NeurIPS’24 & INFORMS Data Mining Paper Competition Finalist

Cost-Aware Bayesian Optimization with Adaptive Stopping via Gittins Indices

Qian Xie 谢倩 (Cornell ORIE)

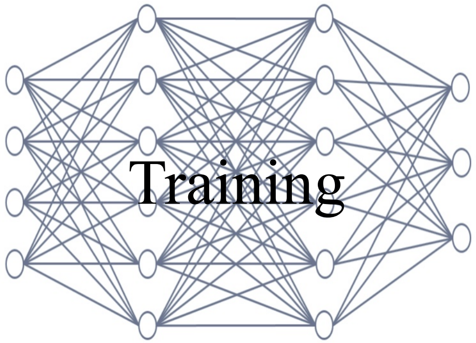
Joint work with Linda Cai (UC Berkeley), Raul Astudillo (MBZUAI), Theodore Brown (UCL), Peter Frazier, Alexander Terenin, Ziv Scully (Cornell), Yu Yu and Li Jin (SJTU)

INFORMS Annual Meeting 2025 Job Market Showcase

Optimization Under Uncertainty

ML model training:

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



$\longrightarrow$ Accuracy

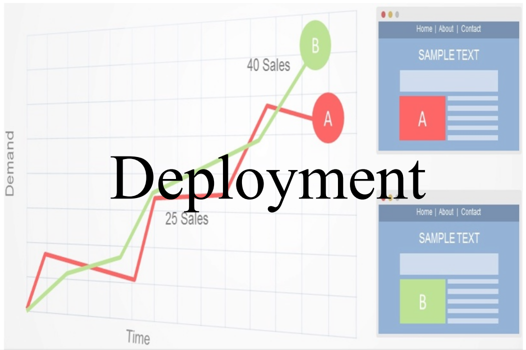
Optimization Under Uncertainty

ML model training:

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

Adaptive experimentation:

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



Optimization Under Uncertainty

Black-box optimization:

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

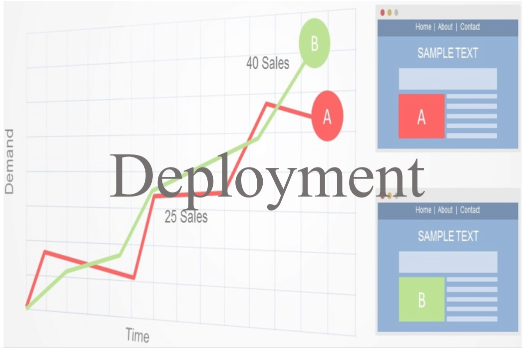
non-analytical & no gradient info

ML model training:

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

⟶ Accuracy

Adaptive experimentation:

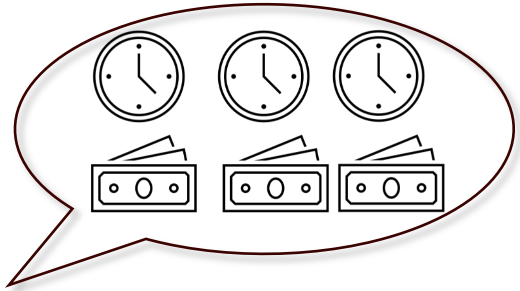
Decision/design variables (e.g., layout, pricing level) ⟶ 

⟶ Revenue

Black-Box Optimization

expensive-to-evaluate

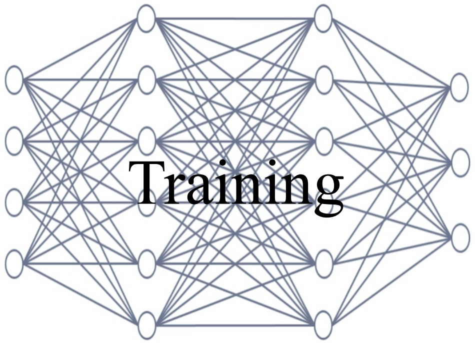
Input x ⟶  ⟶ Performance metric $f(x)$



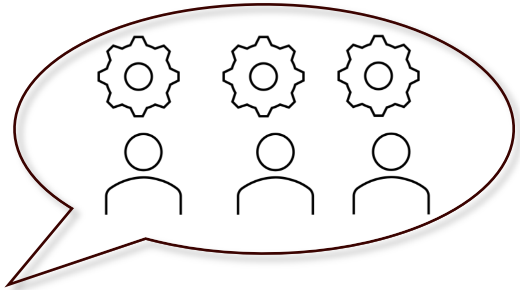
Training time

Compute credits

ML model training:

