NeurIPS'24 & INFORMS Data Mining Paper Competition Finalist

Cost-Aware Bayesian Optimization with Adaptive Stopping via Gittins Indices

Qian Xie 谢倩 (Cornell ORIE)

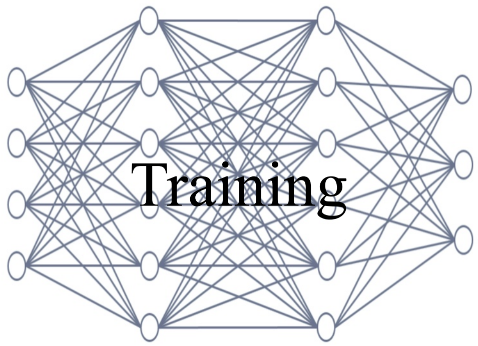
Joint work with Linda Cai (UC Berkeley), Theodore Brown (UCL), Raul Astudillo (MBZUAI), Peter Frazier, Alexander Terenin, and Ziv Scully (Cornell)

INFORMS Annual Meeting 2025 Job Market Showcase

Motivation: World of Optimization under Uncertainty

ML model training:

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



$\longrightarrow$ Accuracy

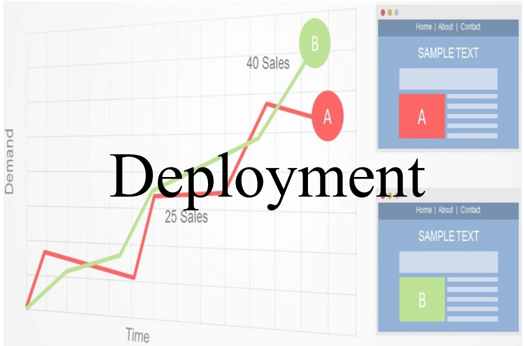
Motivation: World of Optimization under Uncertainty

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:

non-analytical & no gradient info

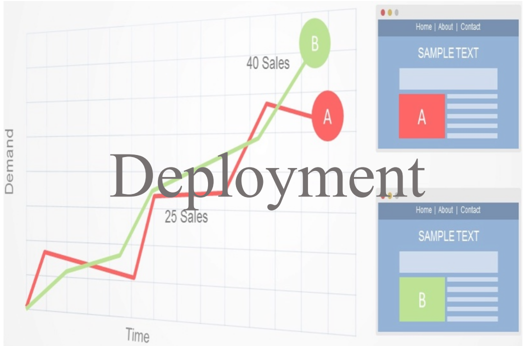
Input x →  → Performance metric $f(x)$

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

Observed outcome $f(x)$

ML model training:

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

Accuracy

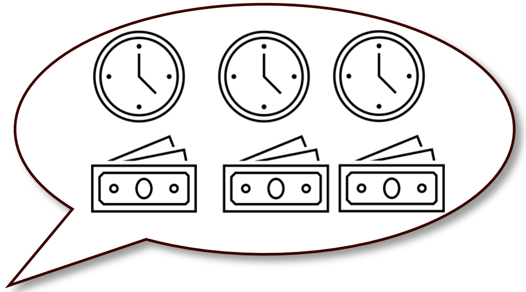
Black-Box Optimization

Black-box optimization:

(gradient-based method not applicable)

Input x ⟶  ⟶ Observed outcome $f(x)$

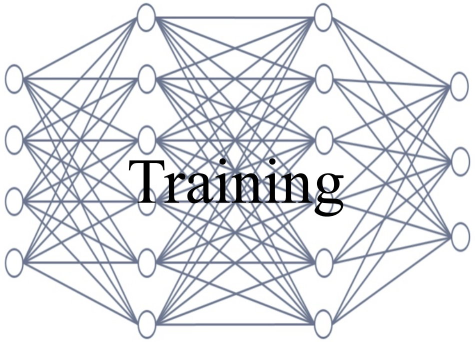
expensive-to-evaluate



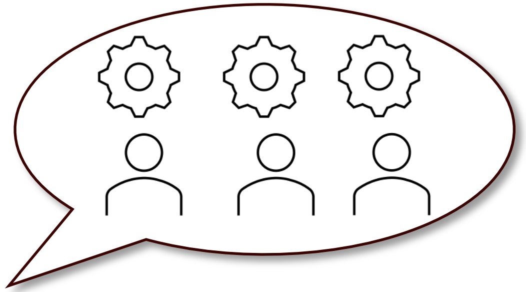
Training time

Compute credits

ML model training:

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

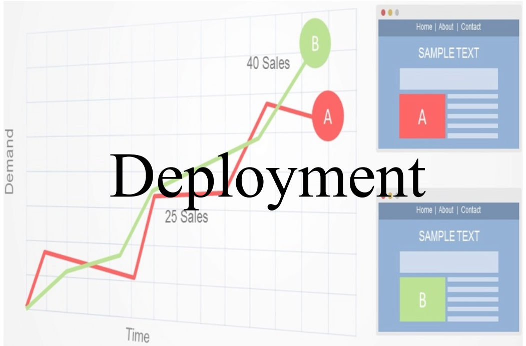
⟶ Accuracy



Operational cost

User experience

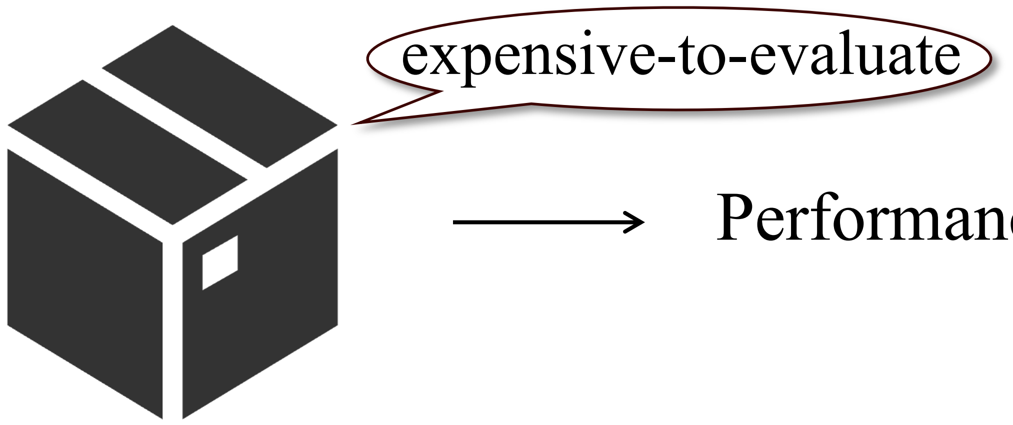
Adaptive experimentation:

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

⟶ Revenue

Black-Box Optimization

Input x $\longrightarrow$



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

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

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

Data-Driven Black-Box Optimization

Input x $\longrightarrow$

expensive-to-evaluate

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

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

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

expensive-to-evaluate

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

$f \sim$Stochastic Process

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

Black-box function

Bayesian Optimization

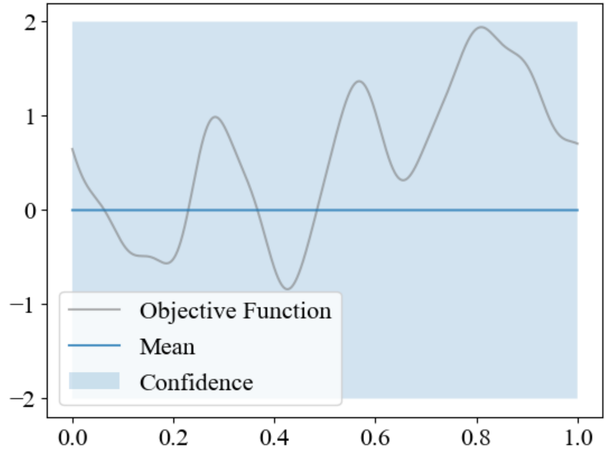
Time 0

$f \sim$ Stochastic Process

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

Black-box function

Model belief



Probabilistic model

(e.g., Gaussian process)

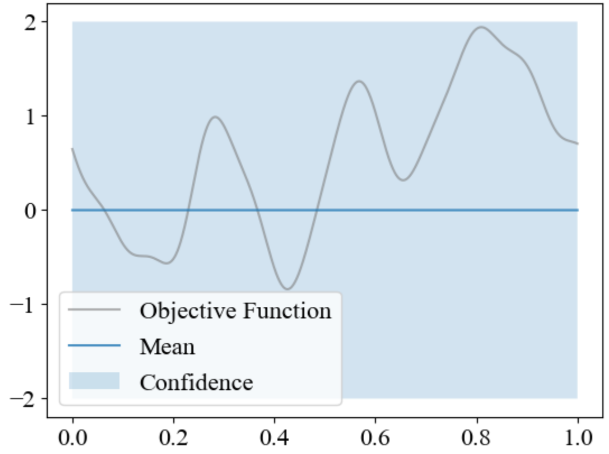
Bayesian Optimization

Time t

$x_1, \ldots, x_t \longrightarrow$ Black-box function $\longrightarrow f(x_1), \ldots, f(x_t)$

$f \sim$Stochastic Process

Model belief



Probabilistic model
(e.g., Gaussian process)

Bayesian Optimization

Time t

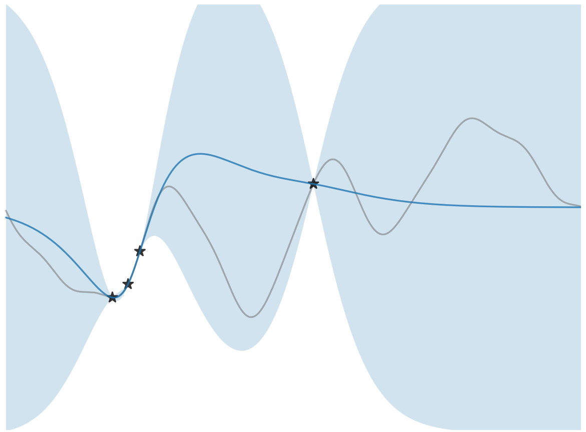
$x_1, \dots, x_t \longrightarrow$

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

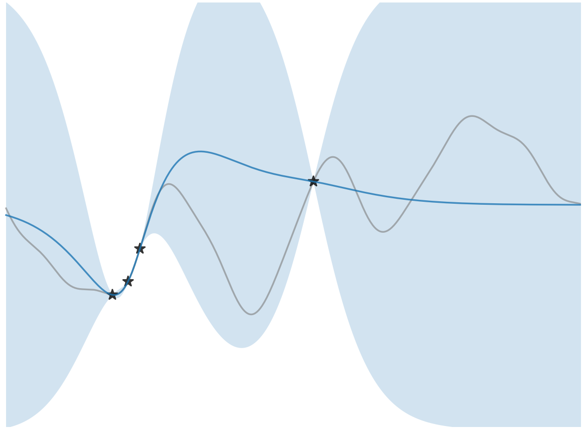
Time t

$x_1, \dots, x_t \longrightarrow$

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

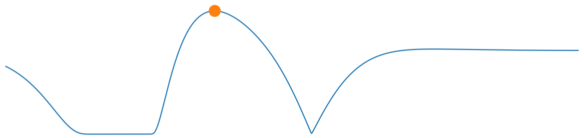
Black-box function

Update belief
(Bayes' rule)



Probabilistic model
(e.g., Gaussian process)

scoring (worth of each point



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

Bayesian Optimization

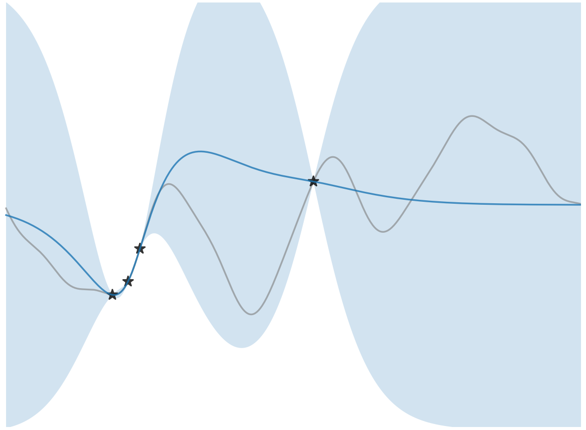
Time t

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

Black-box function

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

Update belief
(Bayes' rule)



Probabilistic model
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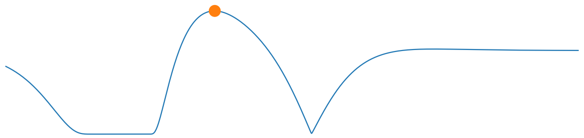


Decision rule
(e.g., EI, UCB, TS)

Decide next input
(gradient-based optimization)

Bayesian Optimization

Time $t + 1$

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

Black-box function

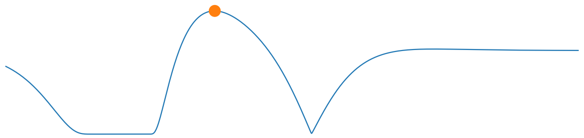
$\longrightarrow f(x_1), \dots, f(x_{t+1})$

Decide next input

(gradient-based optimization)

