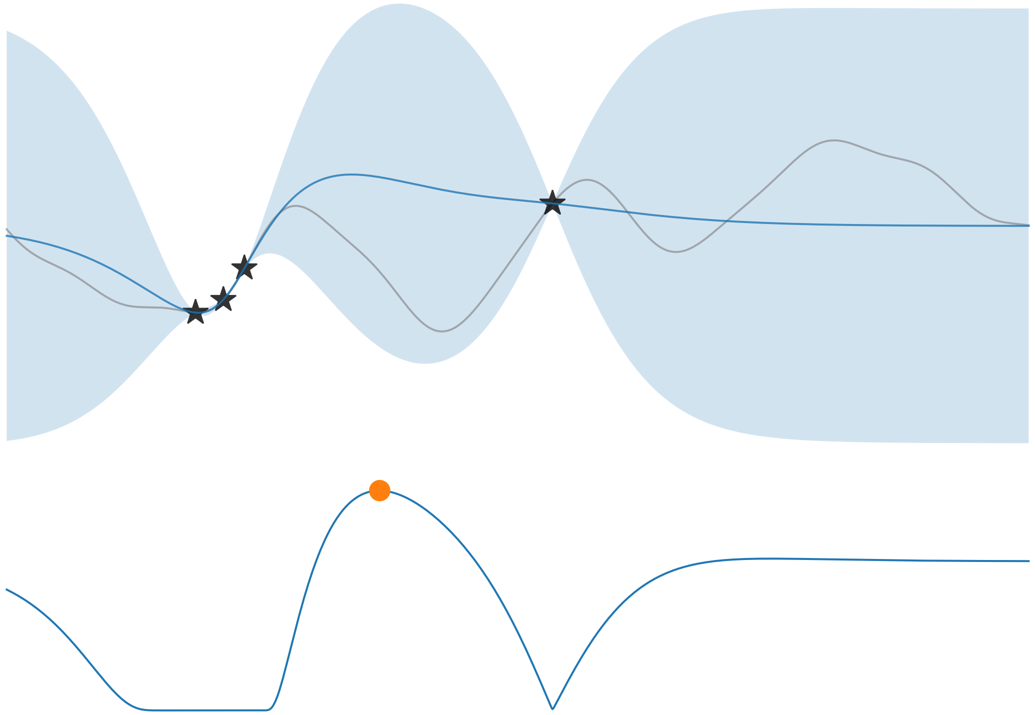


Expected improvement $\mathrm{EI}(x)$

Improvement-based design principle

Existing Design Principles

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

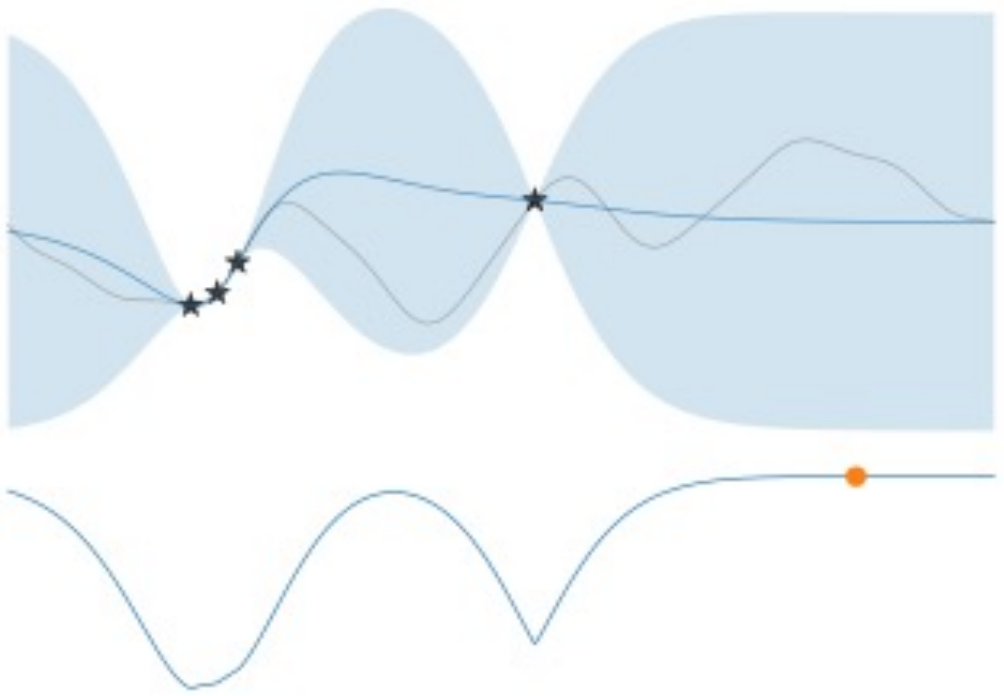


Expected improvement $\mathrm{EI}(x)$

Improvement-based design principle

New Design Principle: Gittins Index

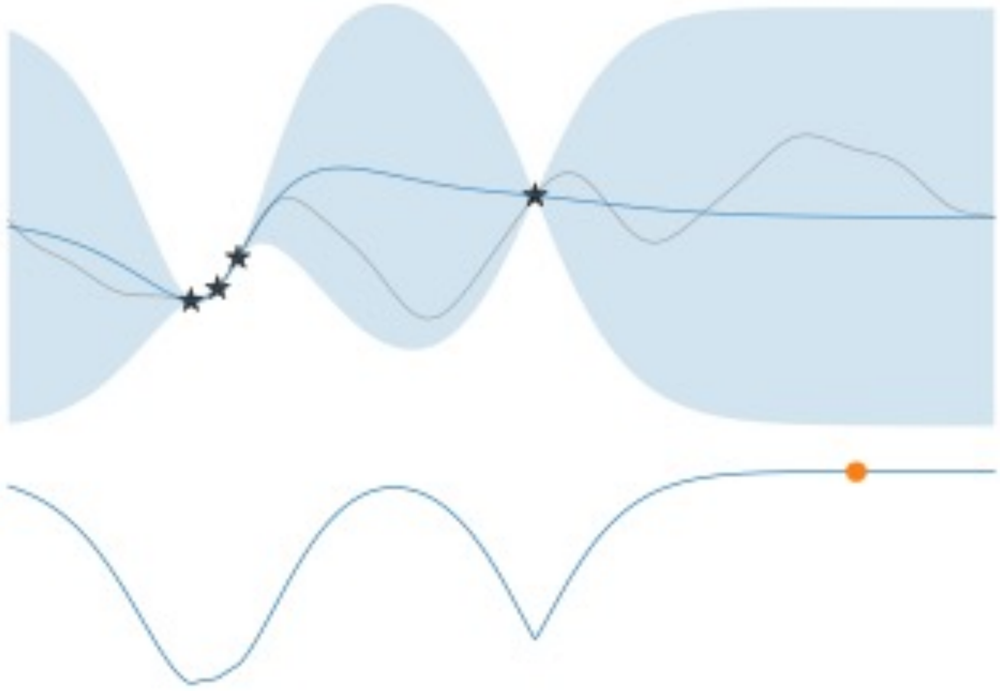
- Improvement-based (e.g., EI)
- Entropy-based
- Confidence bounds (UCB/LCB)
- Thompson sampling (TS)
- Gittins Index



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?

Our Contribution: Gittins Index Principle

? Why another principle?

1. Principled design via problem simplification

2. Natural incorporation of side info and flexibility

3. Competitive performance on benchmarks

4. Theoretical guarantees

Our Contribution: Gittins Index Principle

1. Principled design via problem simplification

2. Natural incorporation of side info and flexibility

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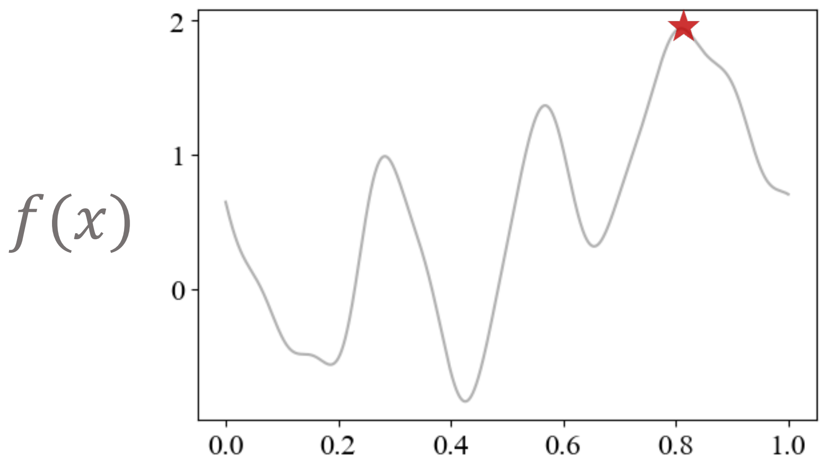
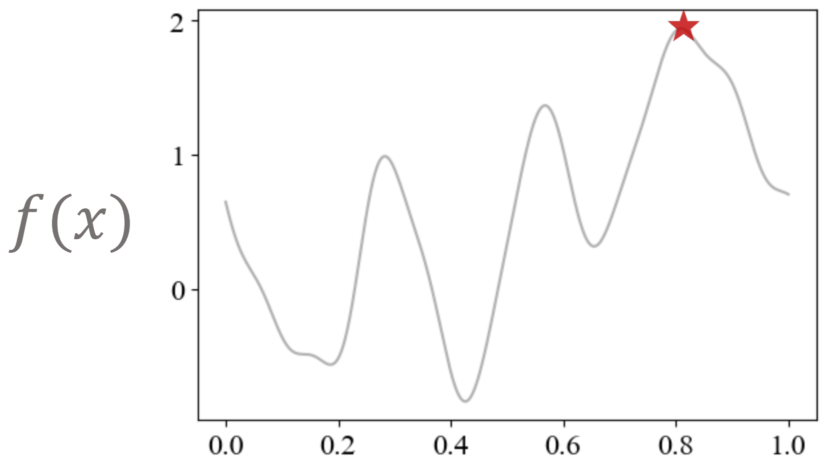
Bayesian Optimization