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

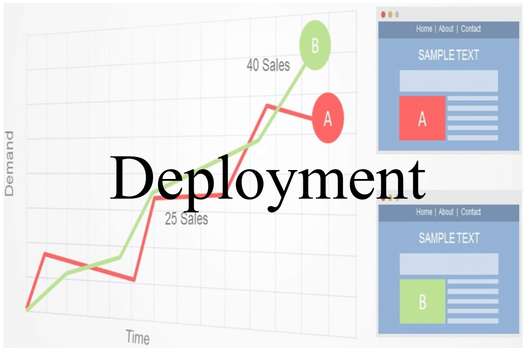
⟶ Accuracy



Operational cost

User experience

Adaptive experimentation:

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

⟶ Revenue

Black-Box Optimization

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

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

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

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Fewer #evaluations

Data-Driven Black-Box Optimization

expensive-to-evaluate

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

adaptively

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

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

Fewer #evaluations

Efficient framework: Bayesian optimization

Bayesian Optimization

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

$f \sim$Stochastic Process

Black-box function

Bayesian Optimization

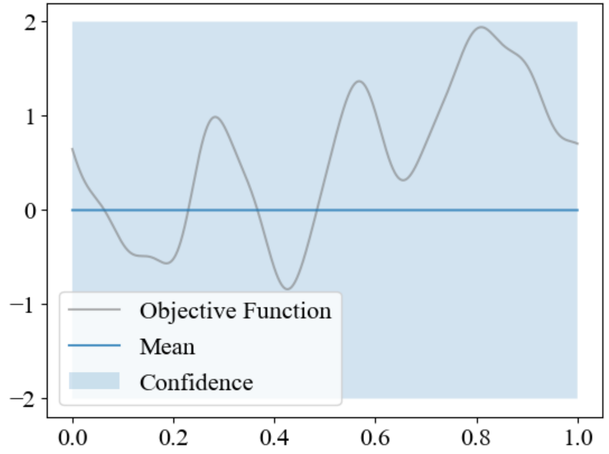
Time 0

$f \sim$Stochastic Process

x →  → $f(x)$

Black-box function

Model belief



Probabilistic model

(e.g., Gaussian process)

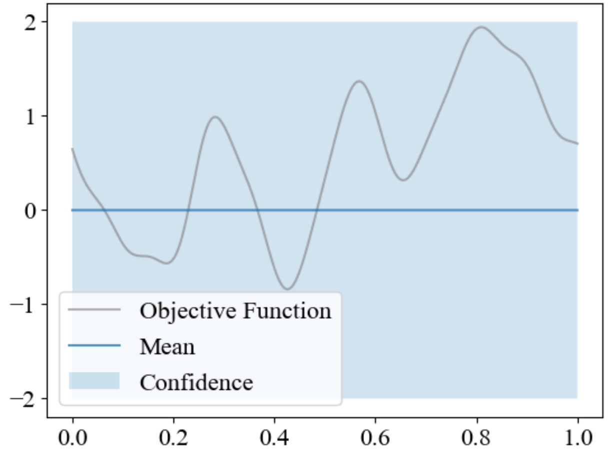
Bayesian Optimization

Time t

$f \sim$Stochastic Process

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

Model belief



Probabilistic model
(e.g., Gaussian process)