Update belief

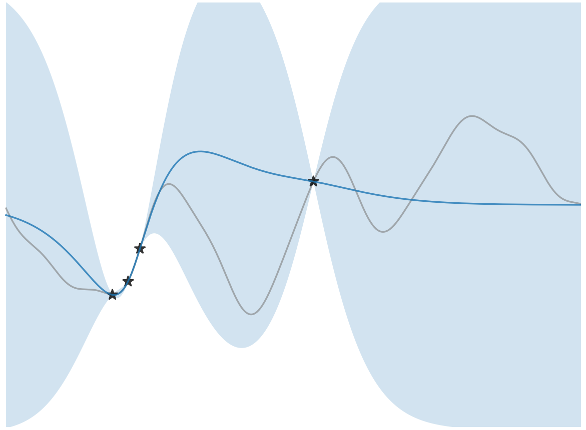
(Bayes' rule)



Decision rule

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

scoring (worth of each point



Probabilistic model

(e.g., Gaussian process)

Bayesian Optimization

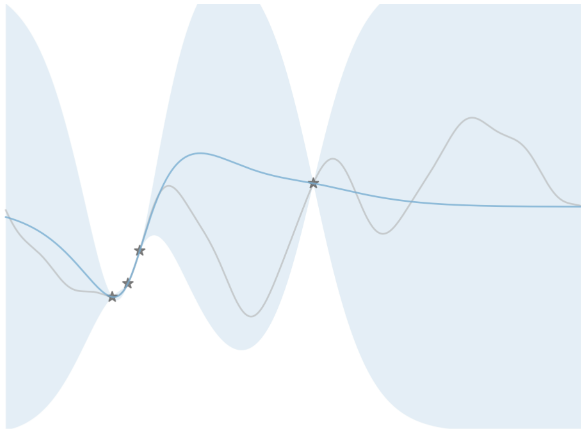
Time $t + 1$

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

Black-box function

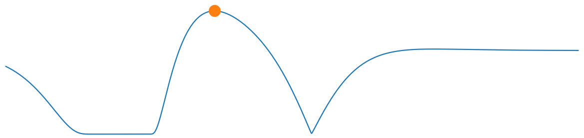
$f(x_1), \ldots, f(x_{t+1})$

Update belief
(Bayes' rule)



Probabilistic model
(e.g., Gaussian process)

scoring (worth of each point

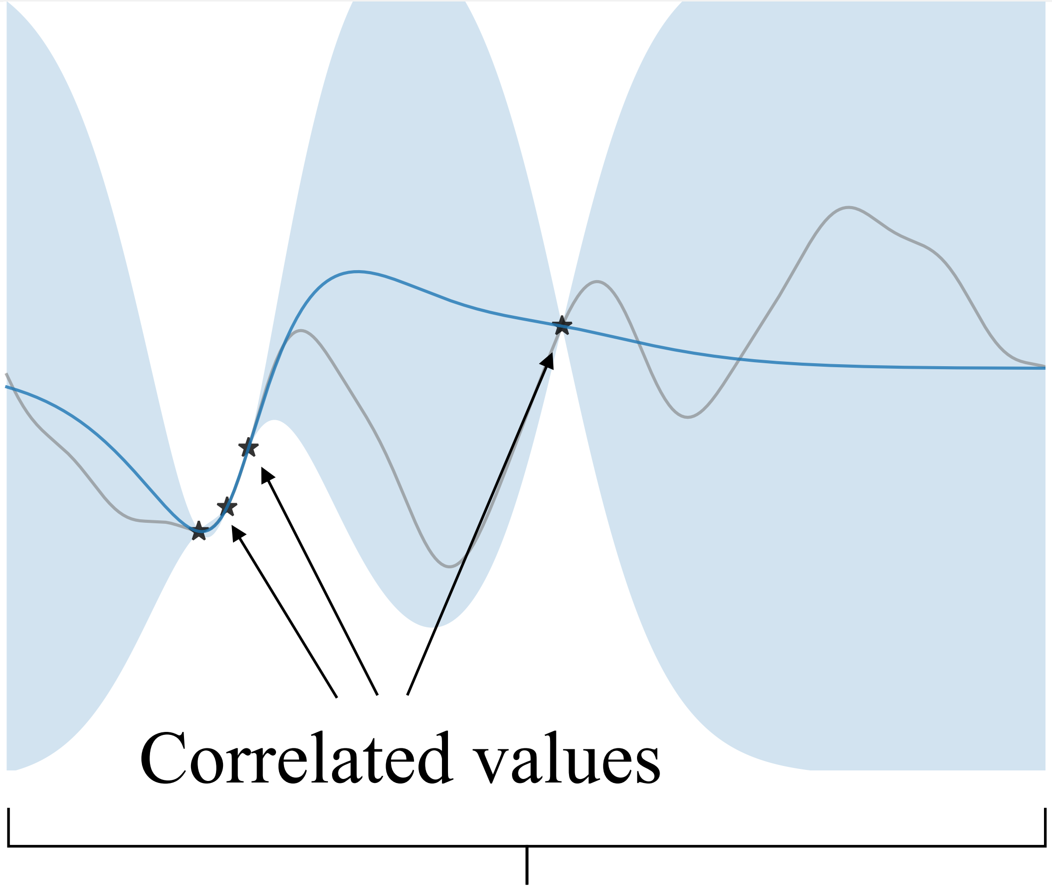


Decision rule
(e.g., EI, UCB, TS)

My focus

Decide next input
(gradient-based optimization)

Challenge in Decision Rule Design



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

Popular Decision Rule: Expected Improvement

current best observed

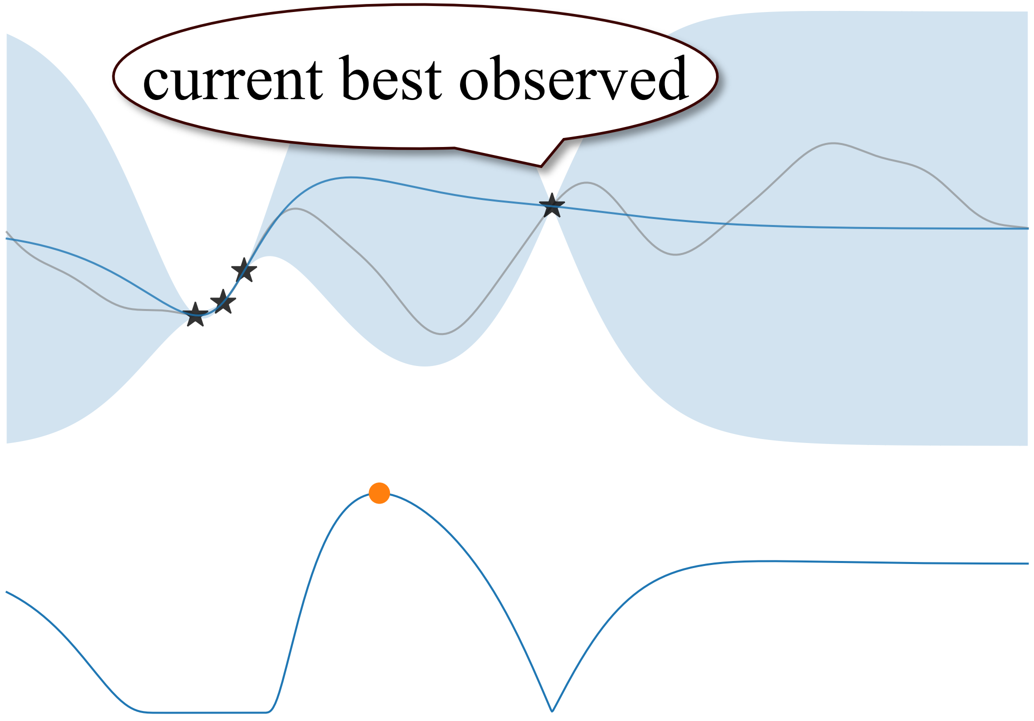
data

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

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

posterior distribution

One-step approximation to MDP



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

Popular Decision Rule: Expected Improvement

current best observed

data

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

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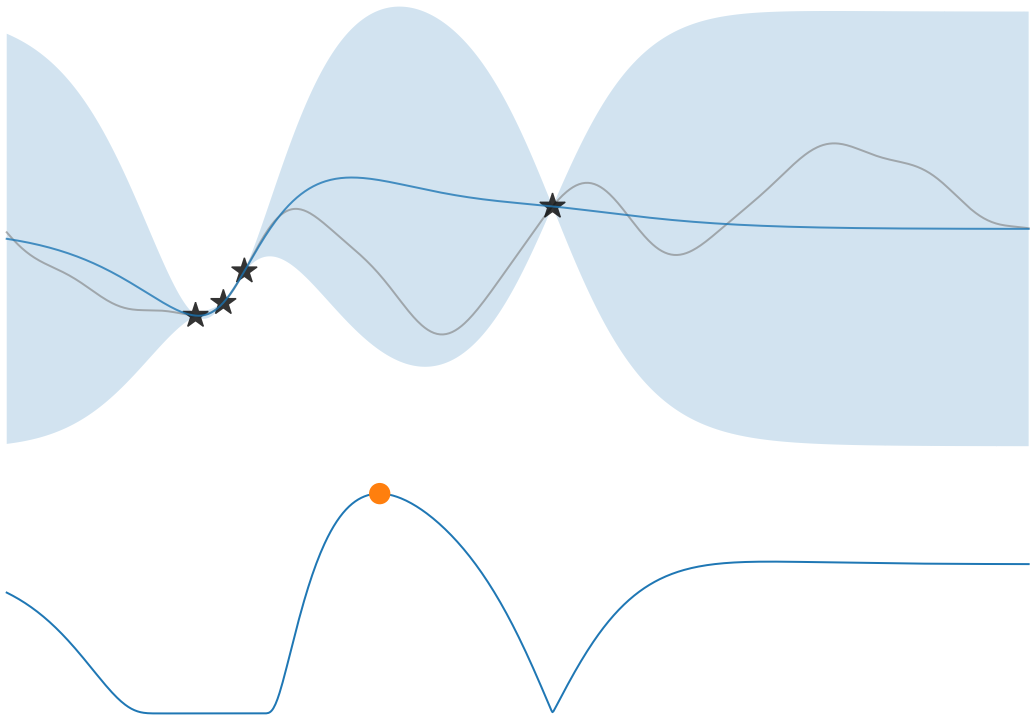
One-step approximation to MDP