Continuous

Correlated

Bayesian Optimization

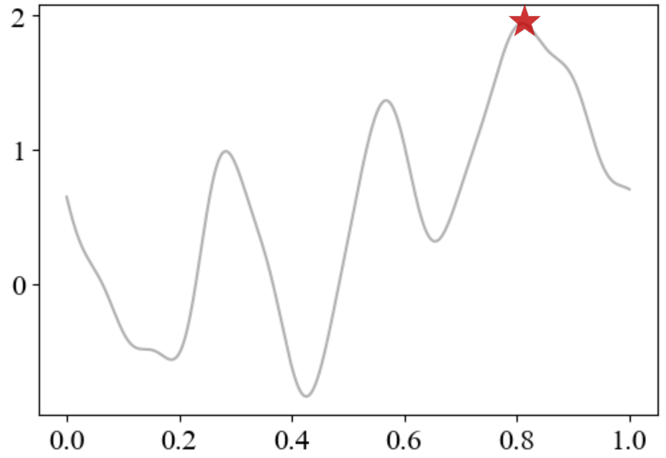


Continuous $\Longrightarrow$ Discrete

Correlated $\Longrightarrow$ Independent

Bayesian Optimization

$f(x)$



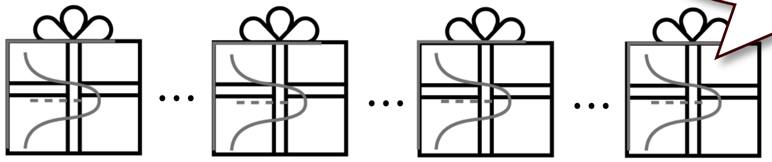
Continuous

Correlated

Pandora's Box

[Weitzman'79]

distribution of hidden reward

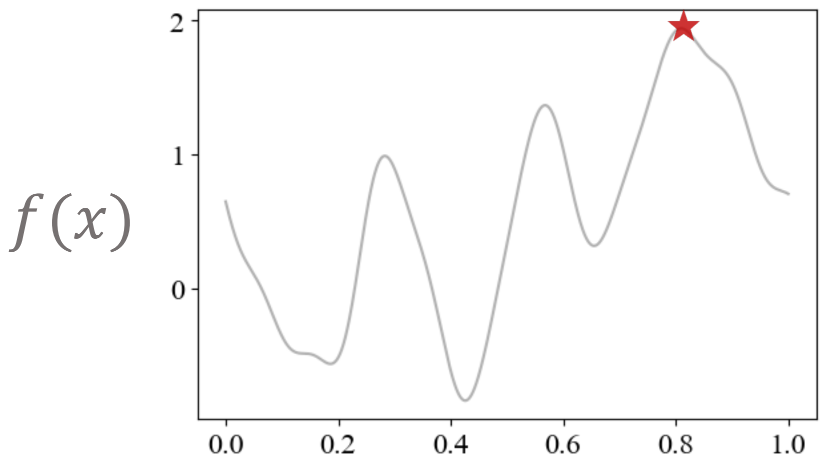


$f(x)$

Discrete

Independent

Bayesian Optimization

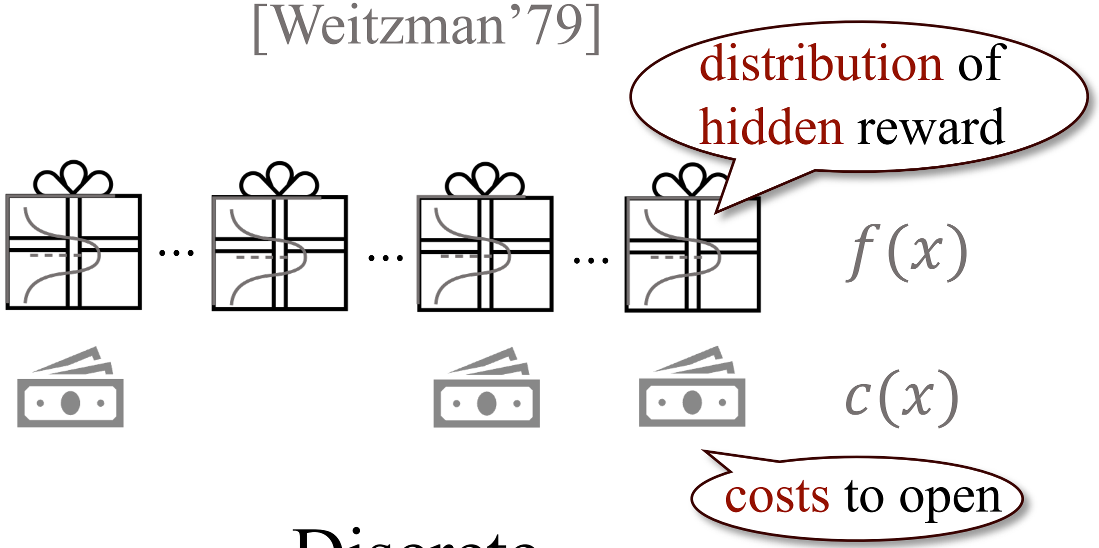


Continuous

Correlated

Pandora's Box

[Weitzman'79]

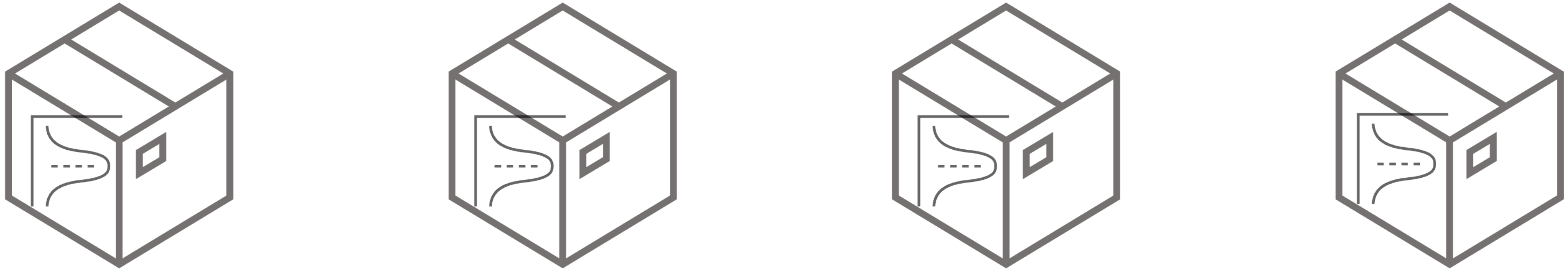


Discrete

Independent

Pandora's Box

$t = 0$

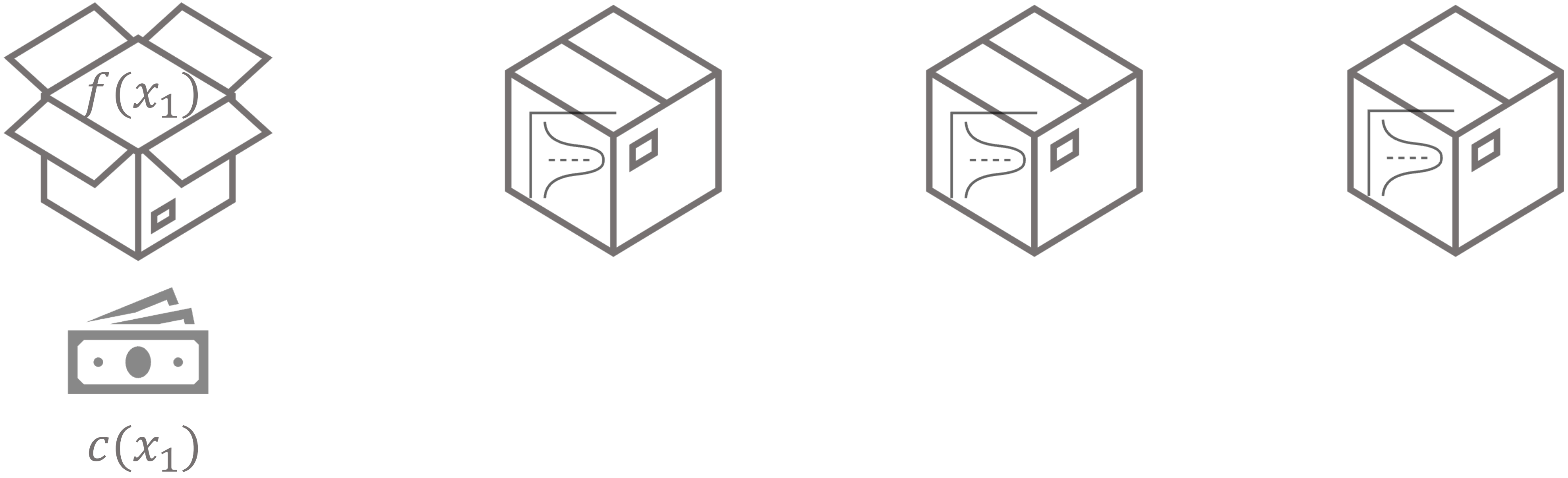


High-level goal: Choose box $x_1, \dots, x_T$ to open to maximize the expected utility

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

Pandora's Box

$t = 1$



High-level goal: Choose box $x_1, \dots, x_T$ to open to maximize the expected utility

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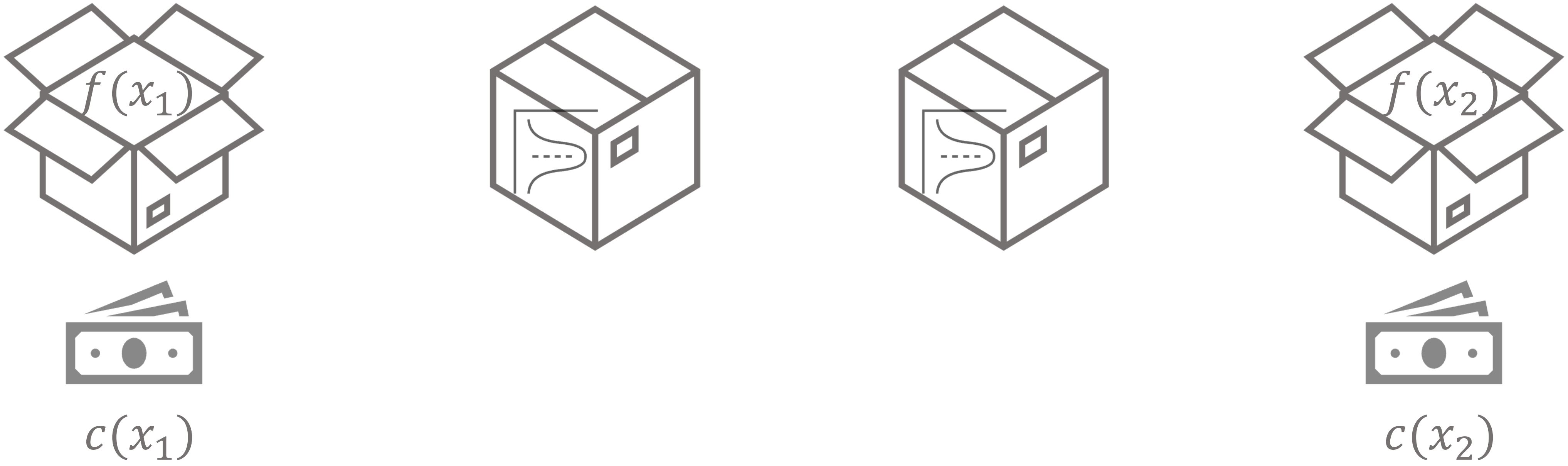
Pandora's Box