Bayesian Optimization

Time t

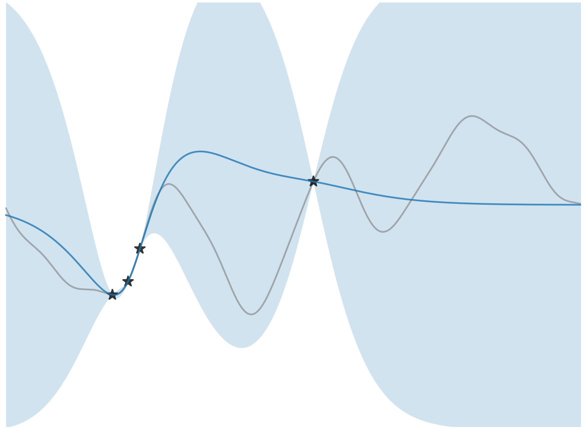
$x_1, \dots, x_t \longrightarrow$

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

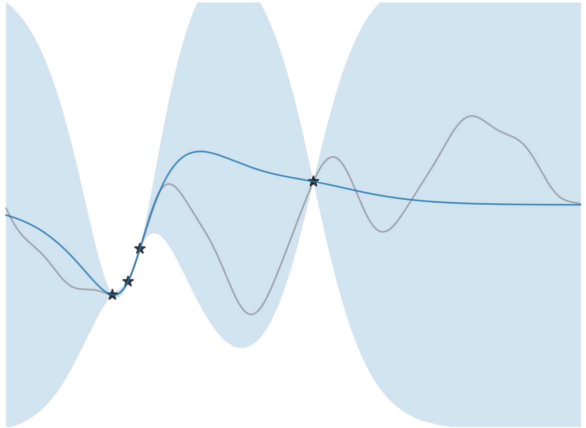
Time t

$x_1, \ldots, x_t \longrightarrow$

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

Black-box function

Update belief
(Bayes' rule)



Probabilistic model
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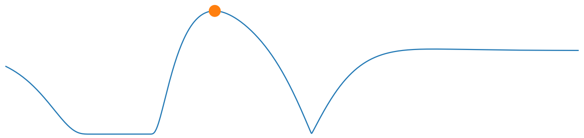


Acquisition function
(e.g., EI, UCB, TS)

scoring (worth of each point

Bayesian Optimization

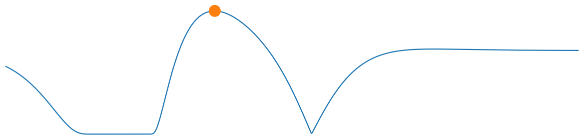
Time t

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

Black-box function

Acquire next input
(gradient-based optimization)

Update belief
(Bayes' rule)



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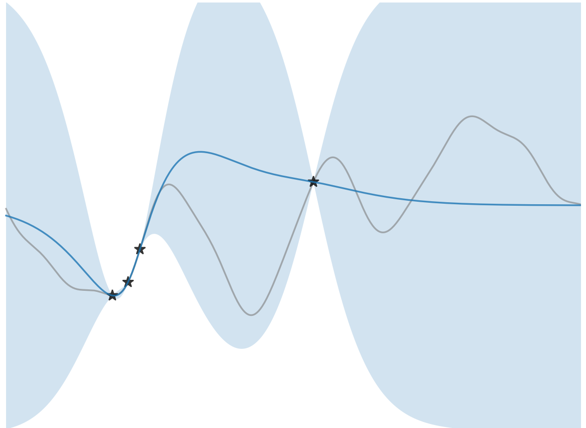


Probabilistic model
(e.g., Gaussian process)

Bayesian Optimization

Time $t + 1$

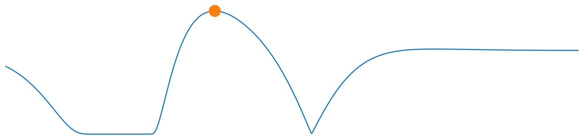
$x_1, \dots, x_{t+1} \longrightarrow$

Black-box function

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

Acquire next input
(gradient-based
optimization)

Update belief
(Bayes' rule)