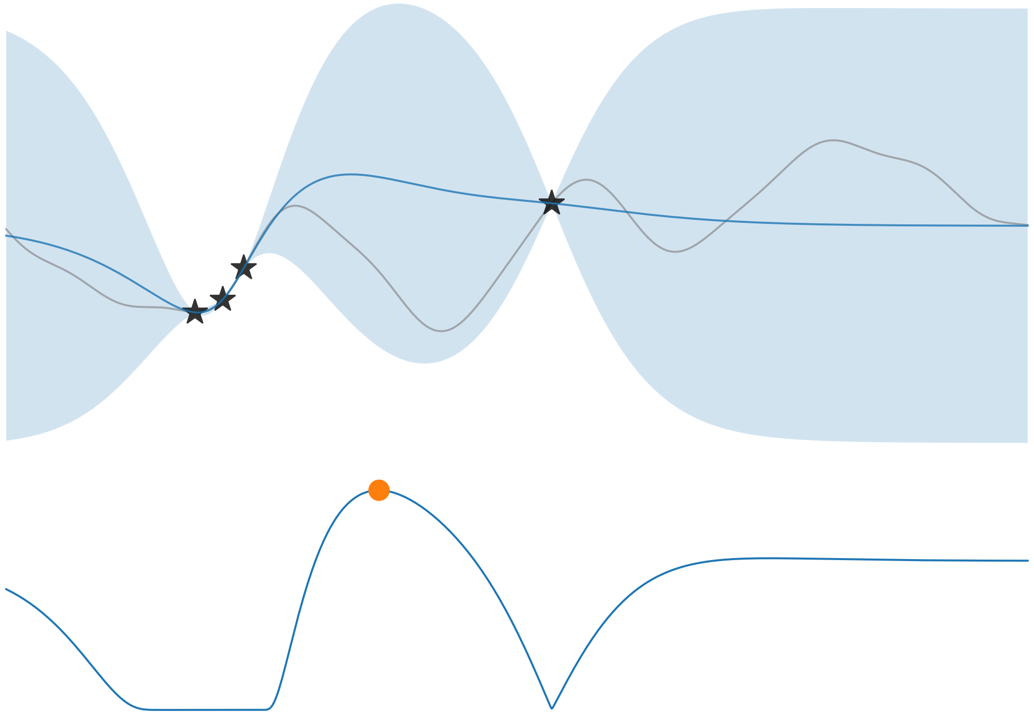


Expected improvement $\mathrm{EI}(x)$

Improvement-based design principle

Existing Design Principles

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

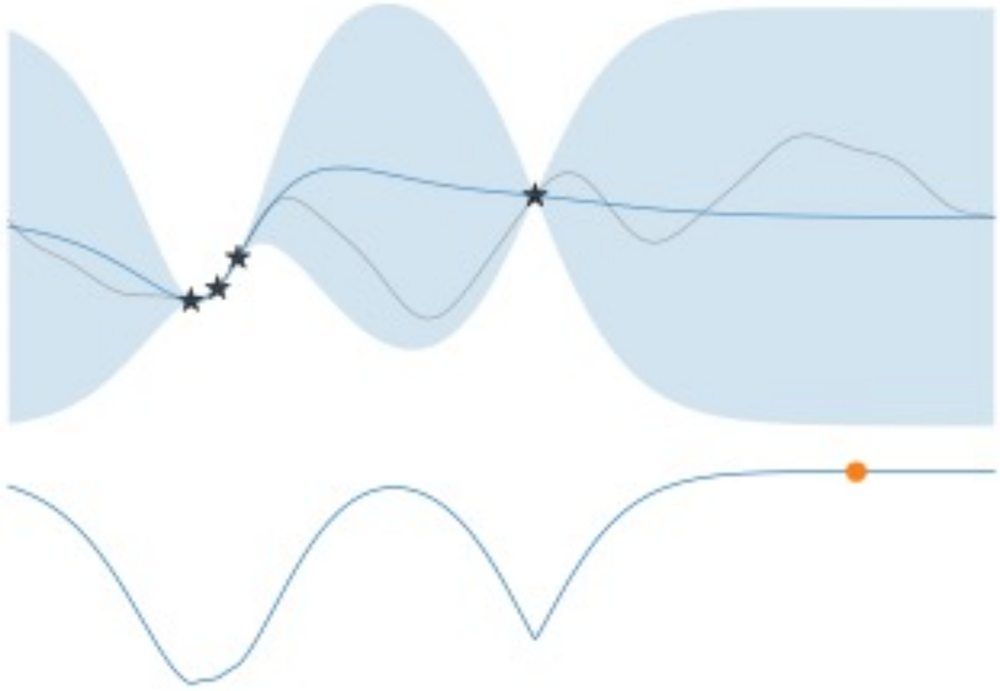


Expected improvement $\mathrm{EI}(x)$

Improvement-based design principle

New Design Principle: Gittins Index

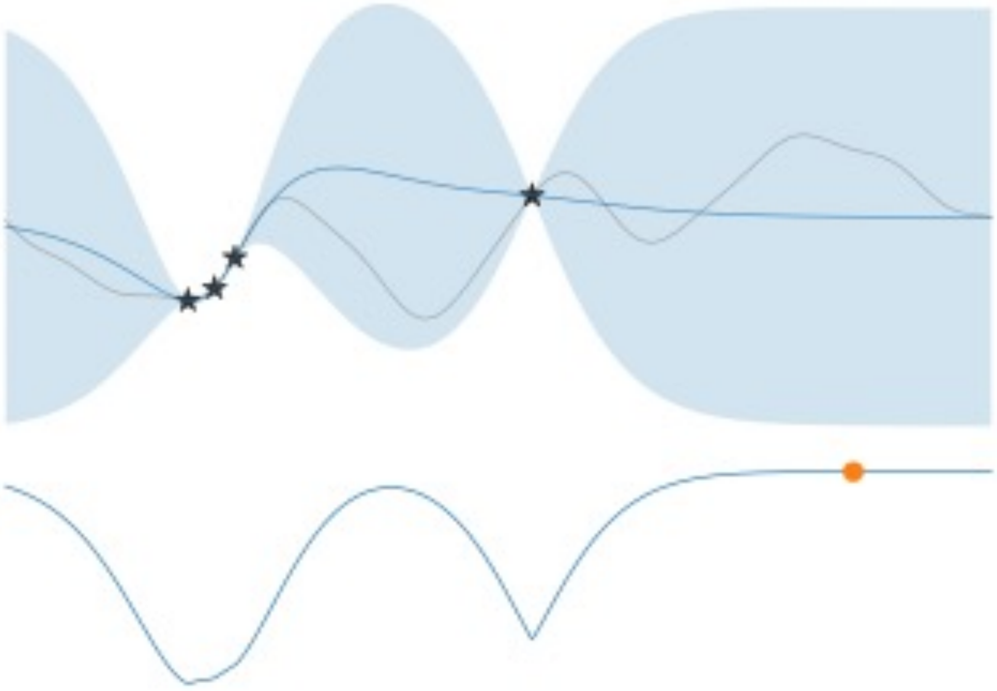
- Improvement-based (e.g., EI)
- Entropy-based
- Confidence bounds (UCB/LCB)
- Thompson sampling (TS)
- Gittins Index



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 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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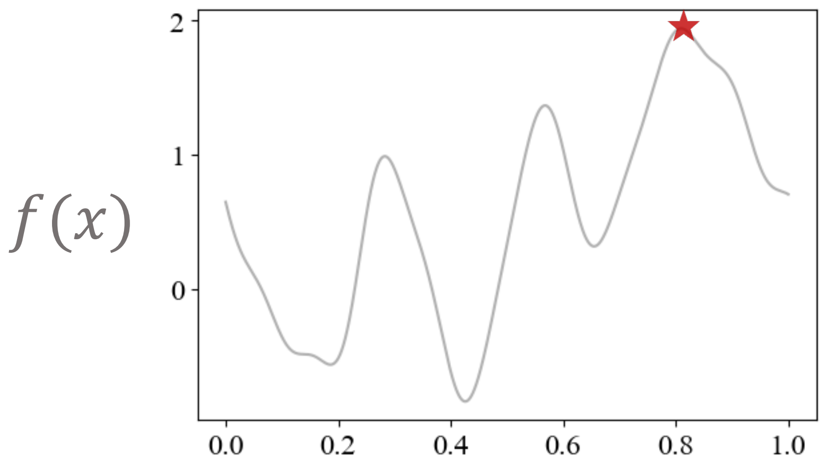
4. Theoretical guarantees

Bayesian Optimization

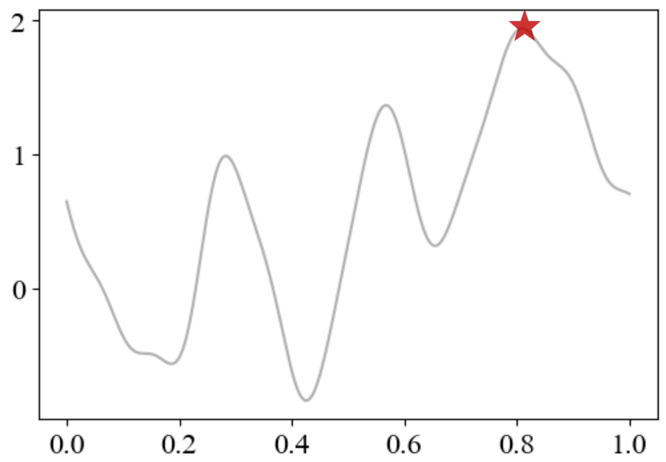


Continuous

Correlated

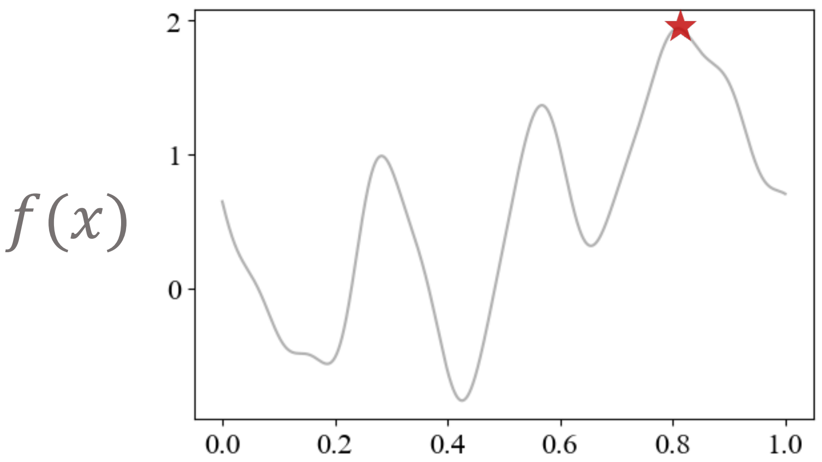
Bayesian Optimization

$f(x)$



Continuous	$\Longrightarrow$	Discrete
Correlated	$\Longrightarrow$	Independent

Bayesian Optimization

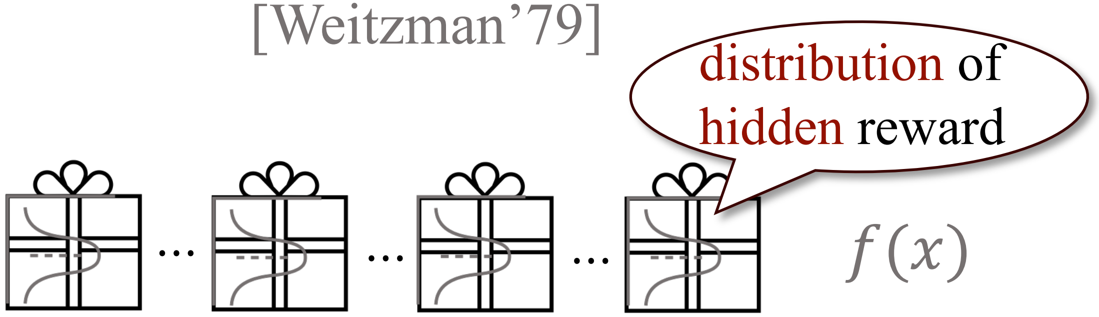


Continuous

Correlated

Pandora's Box

[Weitzman'79]



Discrete

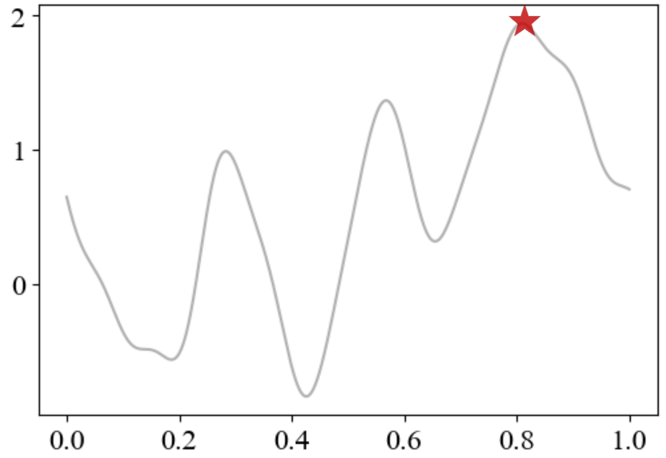
Independent

Bayesian Optimization

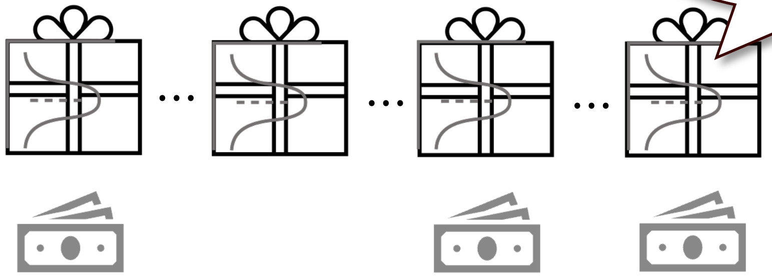
Pandora's Box

[Weitzman'79]