$t = 2$

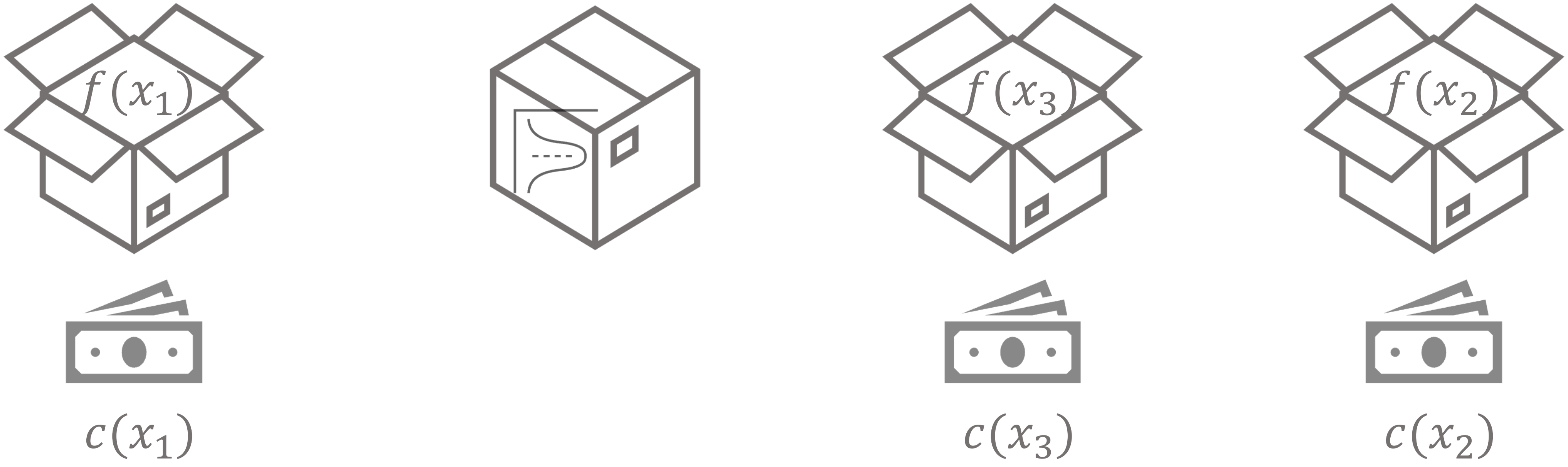


High-level goal: Choose box $x_1, \ldots, x_T$ to open to maximize the expected utility

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

Pandora's Box

$t = 3$

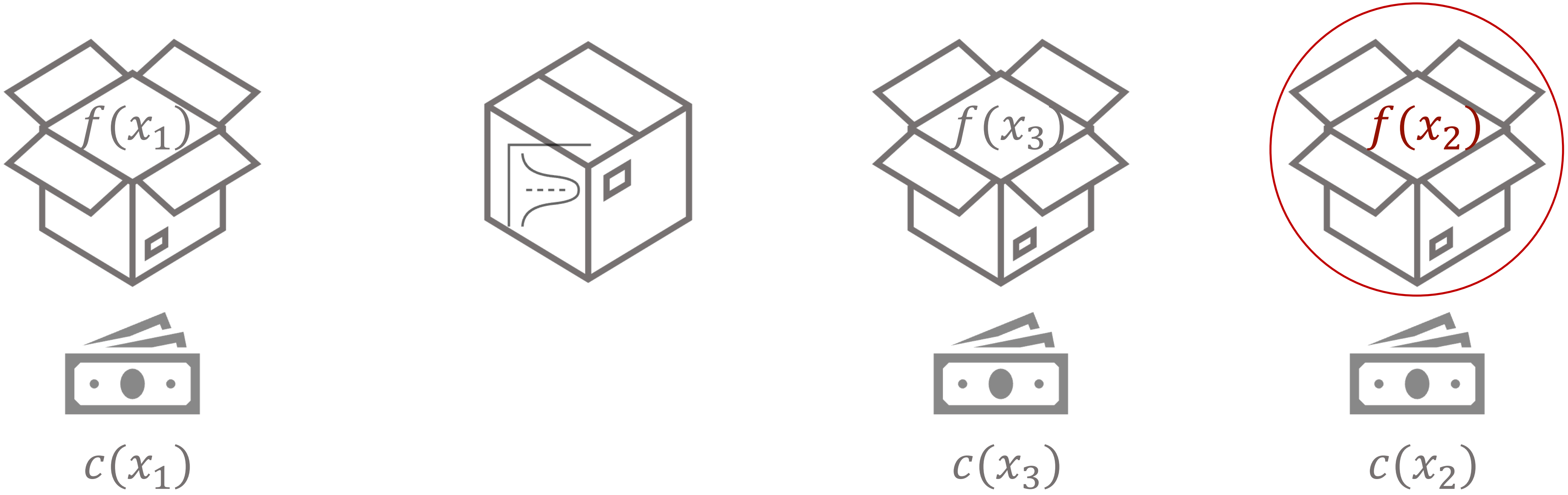


High-level goal: Choose box $x_1, \ldots, x_T$ to open to maximize the expected utility

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

Pandora’s Box

$t = T$, stop

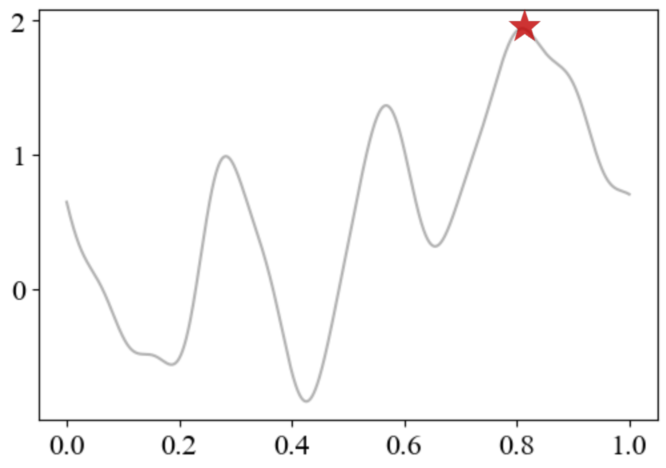


High-level goal: Choose box $x_1, \ldots, x_T$ to open to maximize the expected utility

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

Bayesian Optimization

$f(x)$

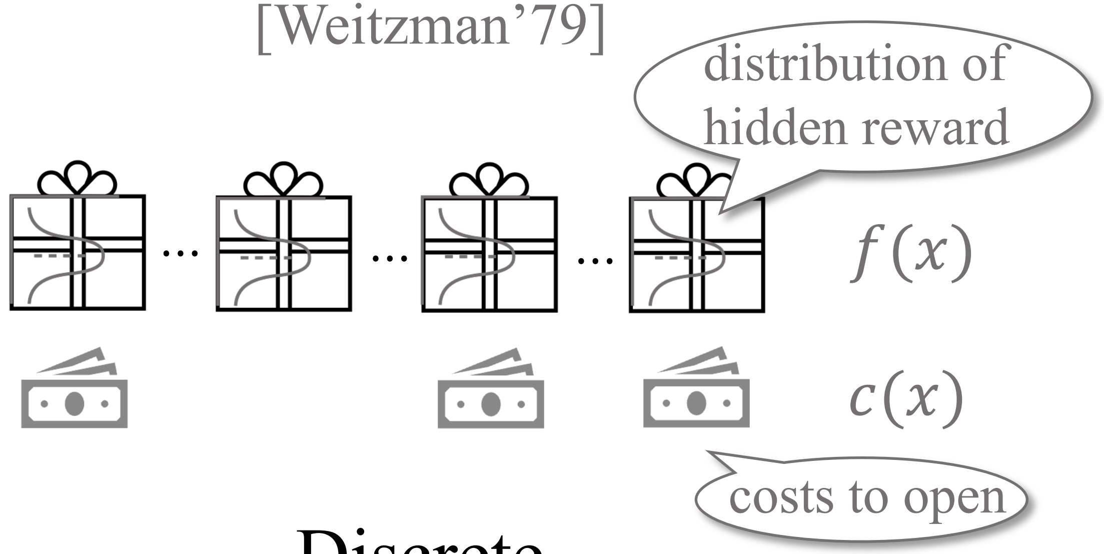


Continuous

Correlated

Pandora's Box

[Weitzman'79]



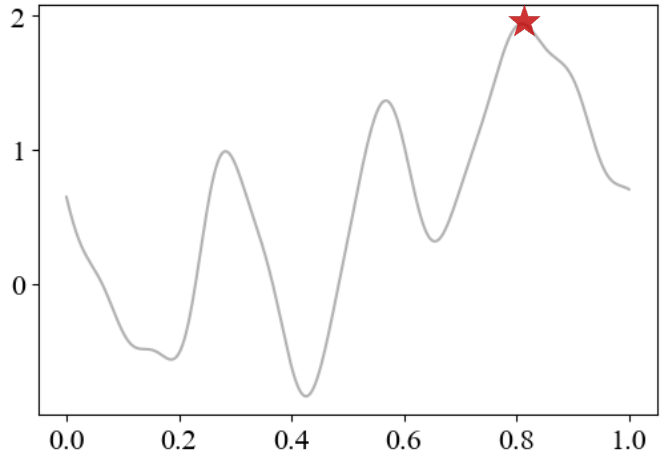
Discrete

Independent

Optimal policy: Gittins index

Bayesian Optimization

$f(x)$

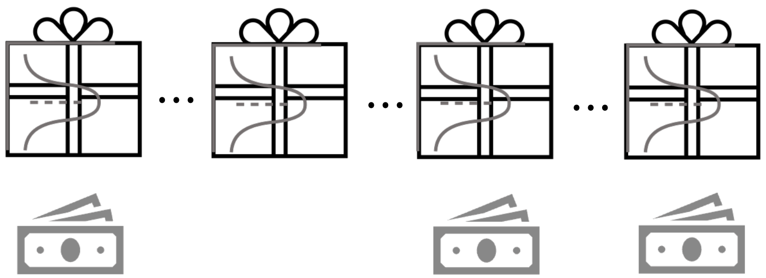


Continuous

Correlated

Pandora's Box

[Weitzman'79]



$f(x)$

$c(x)$

Discrete

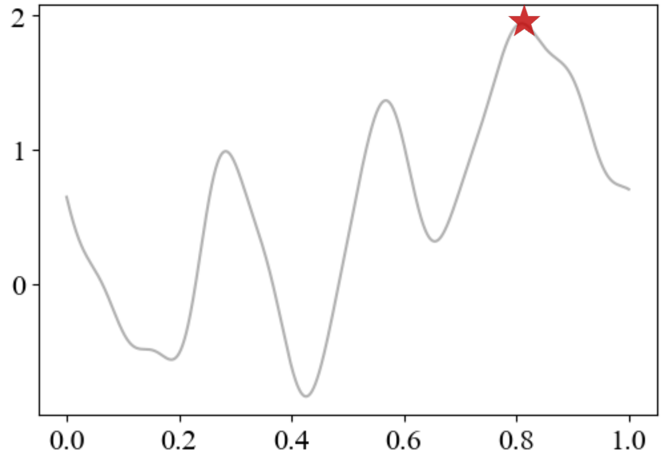
Independent

How to translate?