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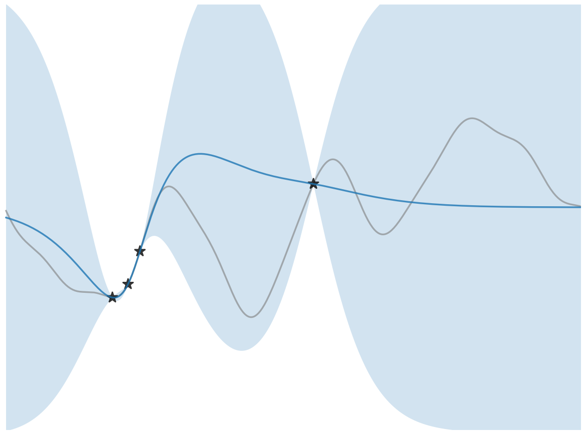


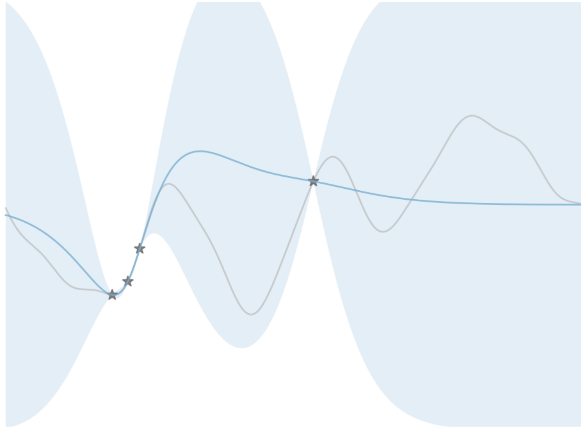
Probabilistic model
(e.g., Gaussian process)

Bayesian Optimization

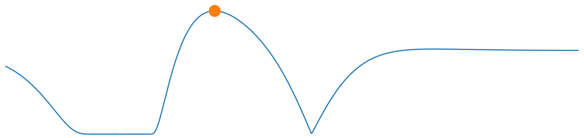
x →  → $f(x)$

Black-box function

Update belief
(Bayes' rule)



Probabilistic model
(e.g., Gaussian process)



My focus

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

scoring (worth of each point

Acquire next input
(gradient-based optimization)

Existing Design Principles

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

New Design Principle: Gittins Index

- Improvement-based (e.g., EI)
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? Why another principle?

Our Contribution: Gittins Index Principle

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

1. Naturally incorporates side info and practical flexibility
2. Performs competitively on benchmarks
3. Comes with theoretical guarantees

Our Contribution: Gittins Index Principle

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2. Performs competitively on benchmarks
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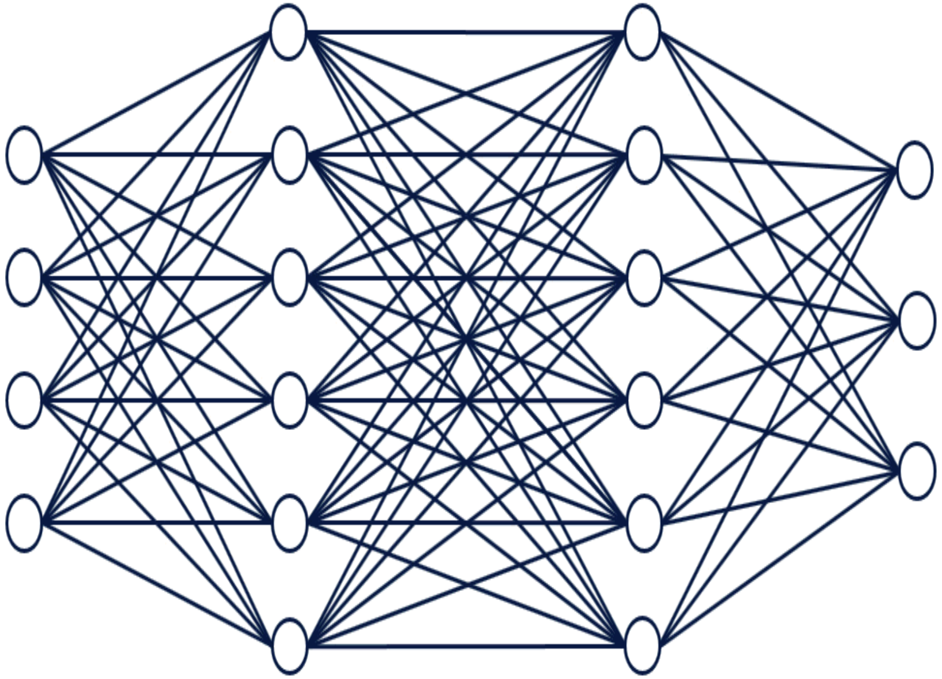
Under-explored Side Info and Flexibility