$f(x)$



distribution of hidden reward



$f(x)$

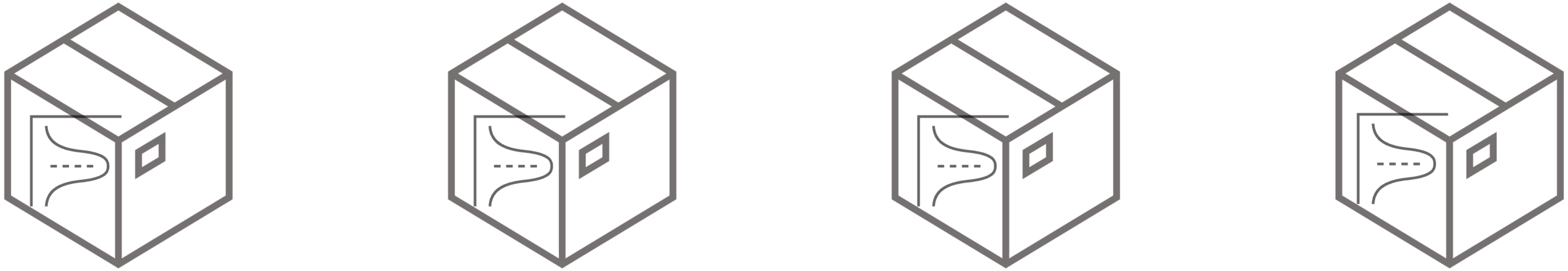
$c(x)$

costs to open

Continuous	Discrete
Correlated	Independent

Pandora’s Box

$t = 0$

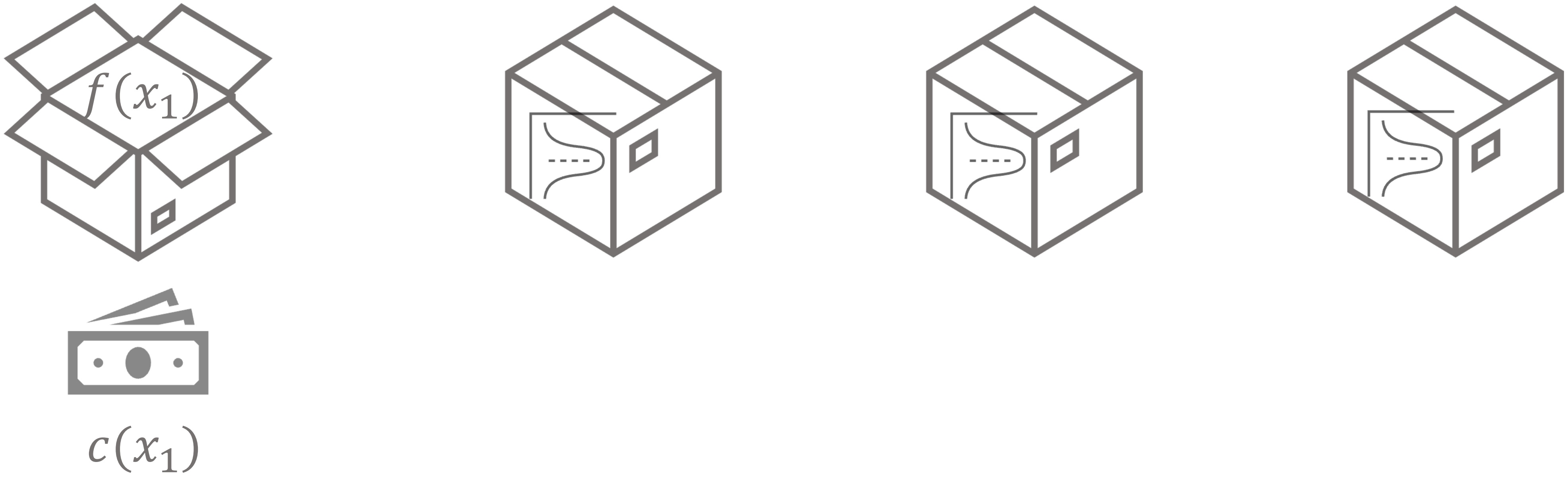


High-level goal: Choose box $x_1, \dots, x_T$ to open to maximize the expected utility

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

Pandora's Box

$t = 1$

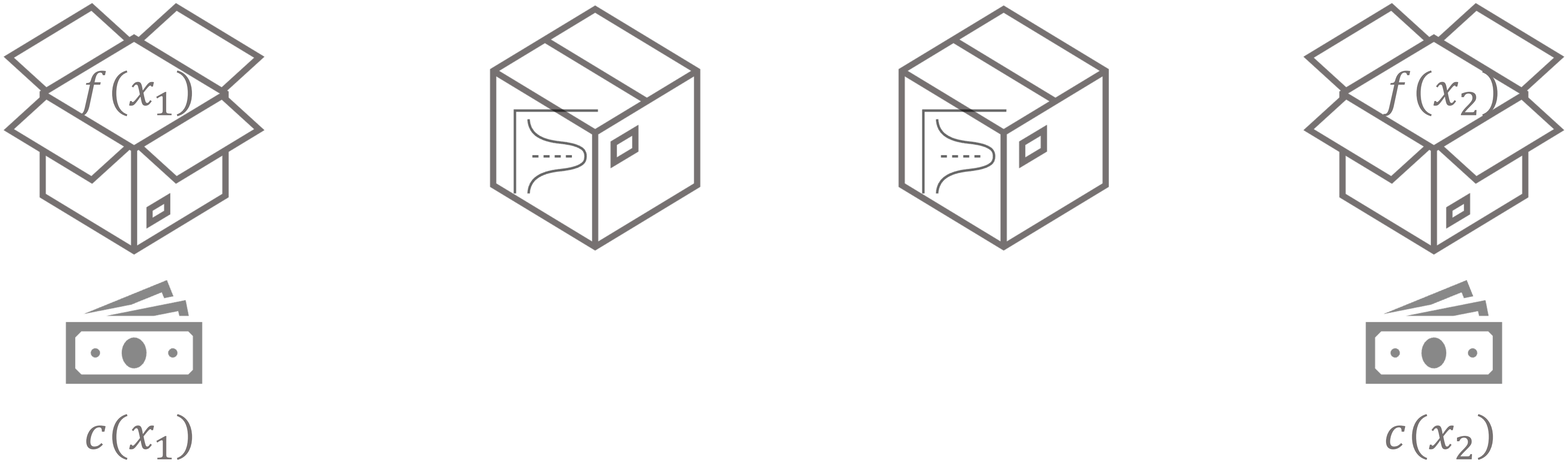


High-level goal: Choose box $x_1, \ldots, x_T$ to open to maximize the expected utility

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

Pandora's Box

$t = 2$

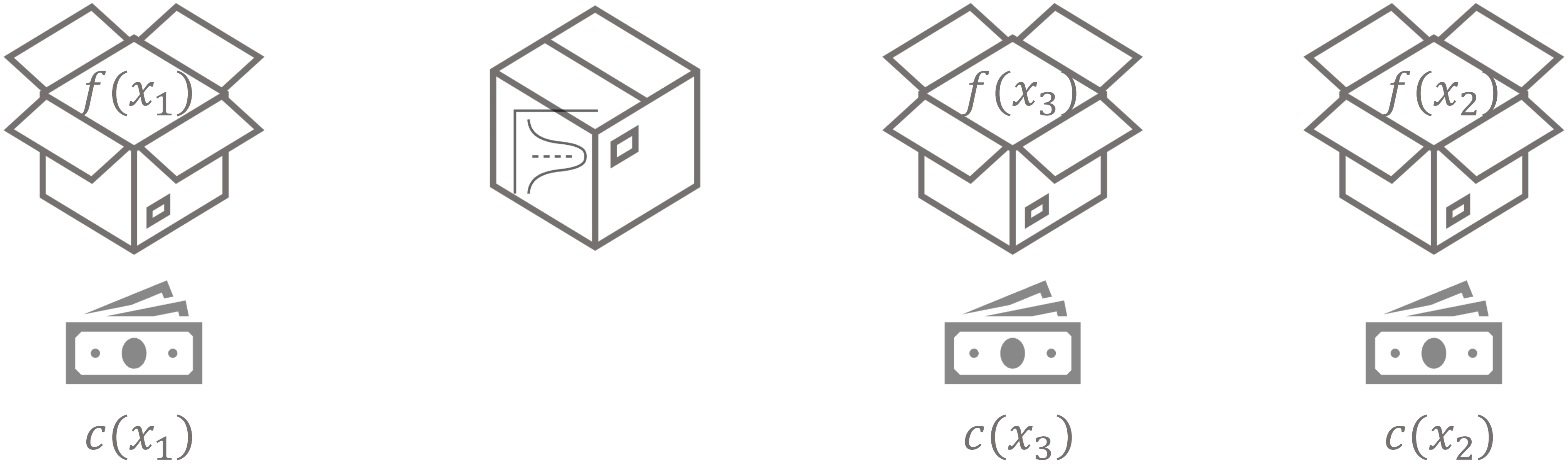


High-level goal: Choose box $x_1, \ldots, x_T$ to open to maximize the expected utility

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

Pandora's Box

$t = 3$

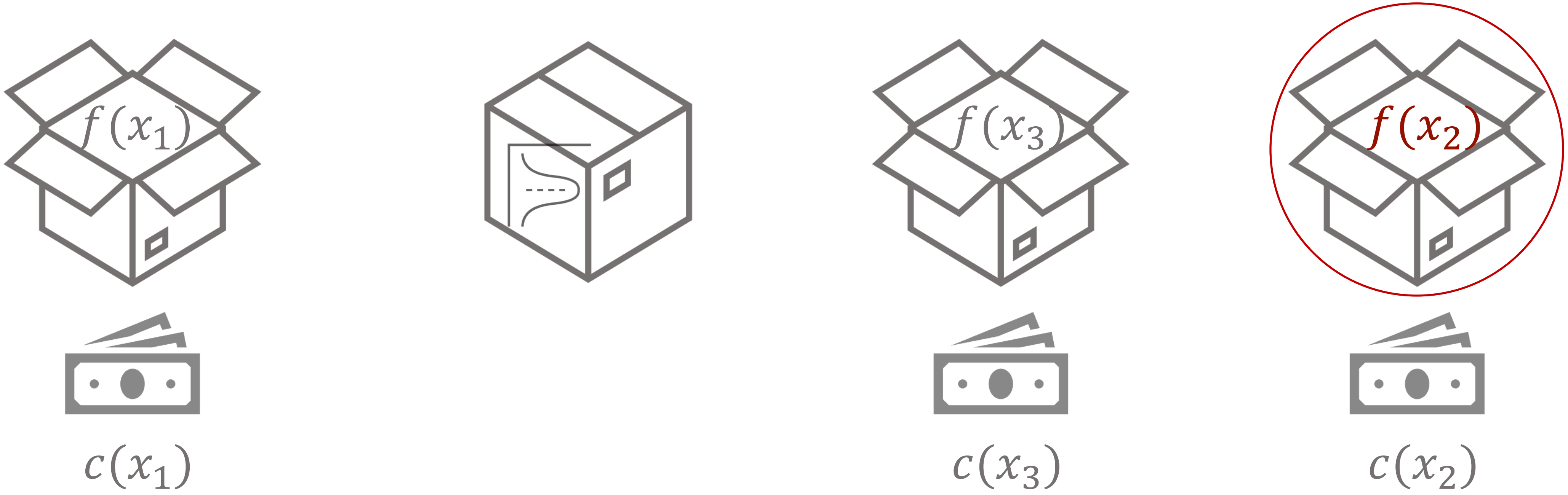


High-level goal: Choose box $x_1, \ldots, x_T$ to open to maximize the expected utility

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

Pandora's Box

$t = T$, stop

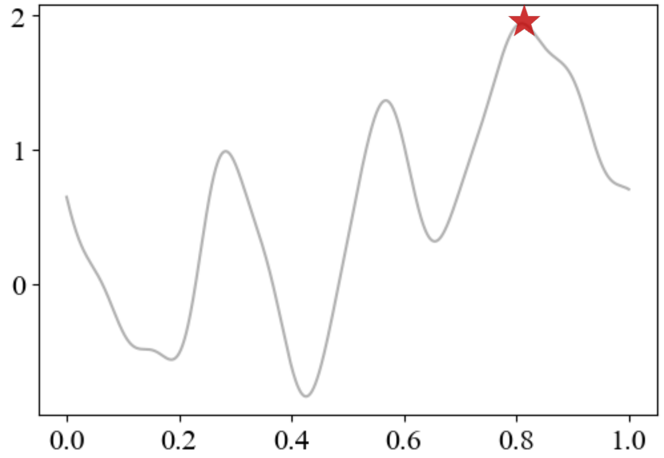


High-level goal: Choose box $x_1, \ldots, x_T$ to open to maximize the expected utility

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

Bayesian Optimization

$f(x)$

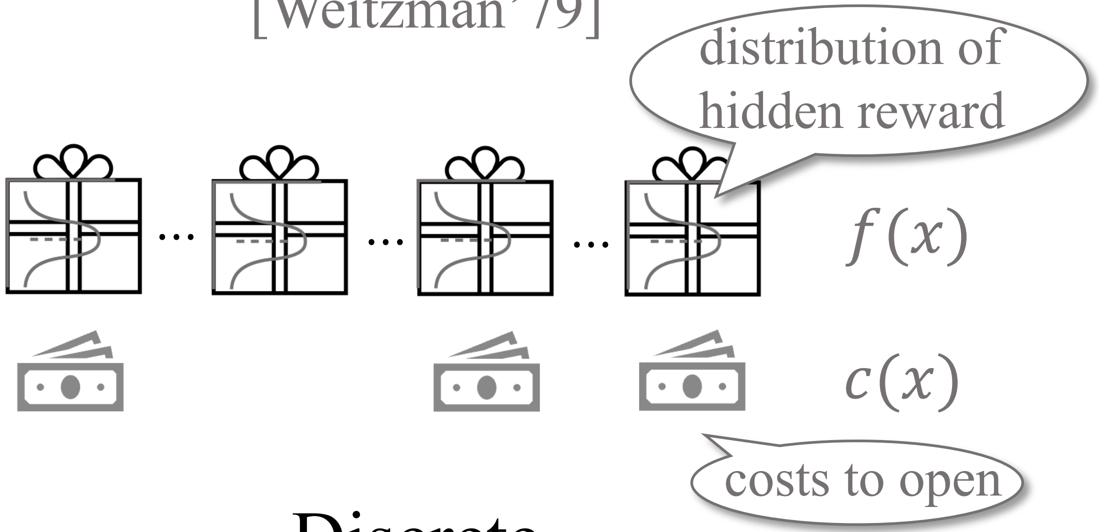


Continuous

Correlated

Pandora's Box

[Weitzman'79]