$\Leftarrow$ Optimal policy: Gittins index

Bayesian Optimization

$f(x)$



Continuous

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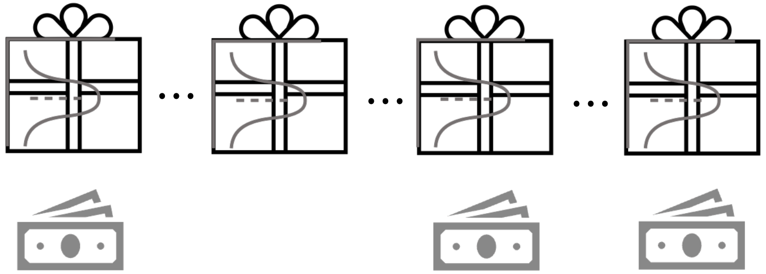
Pandora's Box

[Weitzman'79]



$f(x)$

$c(x)$

Discrete

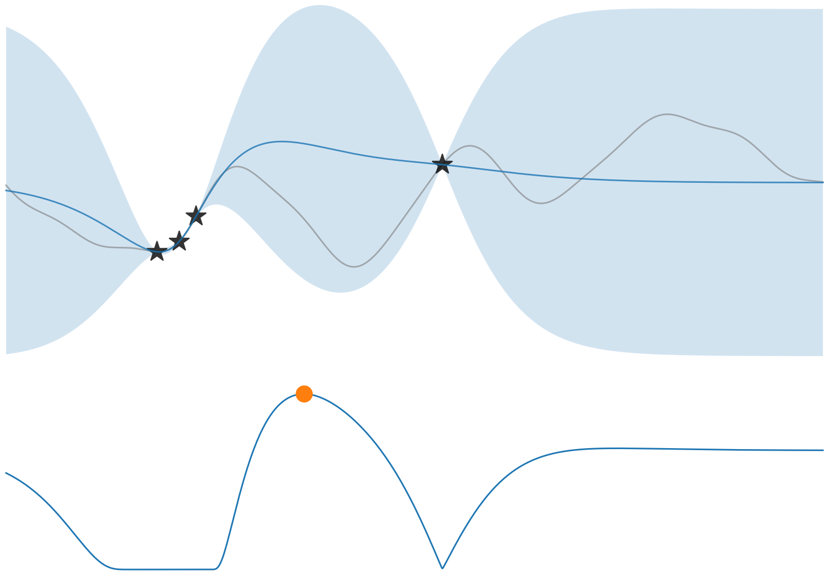
Independent

incorporate posterior

Our policy: $\mathrm{GI}_{f|D}(x; c(x))$ $\Longleftarrow$ Optimal policy: $\mathrm{GI}_f(x; c(x))$

take continuum limit

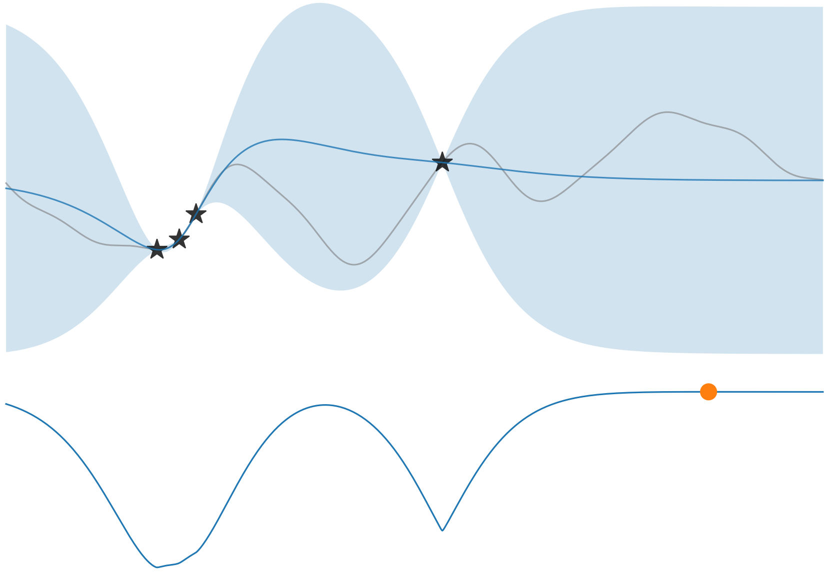
Expected Improvement



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

Temporal simplification to MDP

Gittins Index



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

Spatial simplification to MDP

Our Contribution: Gittins Index Principle

Joint work with Ziv Scully and Alexander Terenin et al.

1. Principled design via problem simplification

2. Natural incorporation of side info and flexibility

3. Competitive performance on benchmarks

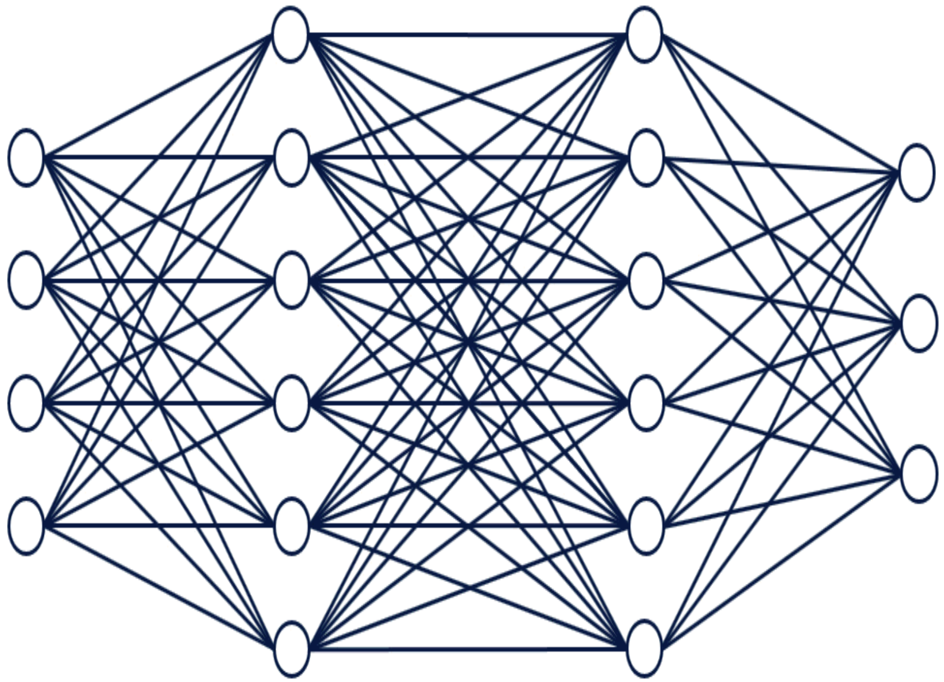
4. Theoretical guarantees

Under-explored Side Info and Flexibility

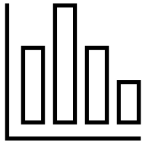
Varying evaluation costs

Smart stopping time

Observable multi-stage feedback



How does existing principle incorporate them?



Varying evaluation costs

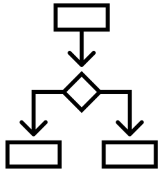
$\mathrm{EI}(x)/c(x)$

Why not subtraction?

Smart stopping time

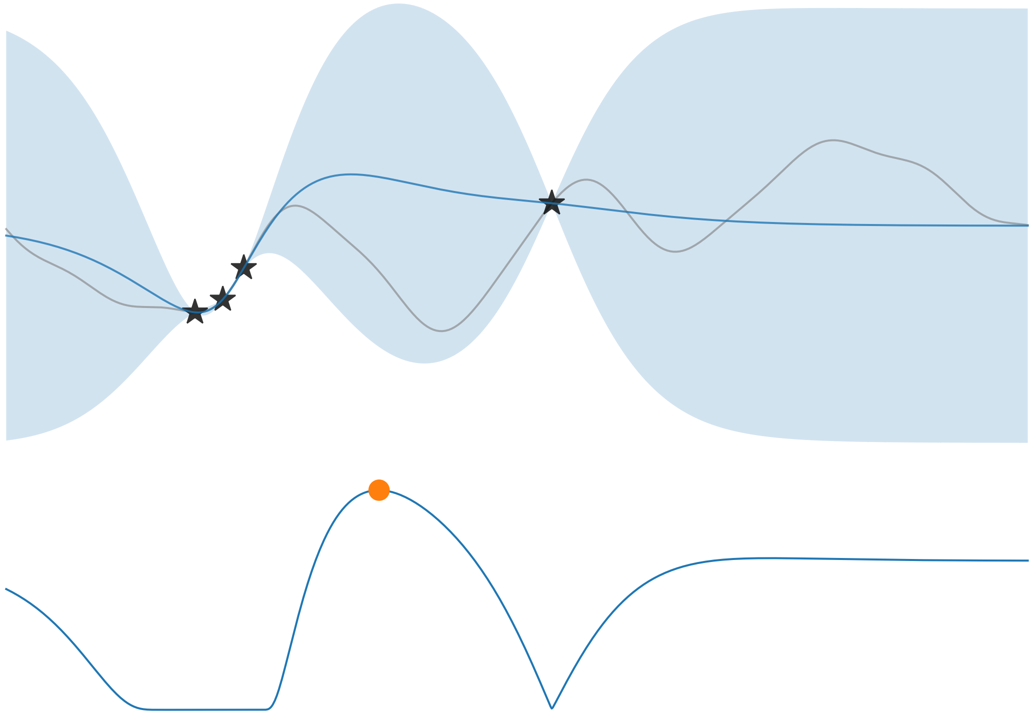
$\mathrm{EI}(x) \leq \theta$

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:
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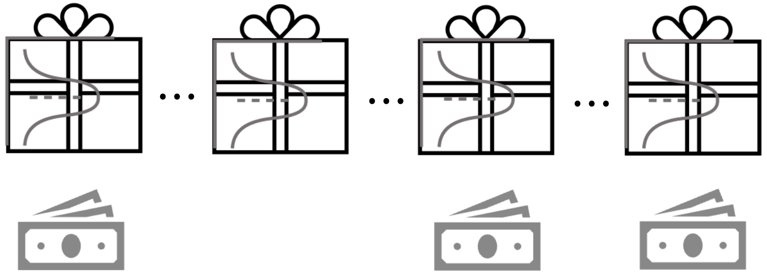
Optimal in related sequential decision problems



Why Gittins index?