Varying evaluation costs

Smart stopping time

Observable multi-stage feedback

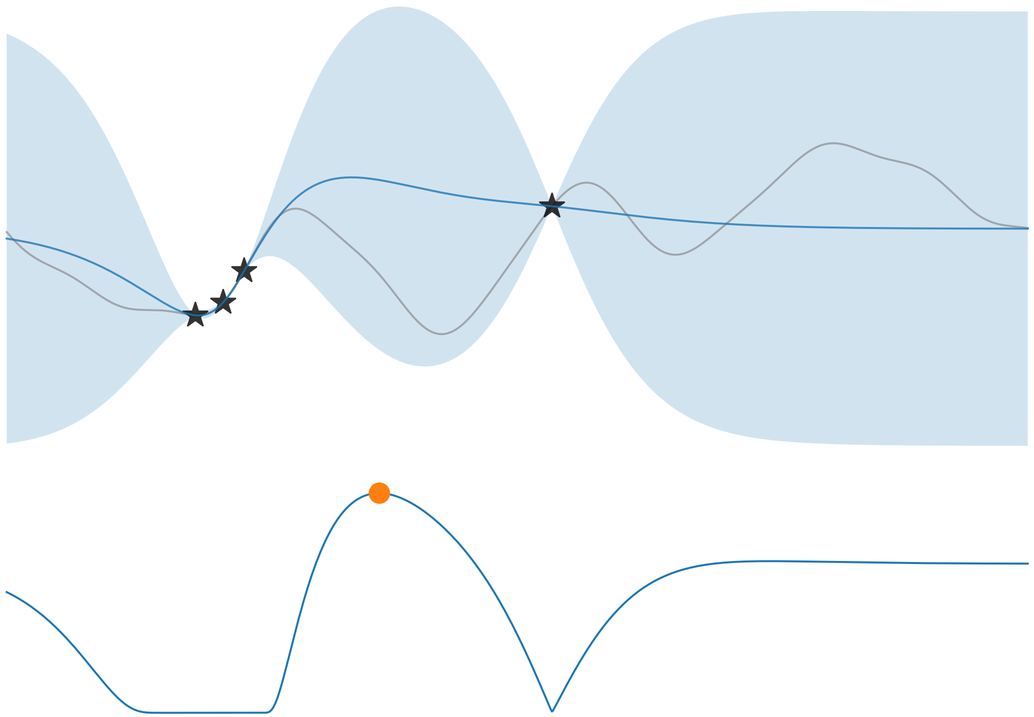


How does existing principle incorporate them?

Varying evaluation costs

Smart stopping time

Observable multi-stage feedback



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

How does existing principle incorporate them?