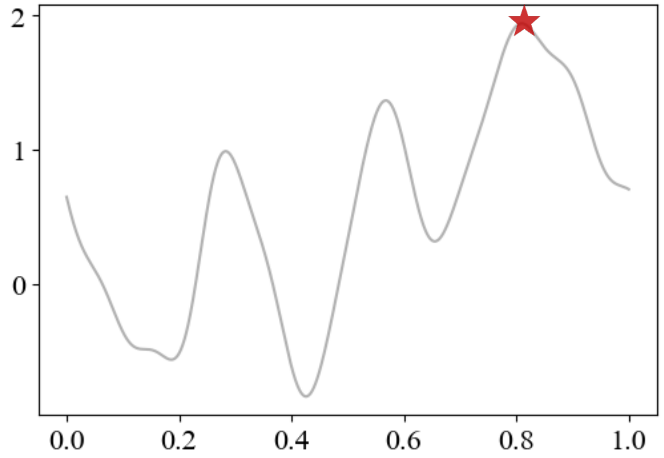
Discrete

Independent

Optimal policy: Gittins index

Bayesian Optimization

$f(x)$

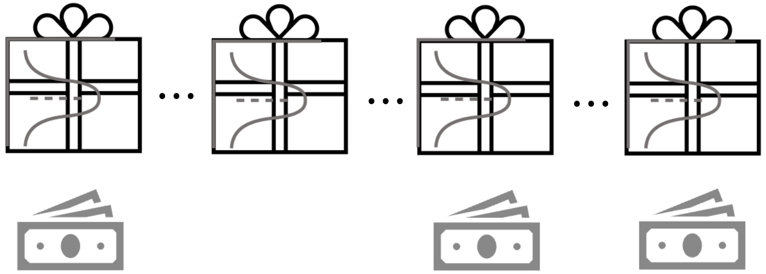


Continuous

Correlated

Pandora's Box

[Weitzman'79]



$f(x)$

$c(x)$

Discrete

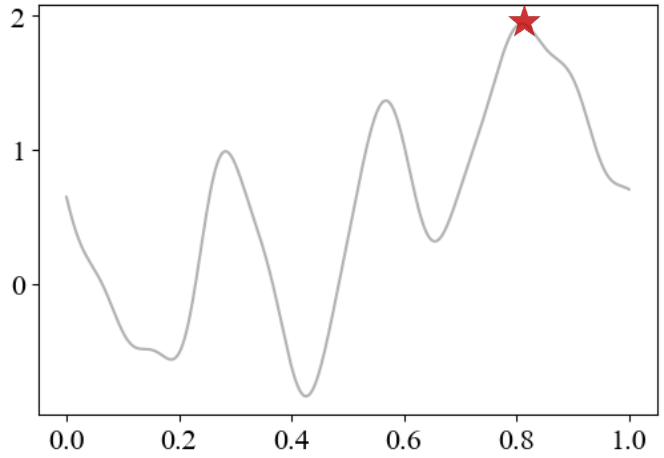
Independent

How to translate?

$\Longleftarrow$ Optimal policy: Gittins index

Bayesian Optimization

$f(x)$



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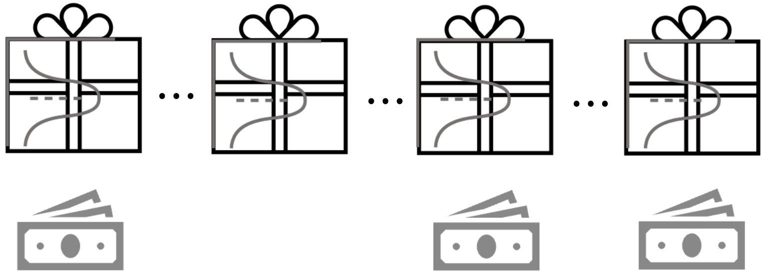


$f(x)$

$c(x)$

Discrete

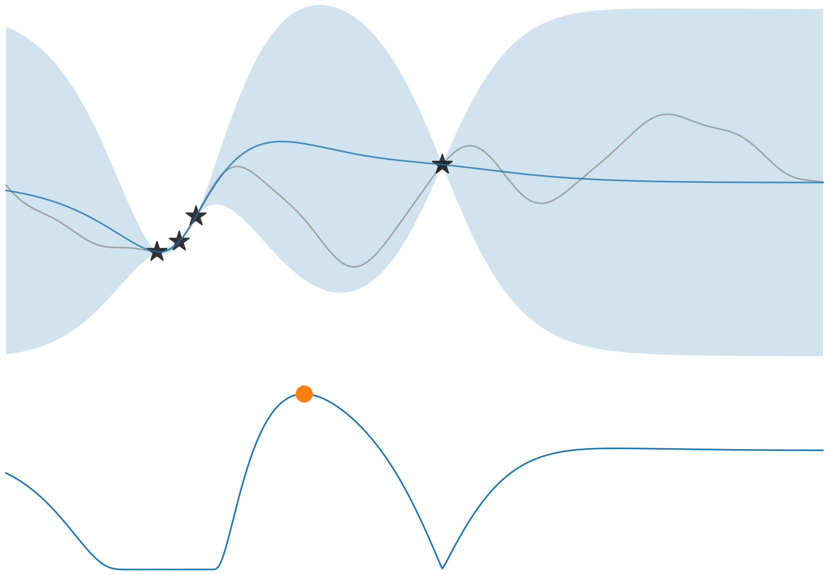
Independent

incorporate posterior

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

take continuum limit

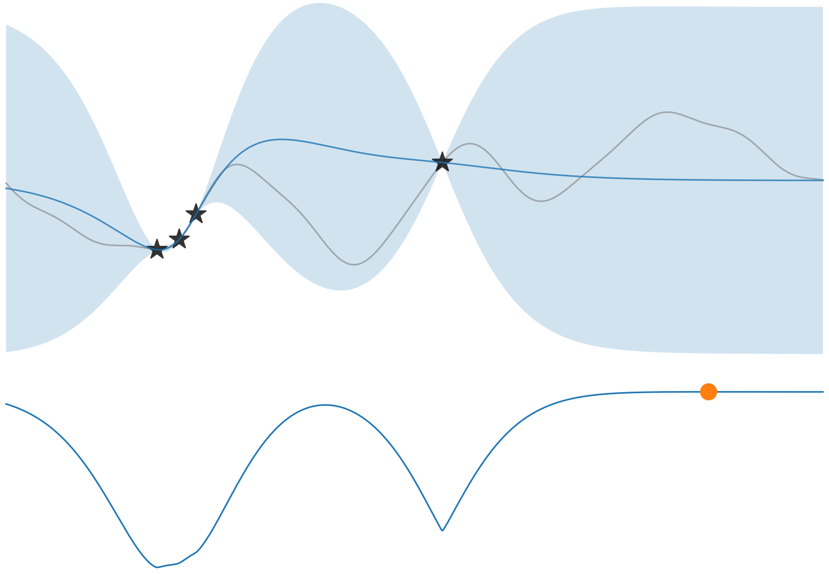
Expected Improvement



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

Temporal simplification to MDP

Gittins Index



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

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

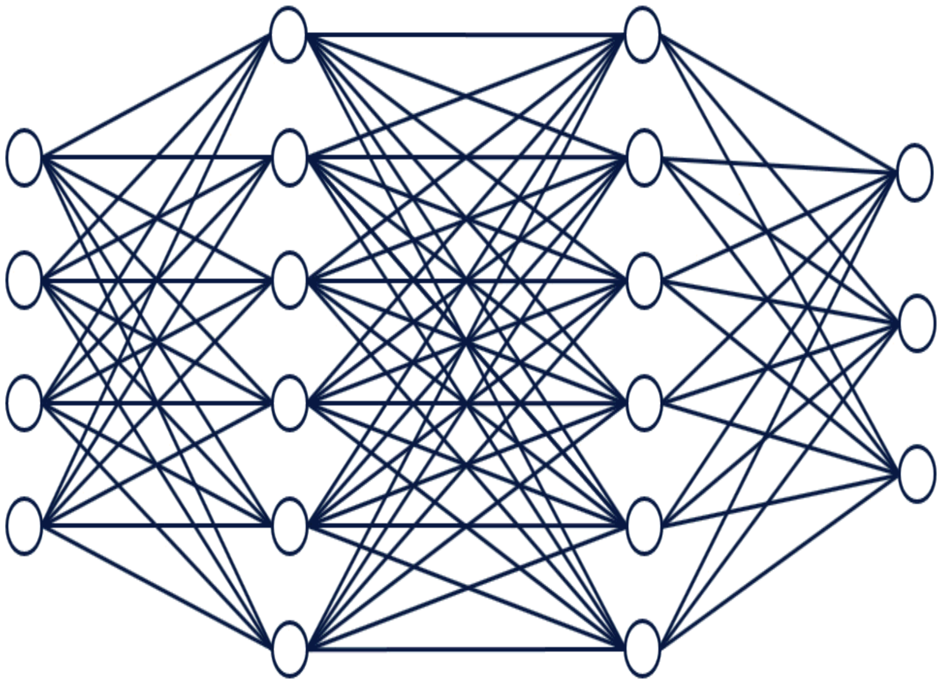
4. Theoretical guarantees

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?

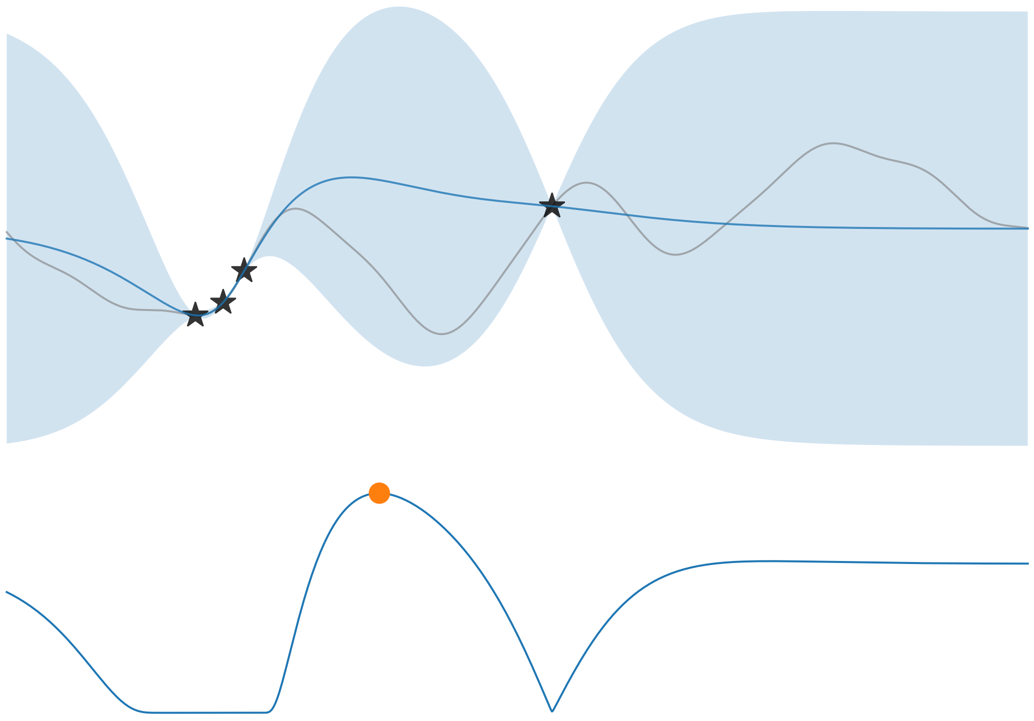
Smart stopping time

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

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

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Features in Pandora's box

Smart stopping time

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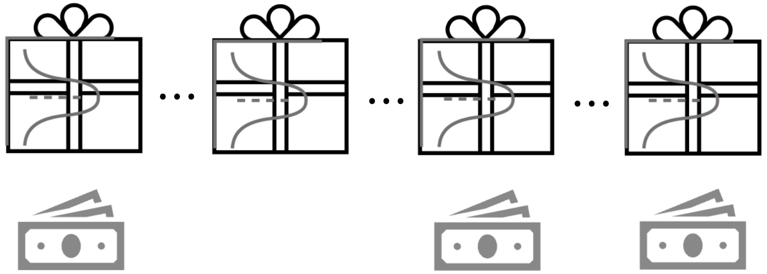
Optimal in related sequential decision problems



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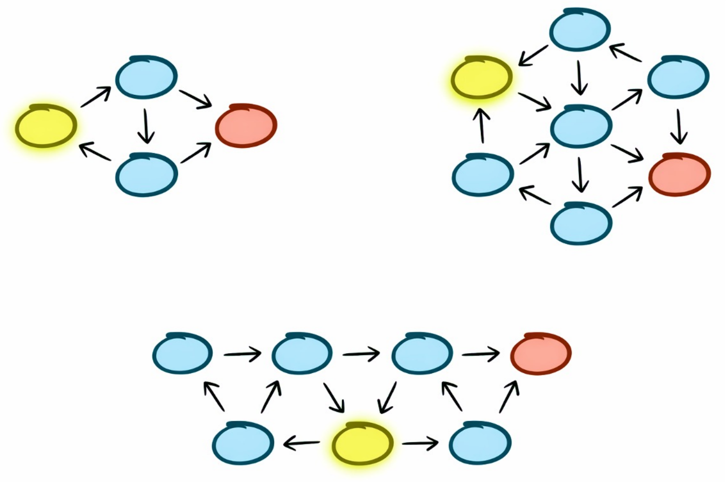

Why Gittins index?