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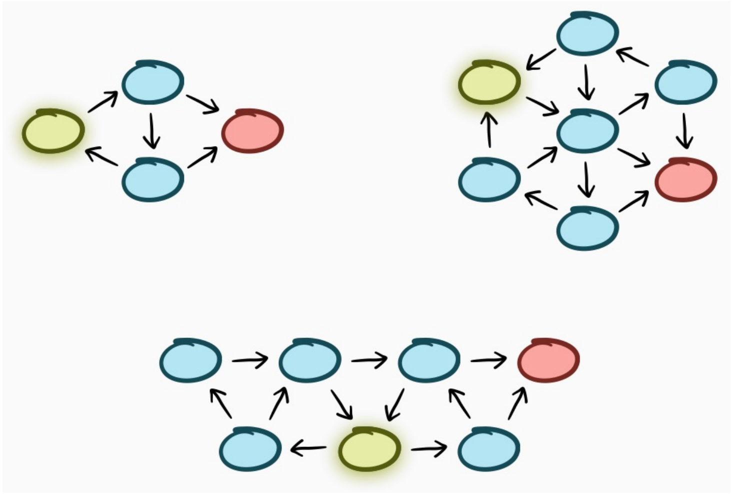


Why Gittins index?

Varying evaluation costs

Features in Pandora's box

This talk's focus

Smart stopping time

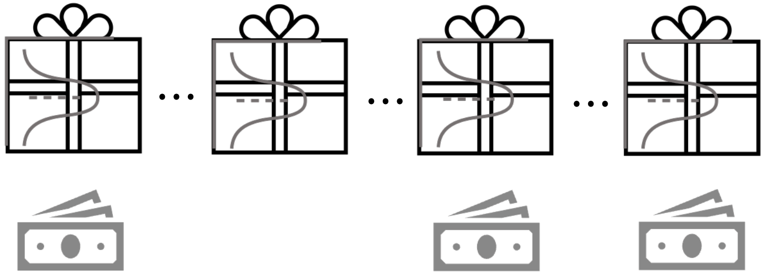
Features in Pandora's box

Observable multi-stage feedback

Features in Markov chain selection

New design principle: Gittins index

Optimal in related sequential decision problems

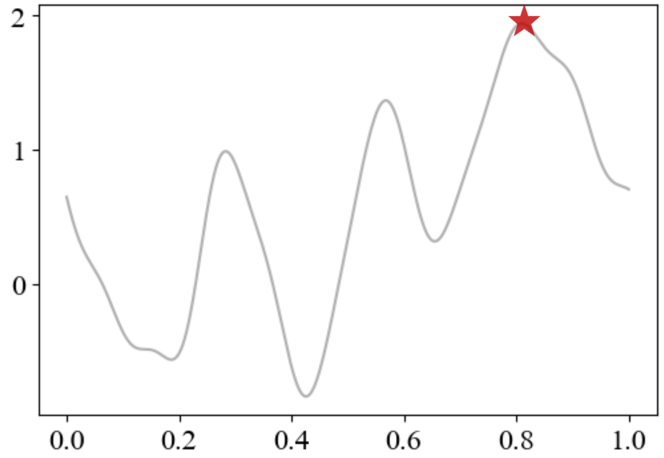


"Cost-aware Bayesian Optimization via the Pandora's Box Gittins Index." NeurIPS'24.

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

Bayesian Optimization

$f(x)$



Continuous

Correlated

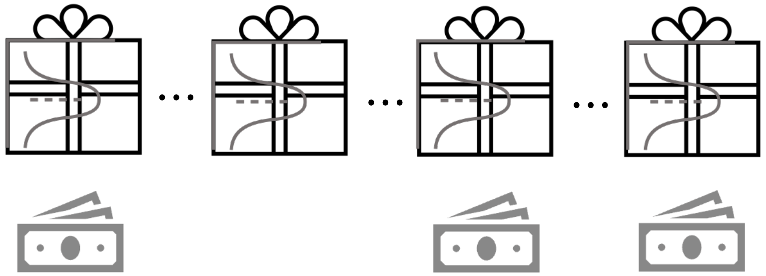
Fixed-iteration

Expected best-observed value

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

Pandora's Box

[Weitzman'79]



$f(x)$

$c(x)$

Discrete

Independent

Flexible-stopping

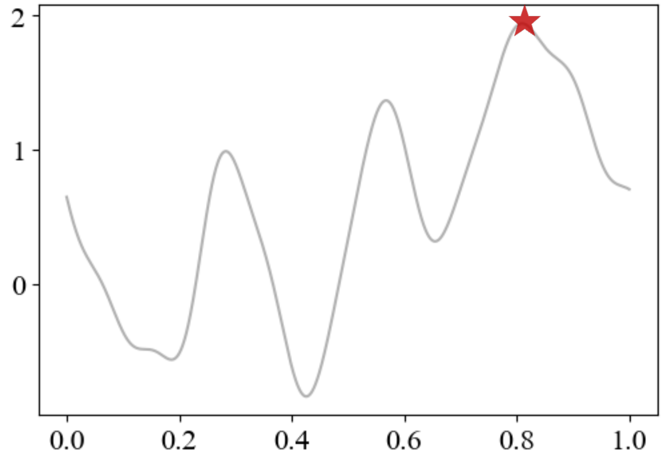
Expected utility

cumulative cost

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

Bayesian Optimization

$f(x)$



Continuous

Correlated

Fixed-iteration

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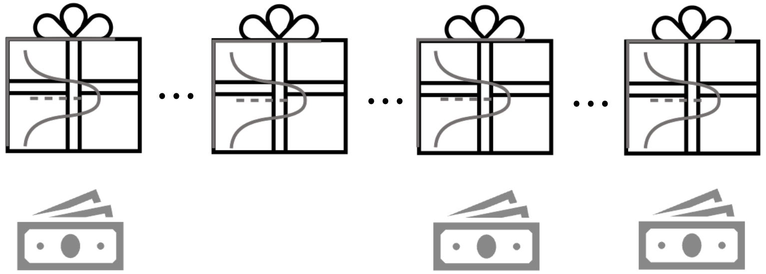
Pandora's Box

[Weitzman'79]



$f(x)$

$c(x)$

Discrete

Independent

Flexible-stopping

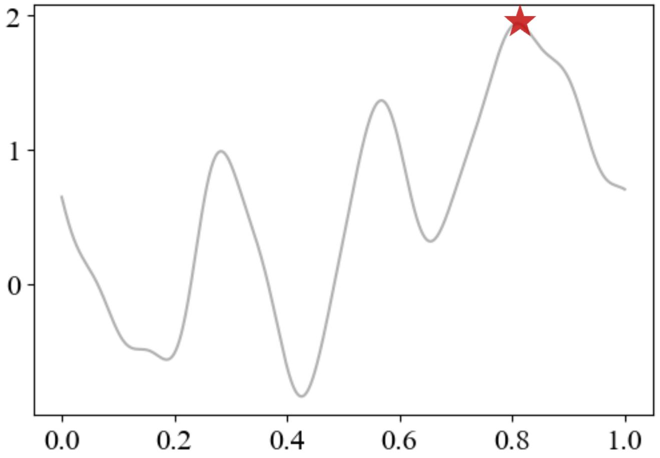
Expected utility

cumulative cost

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

Bayesian Optimization

$f(x)$



Continuous

Correlated

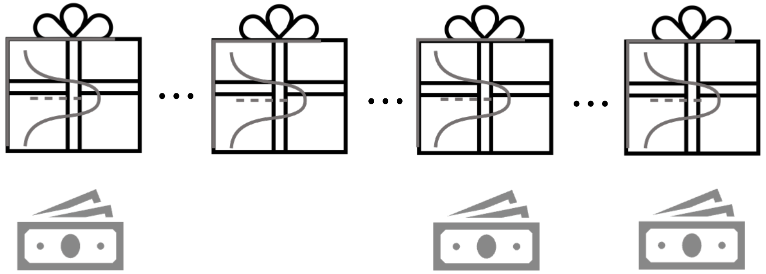
Fixed-iteration

Expected regret

$$\mathbb{E}\max_{x\in\mathcal{X}} f(x) - \mathbb{E}\max_{t=1,2,\ldots,T} f(x_t)$$

Pandora's Box

[Weitzman'79]