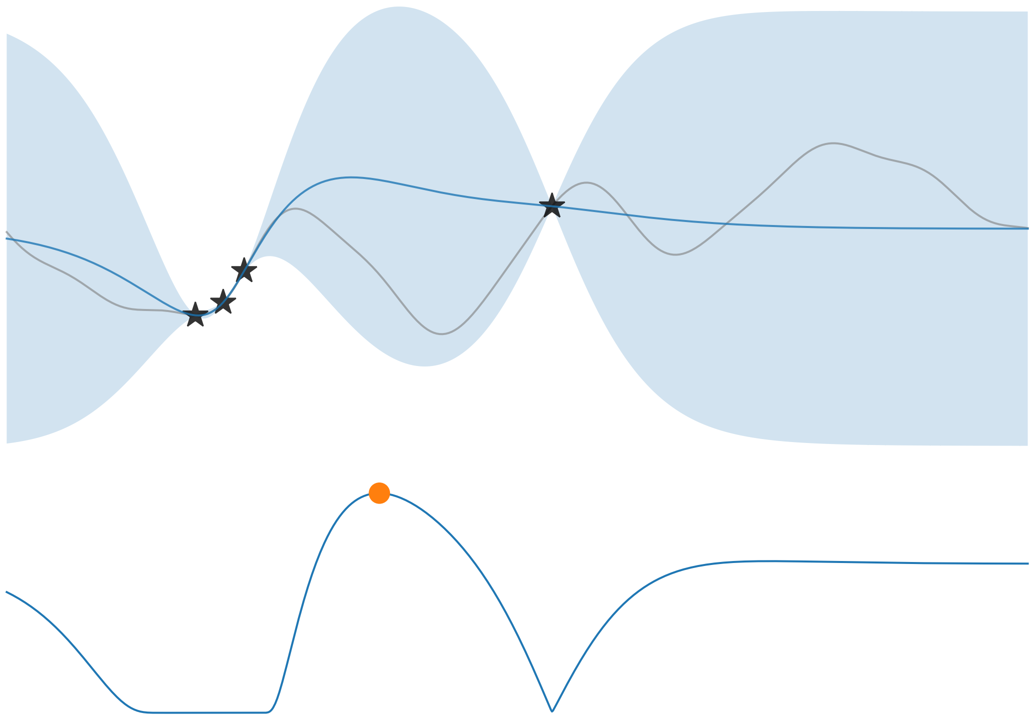
Varying evaluation costs

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

Why divide?

Smart stopping time

Observable multi-stage feedback



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

How does existing principle incorporate them?

Varying evaluation costs

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

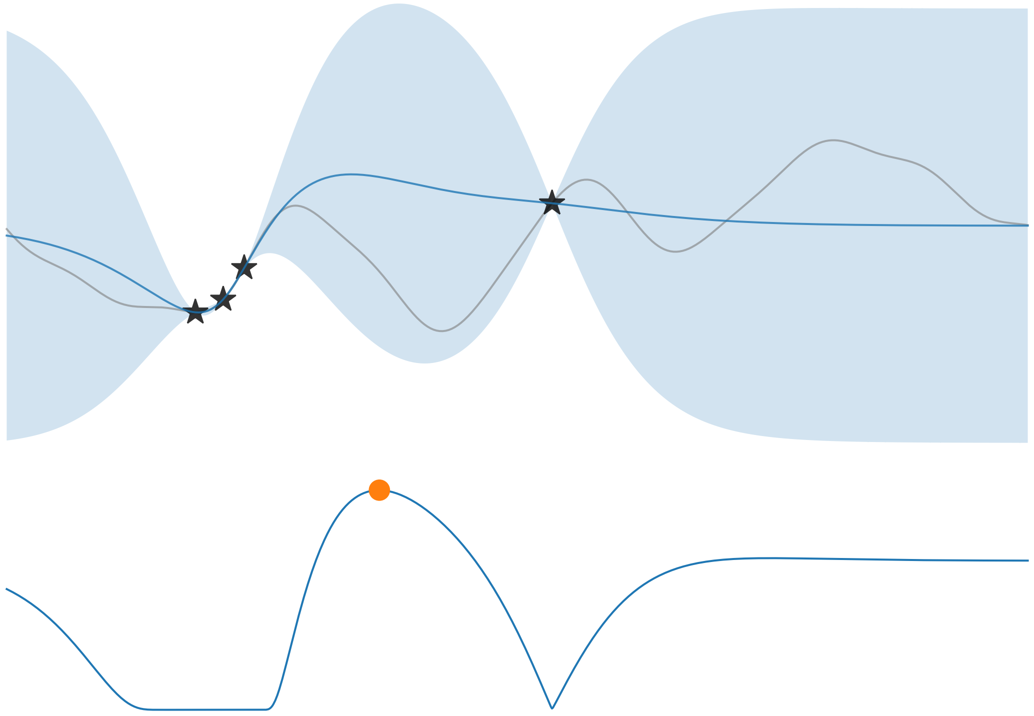
Why divide?

Smart stopping time

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

Which threshold?