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Features in Pandora's box

This talk's focus

Smart stopping time

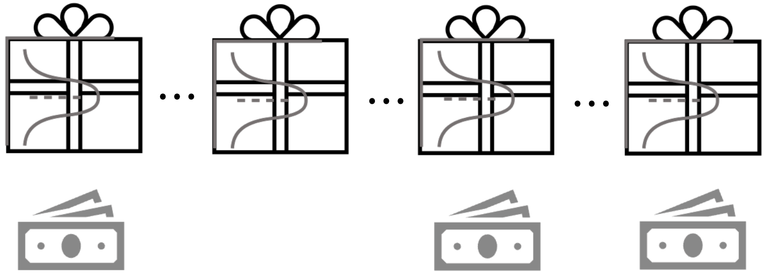
Features in Pandora's box

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.

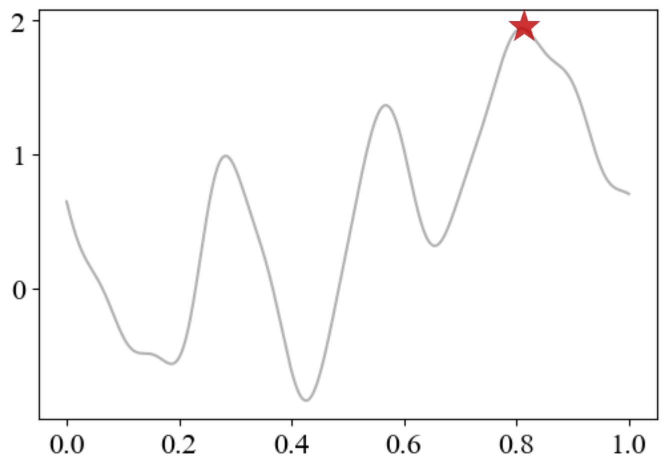
"Cost-aware Stopping for Bayesian Optimization." Under review.

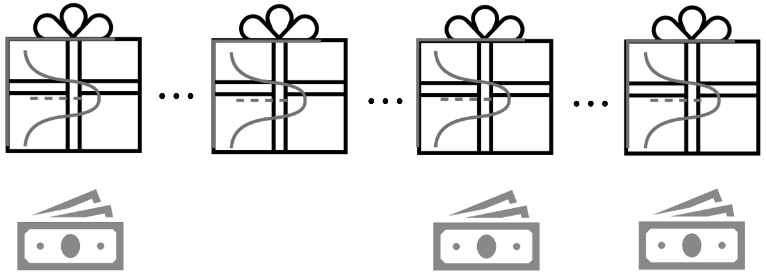
Bayesian Optimization

Pandora's Box

[Weitzman'79]

$f(x)$





$f(x)$

$c(x)$

Continuous

Discrete

Correlated

Independent

Fixed-iteration

Flexible-stopping

Expected best-observed value

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

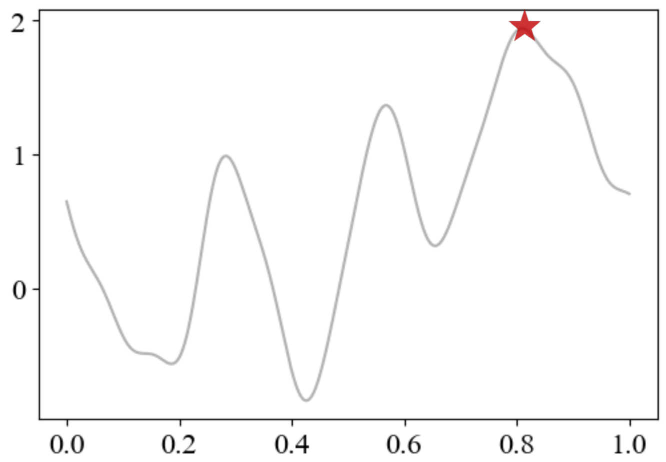
Expected utility

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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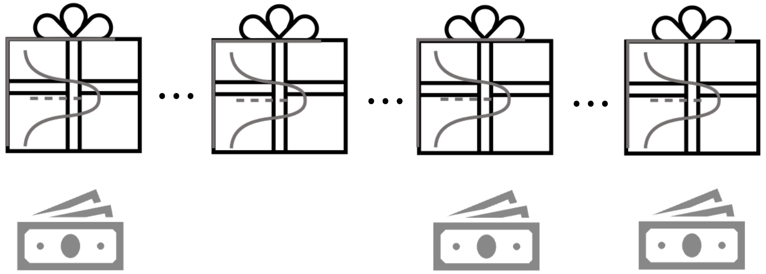
Pandora's Box

[Weitzman'79]



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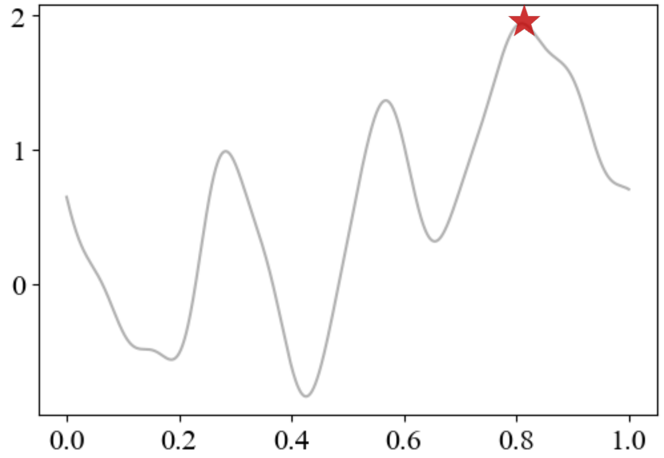
Bayesian Optimization

$f(x)$



Continuous

Correlated

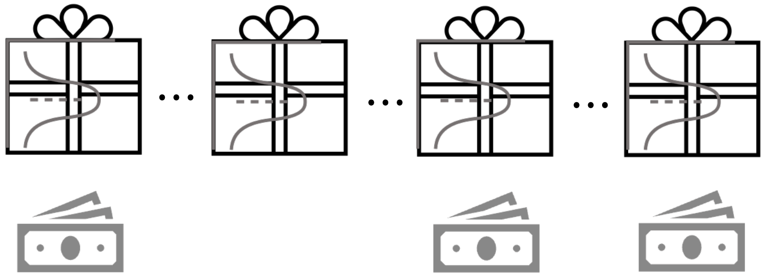
Fixed-iteration

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

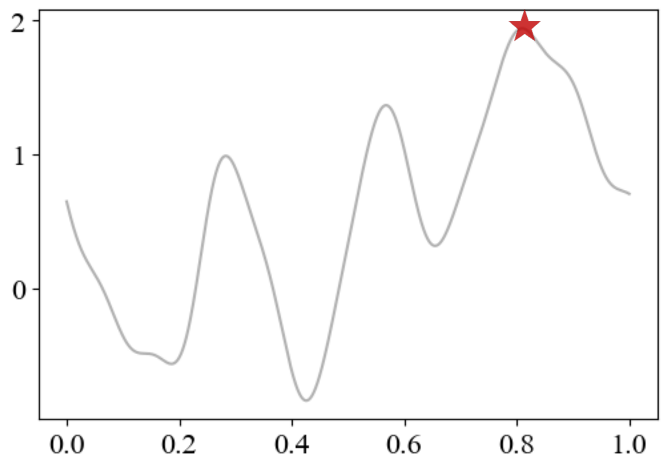
Expected utility

cumulative cost

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

Bayesian Optimization

$f(x)$



Continuous

Correlated

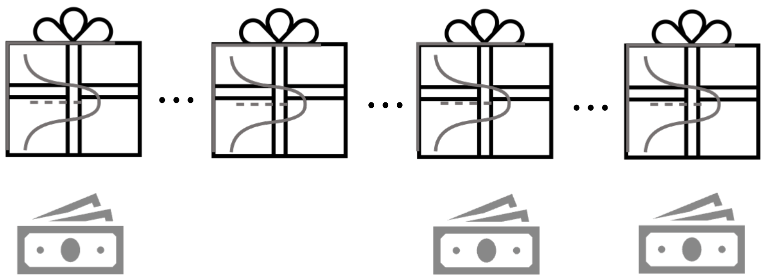
Fixed-iteration

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

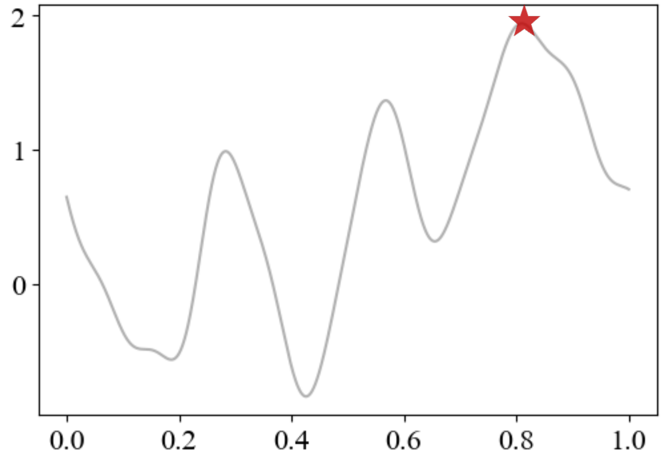
Expected cost-adjusted regret

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

cumulative cost

Bayesian Optimization

$f(x)$



Continuous

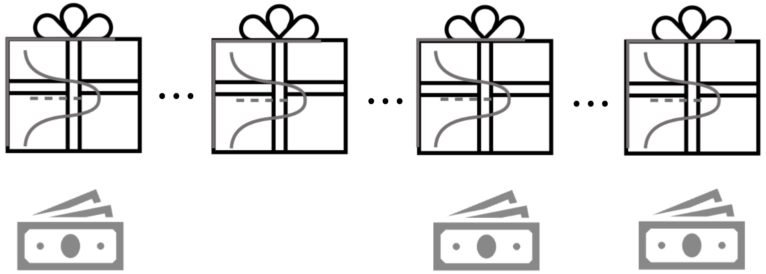
Correlated

Fixed-budget / Flexible-stopping

Expected (cost-adjusted) regret

Pandora's Box

[Weitzman'79]



$f(x)$

$c(x)$

Discrete

Independent

Flexible-stopping

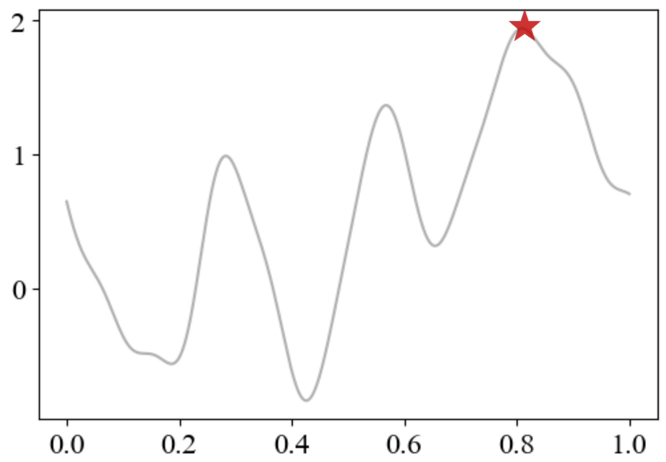
Expected cost-adjusted regret

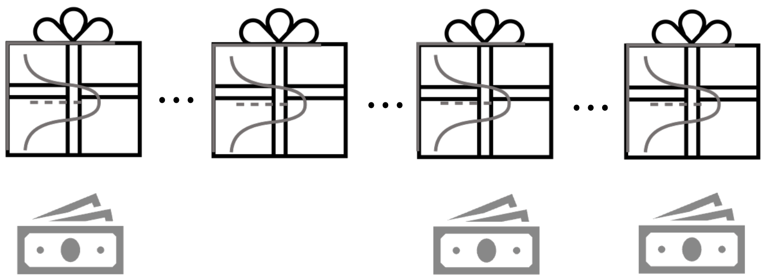
Bayesian Optimization

Pandora's Box

[Weitzman'79]