$f(x)$

$c(x)$

Discrete

Independent

Flexible-stopping

Expected utility

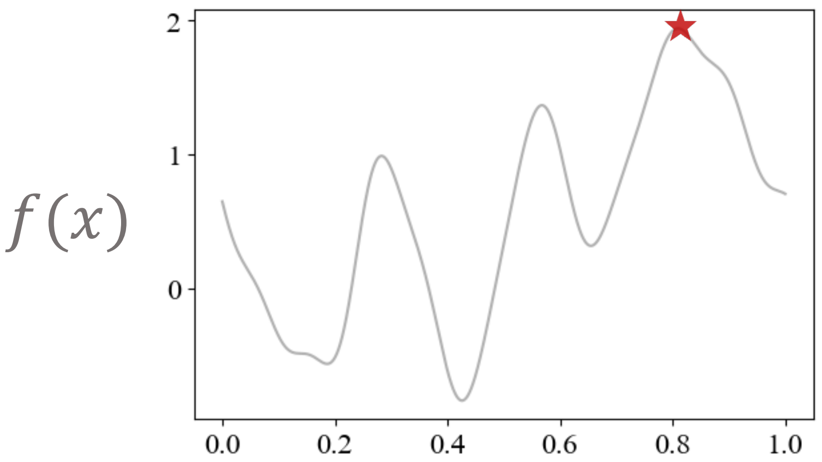
cumulative cost

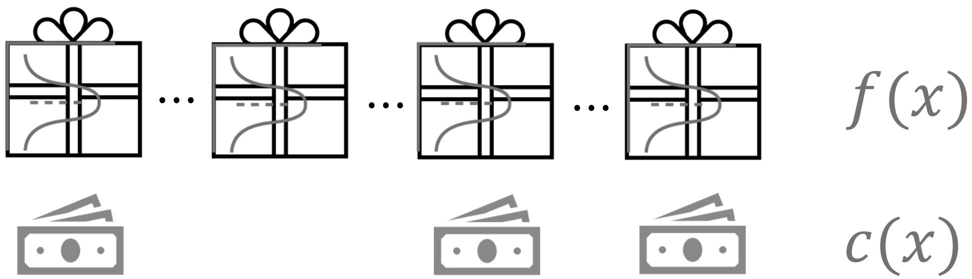
$$\mathbb{E}\max_{t=1,2,\ldots,T} f(x_t) - \mathbb{E}\sum_{t=1}^{T} c(x_t)$$

Bayesian Optimization

Pandora's Box

[Weitzman'79]





Continuous | Discrete

Correlated | Independent

Fixed-iteration | Flexible-stopping

Expected regret

$$\mathbb{E}\max_{x\in\mathcal{X}} f(x) - \mathbb{E}\max_{t=1,2,\ldots,T} f(x_t)$$

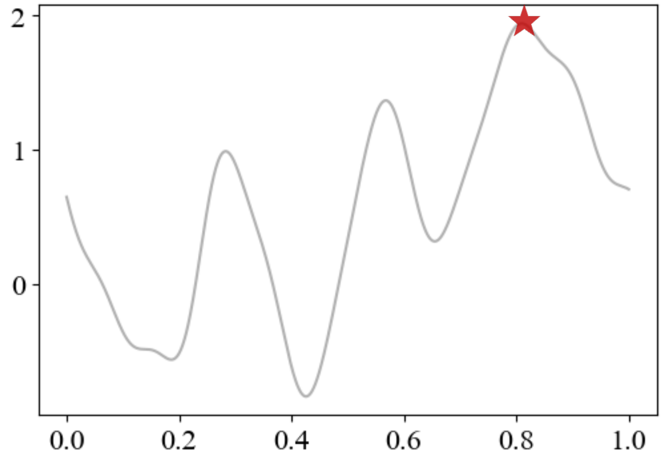
Expected cost-adjusted regret

$$\mathbb{E}\max_{x\in\mathcal{X}} f(x) - \mathbb{E}\max_{t=1,2,\ldots,T} f(x_t) + \mathbb{E}\sum_{t=1}^{T} c(x_t)$$

cumulative cost

Bayesian Optimization

$f(x)$



Continuous

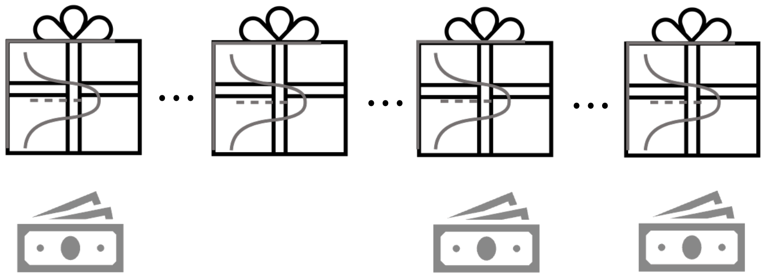
Correlated

Fixed-budget / Flexible-stopping

Expected (cost-adjusted) regret

Pandora's Box

[Weitzman'79]



$f(x)$

$c(x)$

Discrete

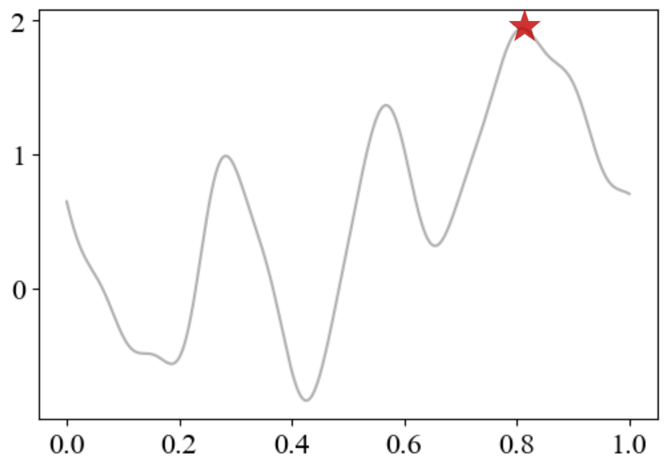
Independent

Flexible-stopping

Expected cost-adjusted regret

Bayesian Optimization

$f(x)$



Continuous

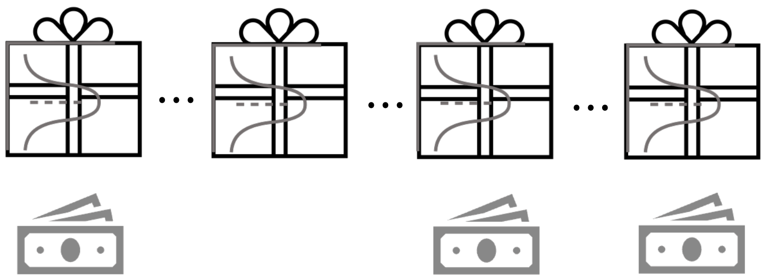
Correlated

Fixed-budget / Flexible-stopping

Expected (cost-adjusted) regret

Pandora's Box

[Weitzman'79]



$f(x)$

$c(x)$

Discrete

Independent

Flexible-stopping

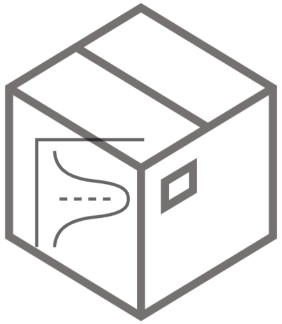
Expected cost-adjusted regret

Optimal policy: Gittins index

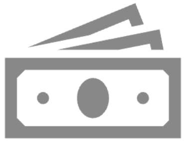
Optimal Policy: Gittins Index

Step 1: Assign each box a Gittins index (higher is better)