$f(x)$





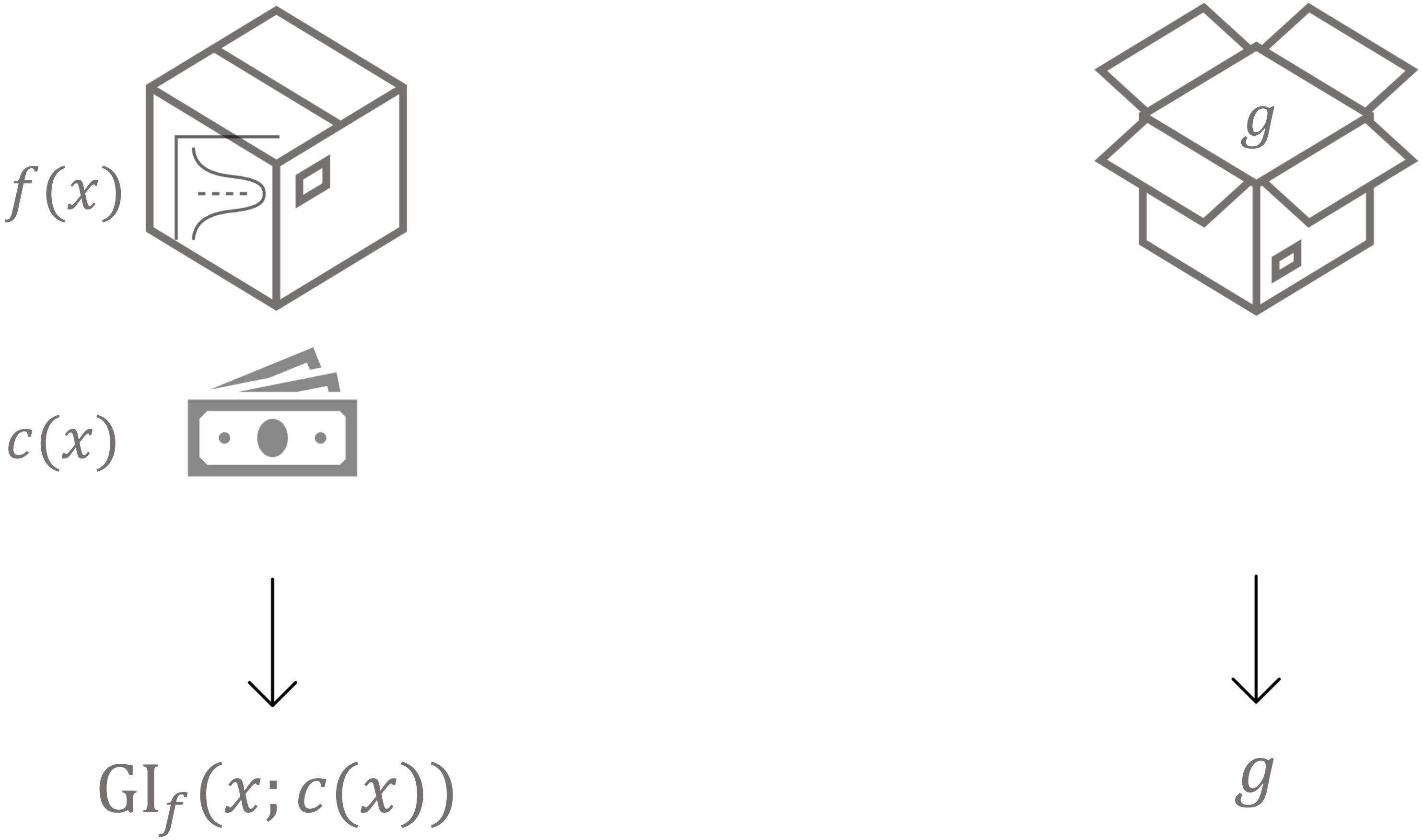
$f(x)$

$c(x)$

Bayesian Optimization	Pandora's Box
Continuous	Discrete
Correlated	Independent
Fixed-budget / Flexible-stopping	Flexible-stopping
Expected (cost-adjusted) regret	Expected cost-adjusted regret
	Optimal policy: Gittins index

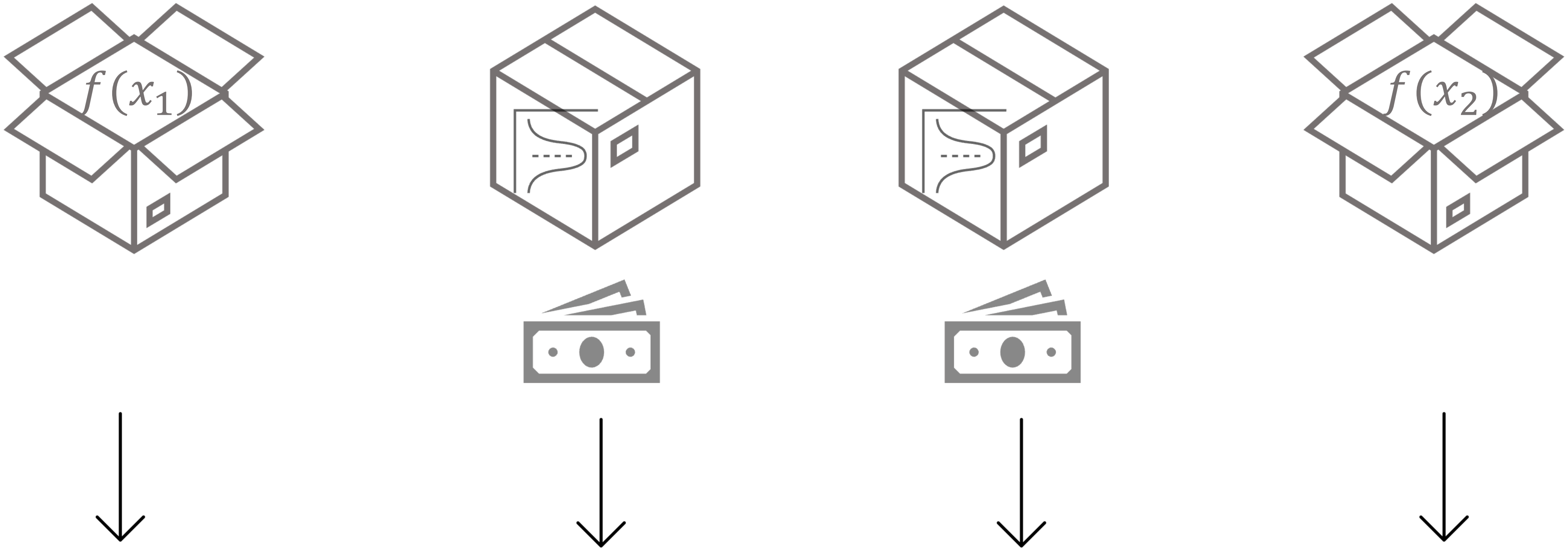
Optimal Policy: Gittins Index

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



Optimal Policy: Gittins Index

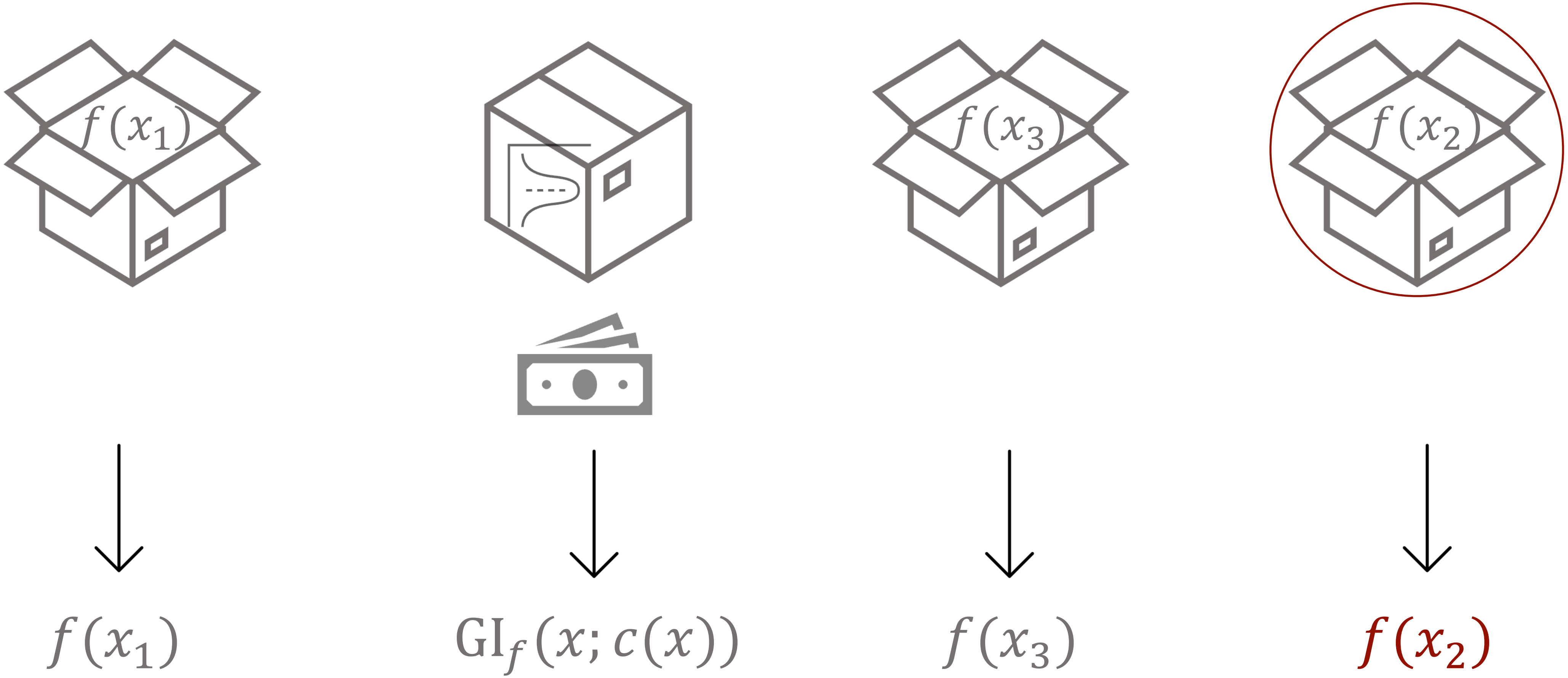
Step 2: Open the box with highest index if it is closed



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

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?

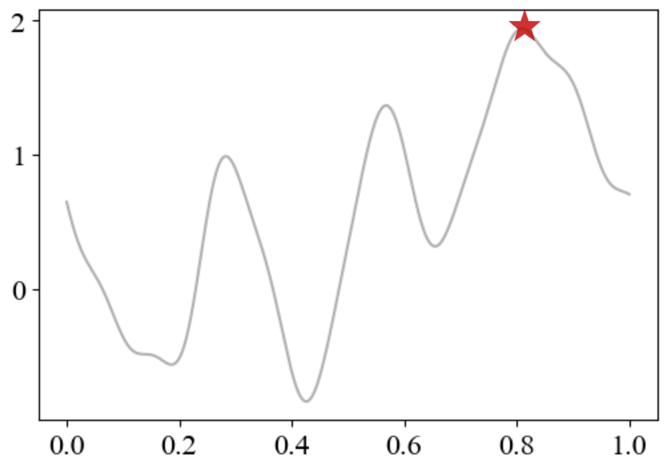
$$\max_x \mathrm{GI}\big(x; c(x)\big) \leq y_{\text{best}}$$

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

derived shared stopping rule

Bayesian Optimization

$f(x)$



Continuous

Correlated

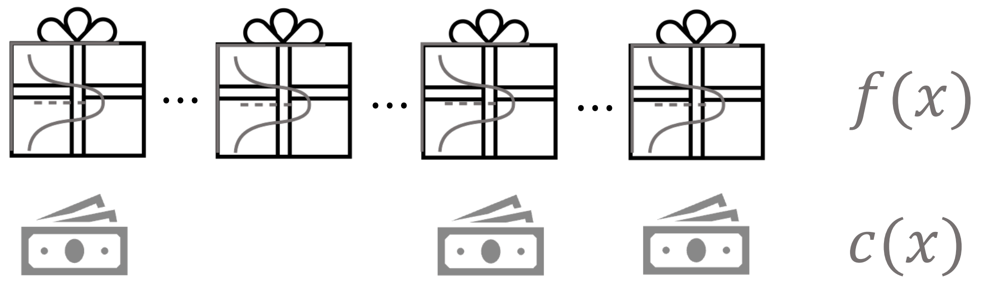
Fixed-budget / Flexible-stopping

Expected (cost-adjusted) regret

Is Gittins index good?

Pandora's Box

[Weitzman'79]



Discrete

Independent

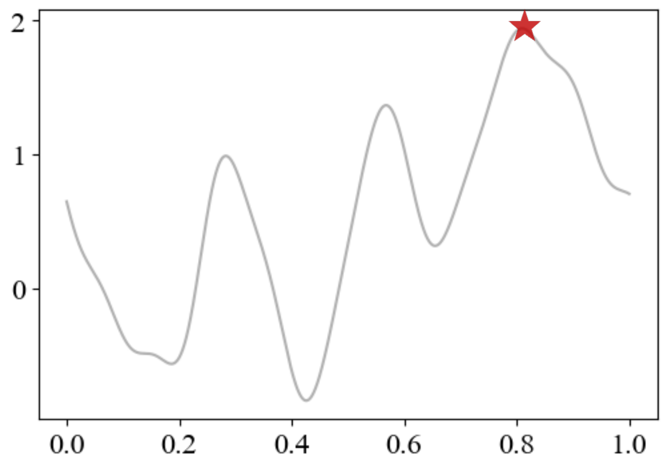
Flexible-stopping

Expected cost-adjusted regret

Gittins index is optimal

Bayesian Optimization

$f(x)$



Continuous

Correlated

Fixed-budget / Flexible-stopping

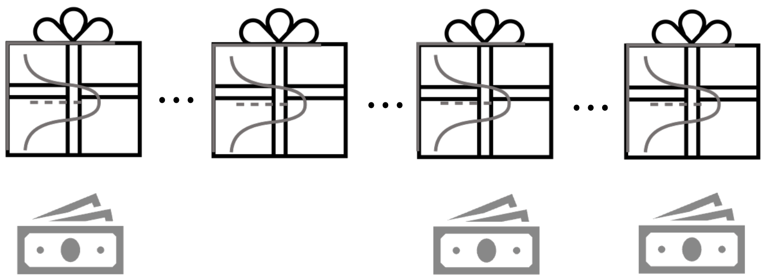
Expected (cost-adjusted) regret

Is Gittins index good?

empirically

Pandora's Box

[Weitzman'79]



$f(x)$

$c(x)$

Discrete

Independent

Flexible-stopping

Expected cost-adjusted regret

Gittins index is optimal

Our Contribution: Gittins Index Principle

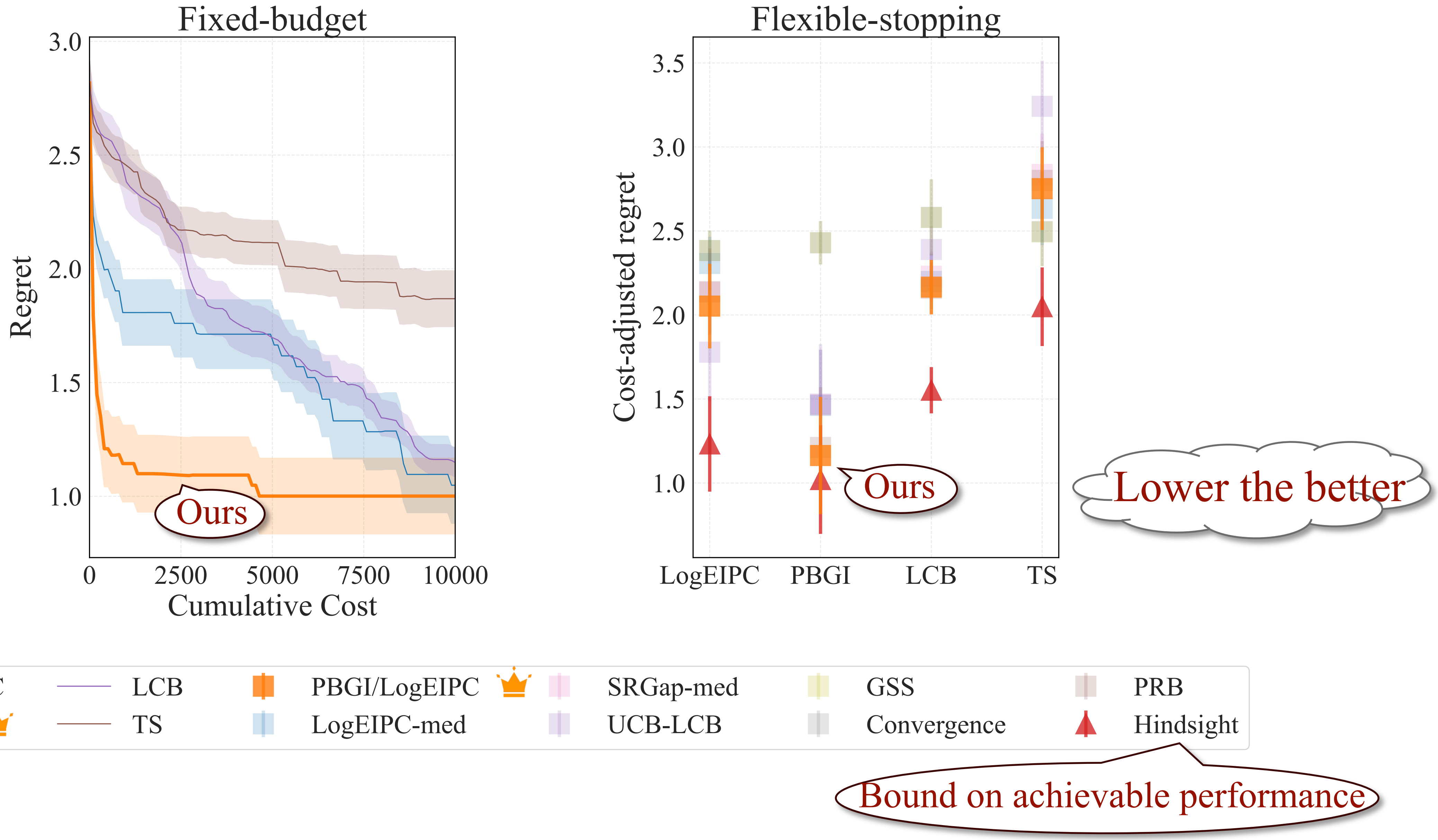
1. Principled design via problem simplification

2. Natural incorporation of side info and flexibility

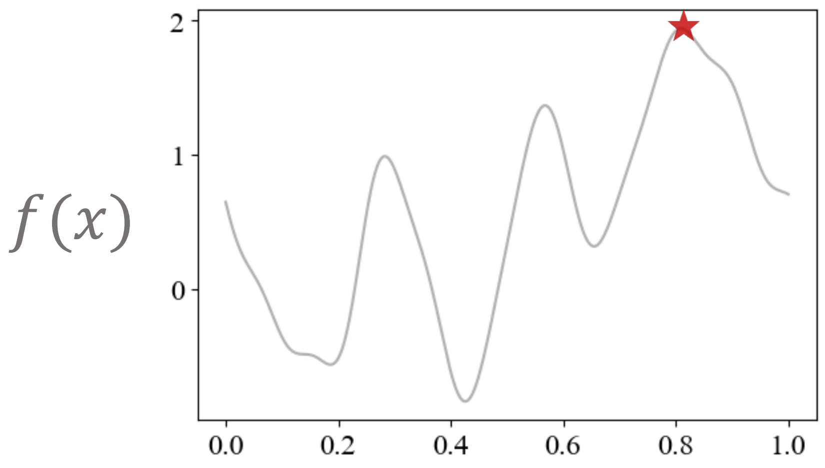
3. Competitive performance on benchmarks

4. Theoretical guarantees

Gittins Index vs Baselines on AutoML Benchmark



Bayesian Optimization



Continuous

Correlated

Fixed-budget / Flexible-stopping

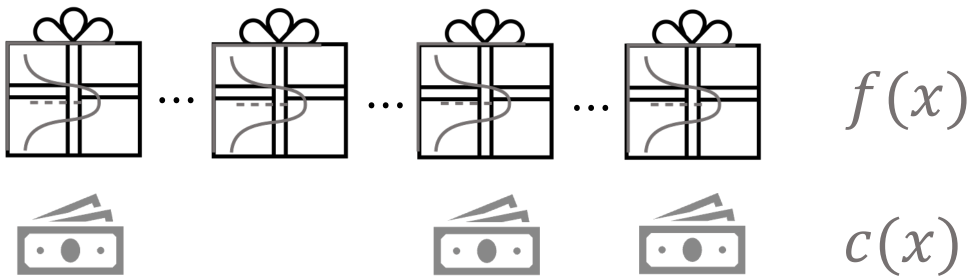
Expected (cost-adjusted) regret

Is Gittins index good?

theoretically

Pandora's Box

[Weitzman'79]



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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)

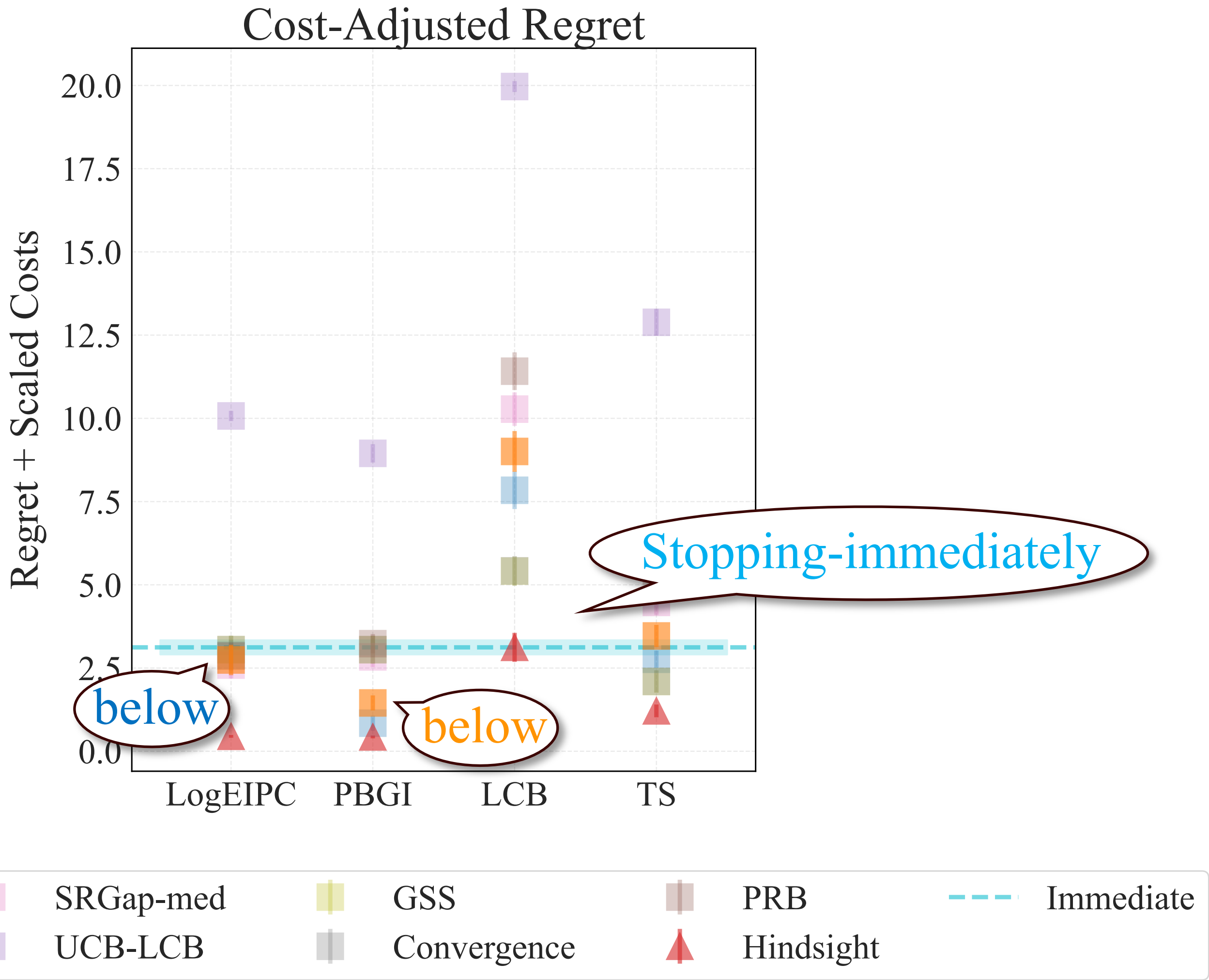
$\mathbb{E}[R(\text{ours; PBGI})] \leq R[\text{stopping immediately}]$

or LogEIPC   cost-adjusted regret

Implication:

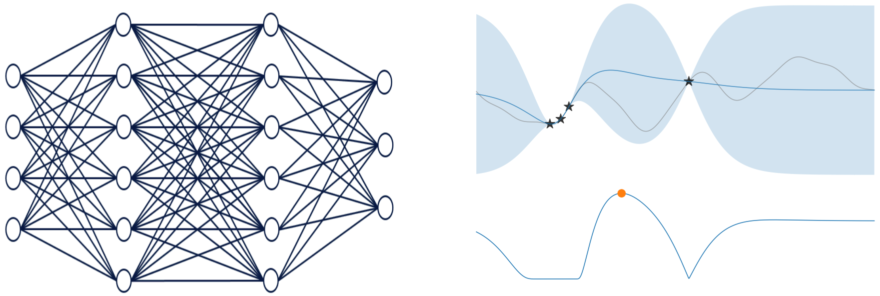
- Matches the best achievable performance in the worst case (evaluations are all very costly).

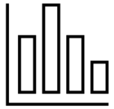
- Avoids over-spending — a property many cost-unaware stopping rules lack.



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

Studied problem

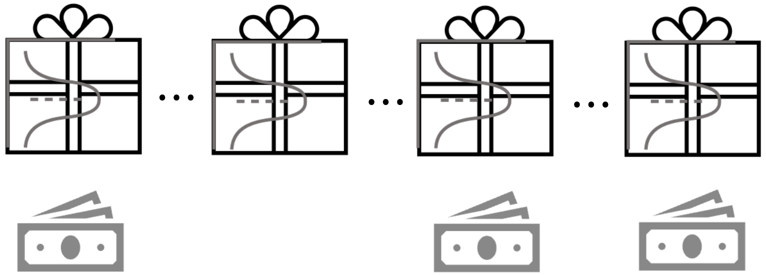




Varying evaluation costs

Adaptive stopping time

Key idea



Link to Pandora's Box problem
& Gittins index theory

Impact

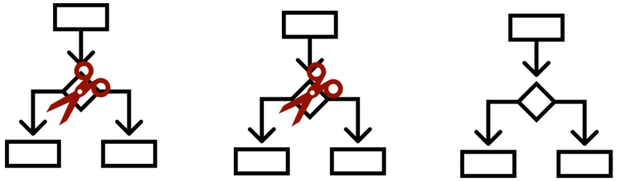
Meta

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

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Find our papers on arXiv!

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