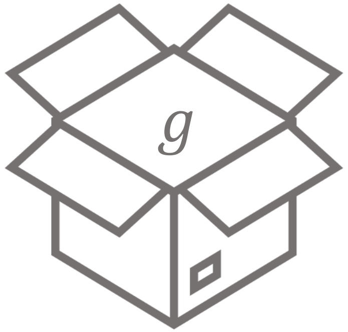
$f(x)$



$c(x)$



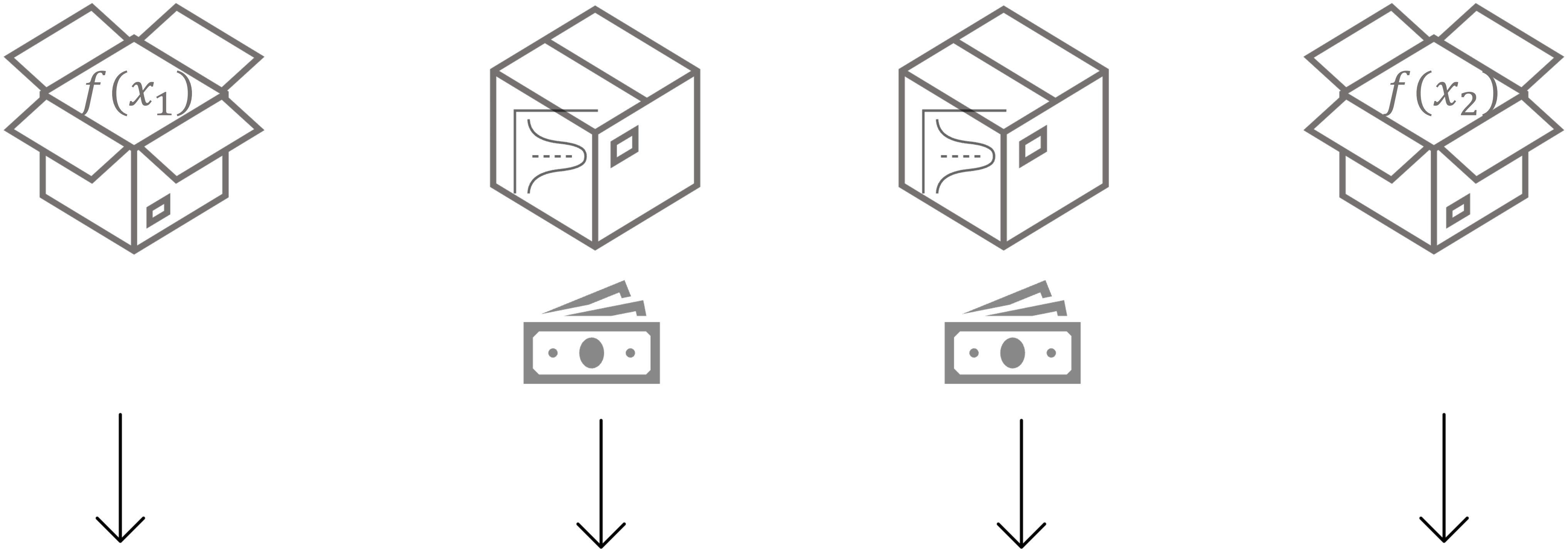
$\mathrm{GI}_f(x; c(x))$



g

Optimal Policy: Gittins Index

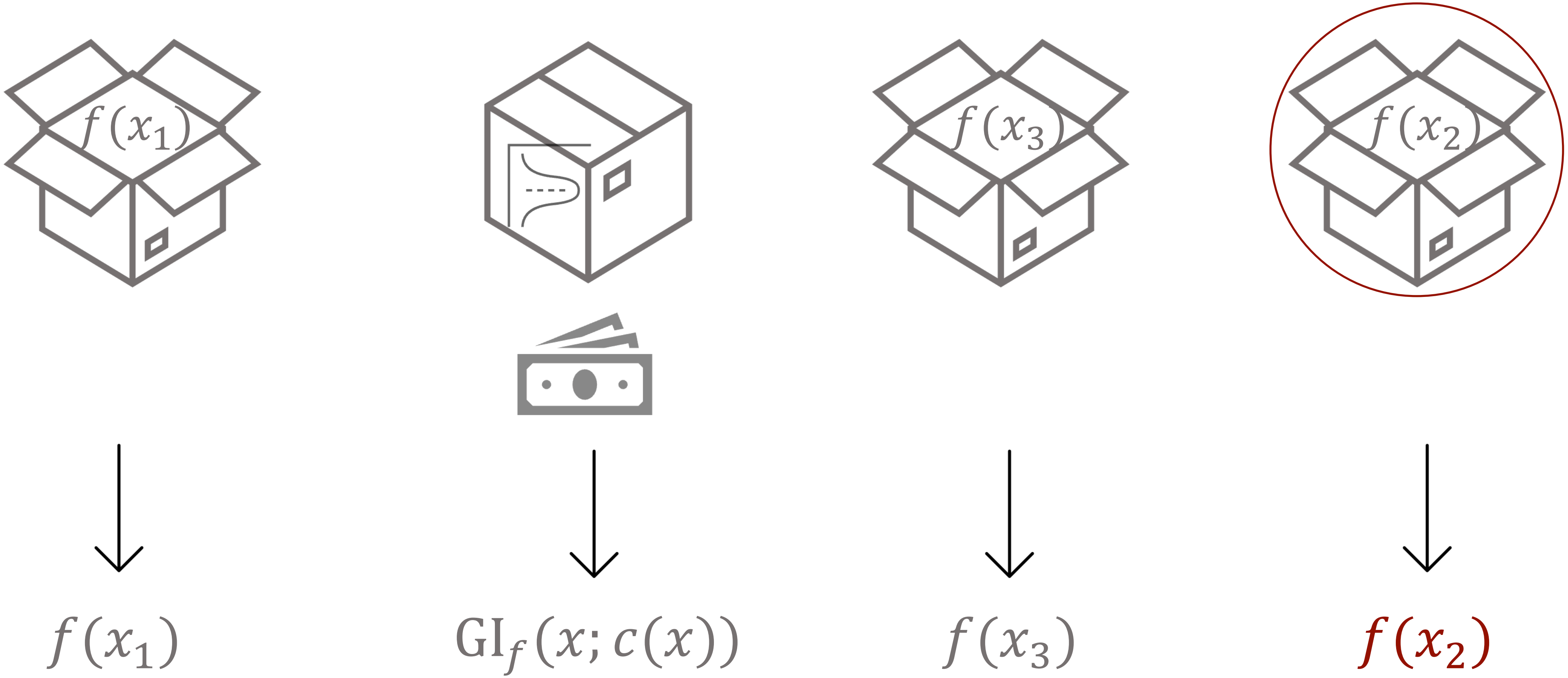
Step 2: Open the box with highest index if it is closed



$f(x_1)$ $\mathrm{GI}_f(x; c(x))$ $\mathrm{GI}_f(x'; c(x'))$ $f(x_2)$

Optimal Policy: Gittins Index

Step 2’: Select the box with highest index if it is opened and stop



Expected Improvement vs Gittins Index

Varying evaluation costs

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

Why not subtraction?

$\mathrm{GI}\big(x; c(x)\big)$

naturally incorporates costs

Smart stopping time

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

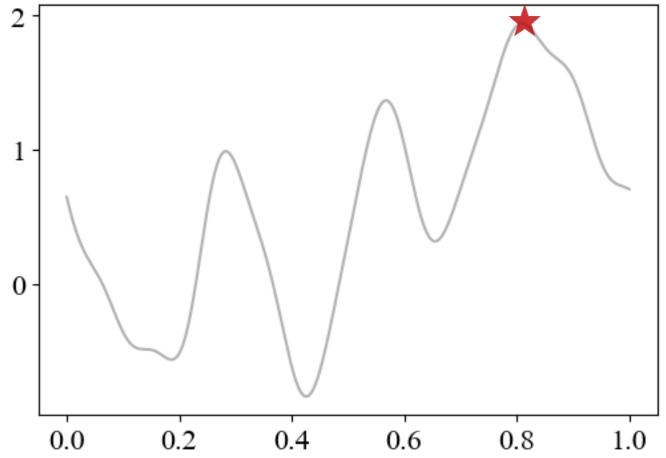
Which threshold?

$$\max_x \mathrm{GI}\big(x; c(x)\big) \leq y_{\text{best}}$$

$$\Longleftrightarrow \max_x \mathrm{EI}(x)/c(x) \leq 1$$

derived shared stopping rule

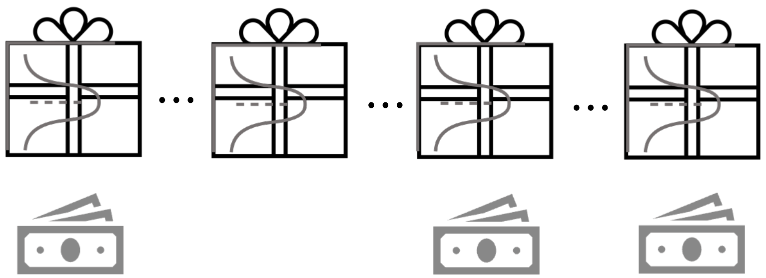
Bayesian Optimization



$f(x)$

Pandora's Box

[Weitzman'79]

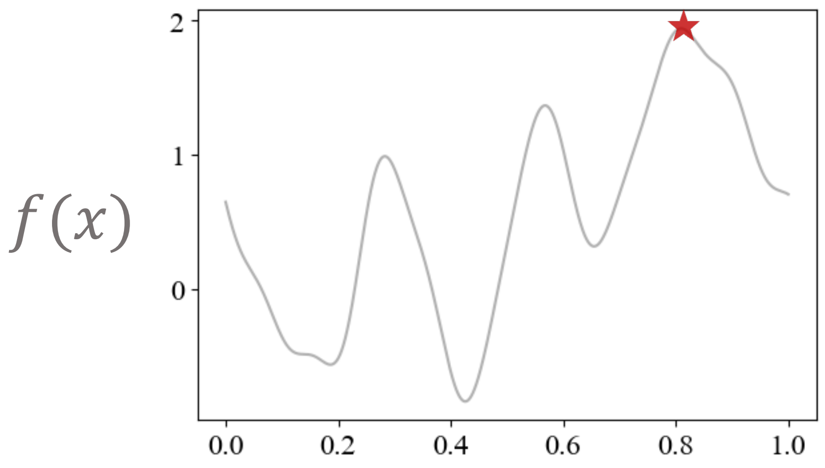


$f(x)$

$c(x)$

Bayesian Optimization	Pandora's Box
Continuous	Discrete
Correlated	Independent
Fixed-budget / Flexible-stopping	Flexible-stopping
Expected (cost-adjusted) regret	Expected cost-adjusted regret
Is Gittins index good?	Gittins index is optimal

Bayesian Optimization



Continuous

Correlated

Fixed-budget / Flexible-stopping

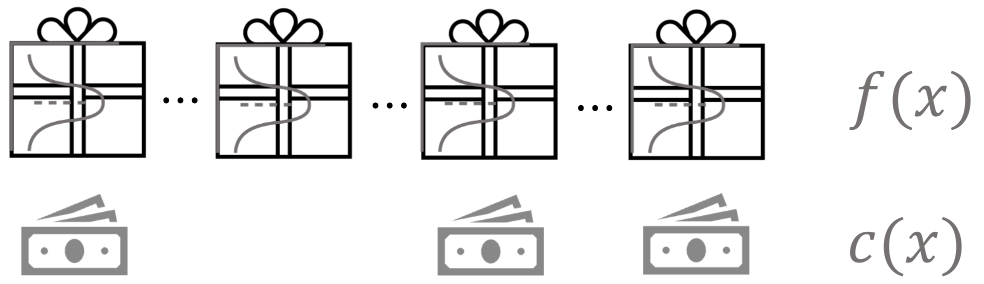
Expected (cost-adjusted) regret

Is Gittins index good?

empirically

Pandora's Box

[Weitzman'79]



Discrete

Independent

Flexible-stopping

Expected cost-adjusted regret

Gittins index is optimal

Our Contribution: Gittins Index Principle

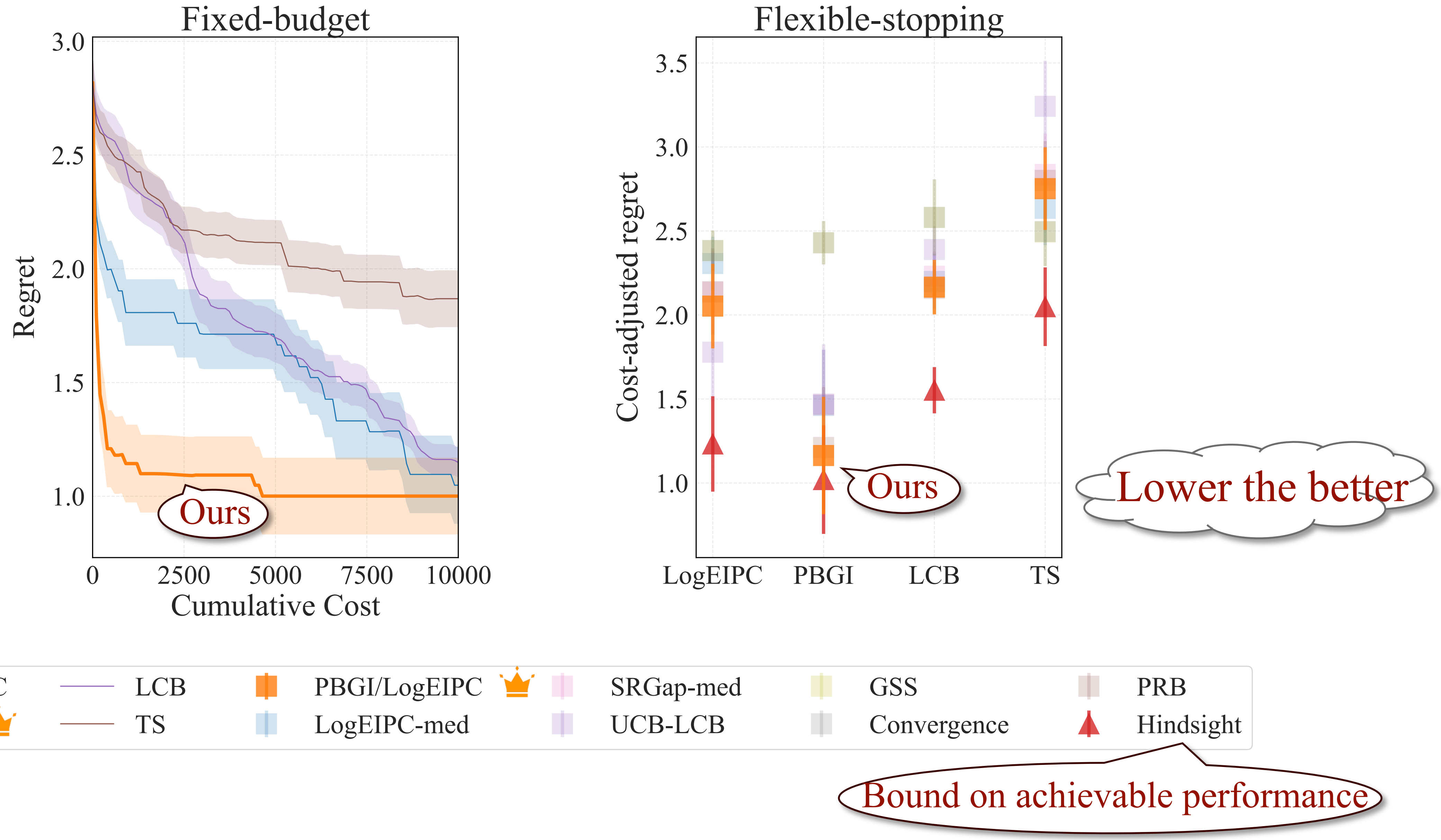
1. Principled design via problem simplification

2. Natural incorporation of side info and flexibility

3. Competitive performance on benchmarks

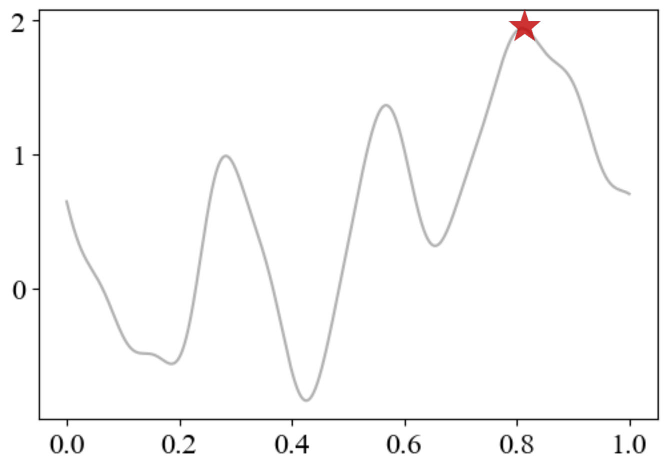
4. Theoretical guarantees

Gittins Index vs Baselines on AutoML Benchmark



Bayesian Optimization

$f(x)$



Continuous

Correlated

Fixed-budget / Flexible-stopping

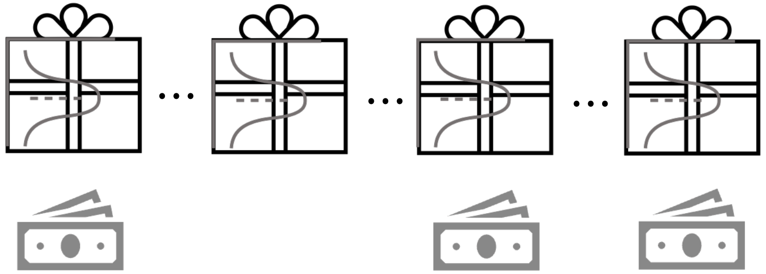
Expected (cost-adjusted) regret

Is Gittins index good?

theoretically

Pandora's Box

[Weitzman'79]



$f(x)$

$c(x)$

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Expected cost-adjusted regret

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Our Contribution: Gittins Index Principle

Joint work with Ziv Scully and Alexander Terenin et al.

1. Principled design via problem simplification

2. Natural incorporation of side info and flexibility

3. Competitive performance on benchmarks

4. Theoretical guarantees

Theoretical Guarantee and Empirical Validation

Theorem (Safeguard Guarantee)

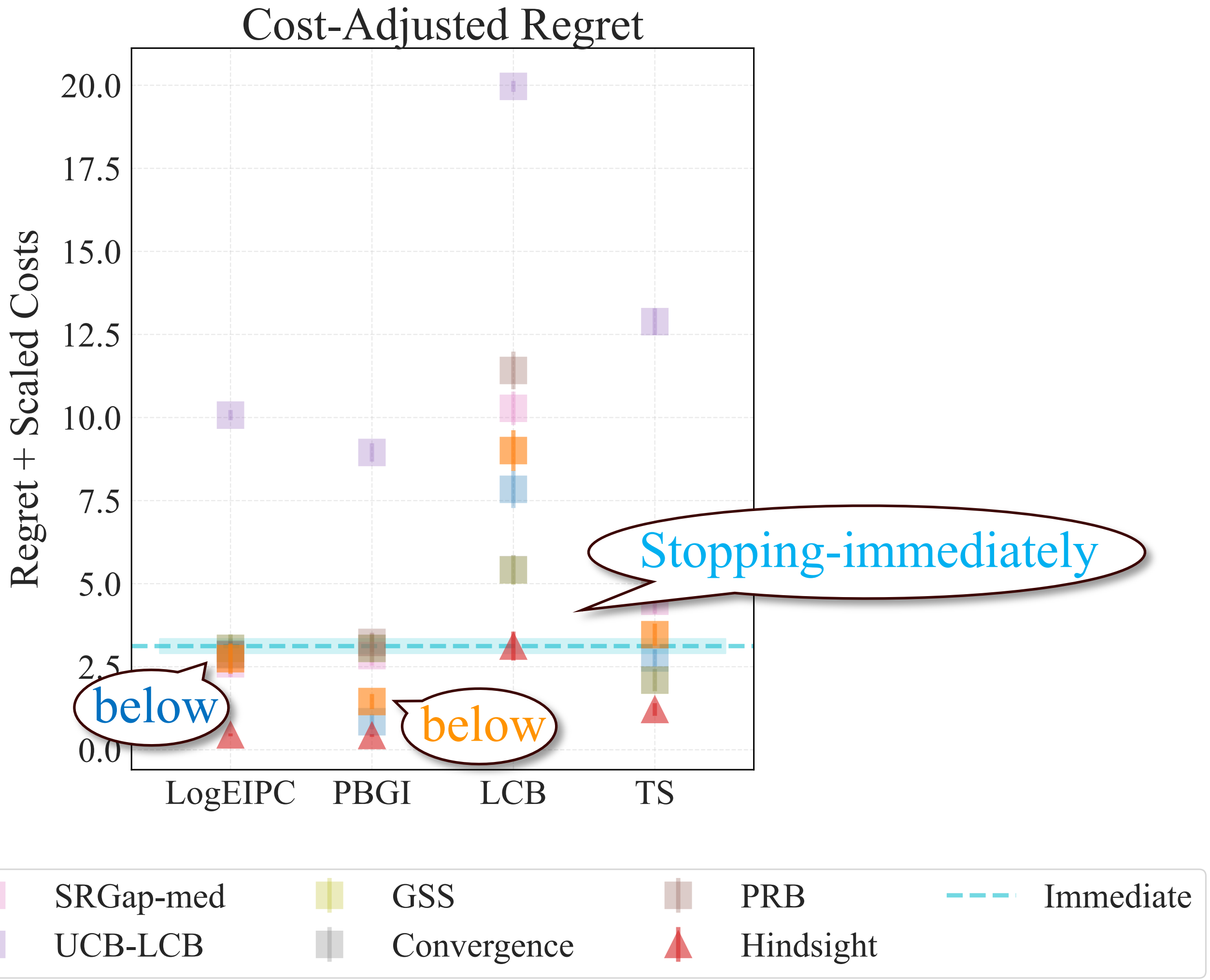
$\mathbb{E}[R(\text{ours; PBGI})] \leq R[\text{stopping immediately}]$

or LogEIPC　　cost-adjusted regret

Implication:

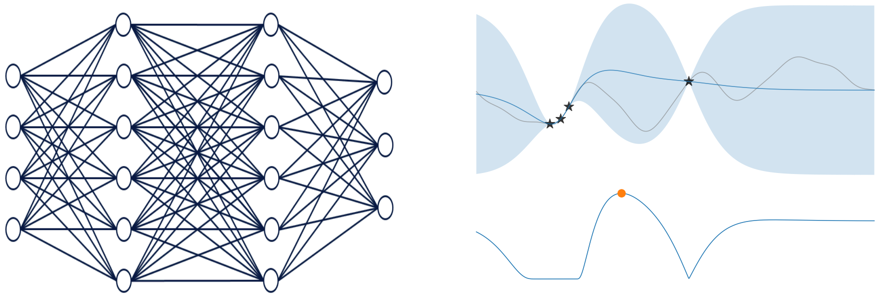
- Matches the best achievable performance in the worst case (evaluations are all very costly).

- Avoids over-spending — a property many cost-unaware stopping rules lack.



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

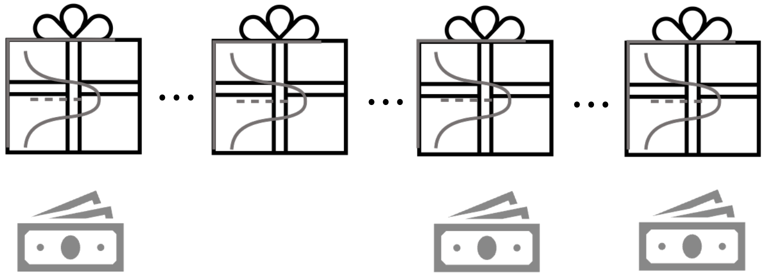
Studied problem



Varying evaluation costs

Adaptive stopping time

Key idea



Link to Pandora's Box problem
& Gittins index theory

Impact

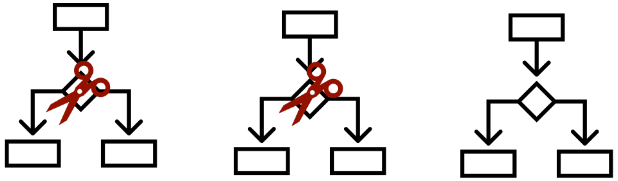
Meta

BoTorch Ax

Competitive empirical performance &
interests from practitioners

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

Ongoing work



Sharper theoretical guarantees & black-box optimization w/ multi-stage feedback

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

Find our papers on arXiv!

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

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