Observable multi-stage feedback



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

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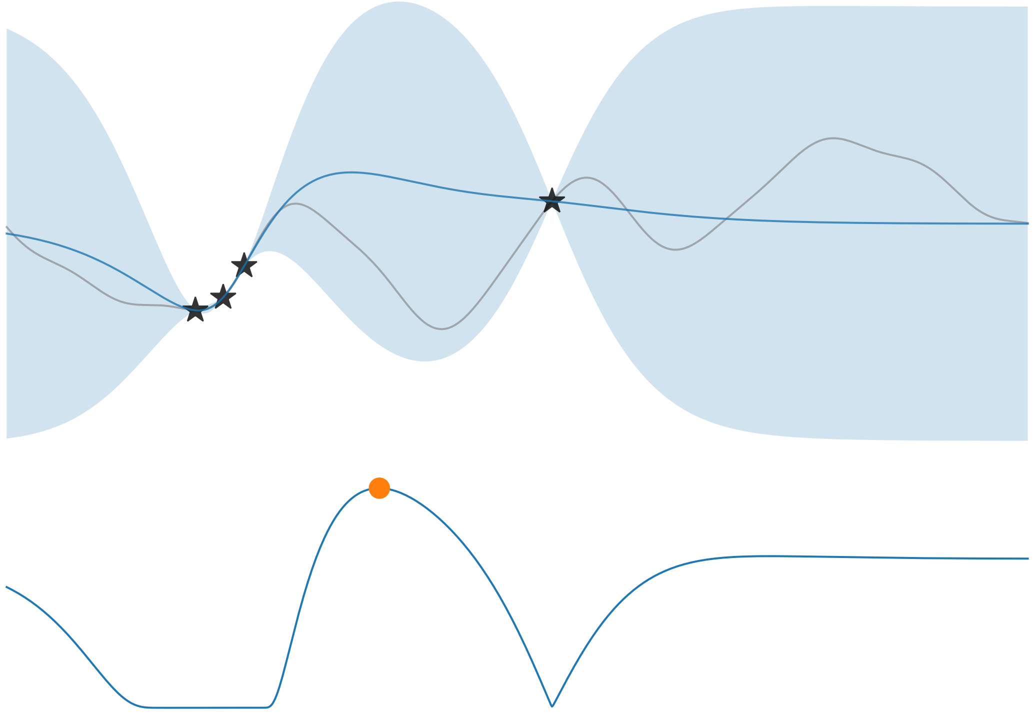
?



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

Under-explored Side Info and Flexibility

Varying evaluation costs

Smart stopping time

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New design principle:
Gittins index

Why Gittins index?

Varying evaluation costs

Smart stopping time

Observable multi-stage feedback

New design principle:
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Why Gittins index?

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New design principle:
Gittins index

Optimal in related sequential decision problems

Why Gittins index?

Varying evaluation costs

Features in Pandora's box

Smart stopping time

Features in Pandora's box

Observable multi-stage feedback

New design principle:
Gittins index

Optimal in related sequential decision problems

Why Gittins index?

Varying evaluation costs

Features in Pandora's box

Smart stopping time

Features in Pandora's box

Observable multi-stage feedback

Features in Markovian bandits

New design principle:
Gittins index

Optimal in related sequential decision problems

What is Pandora’s Box?

Varying evaluation costs

Features in Pandora’s box

Smart stopping time

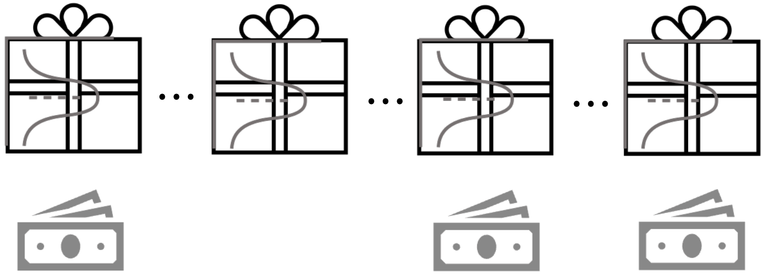
Features in Pandora’s box

Observable multi-stage feedback

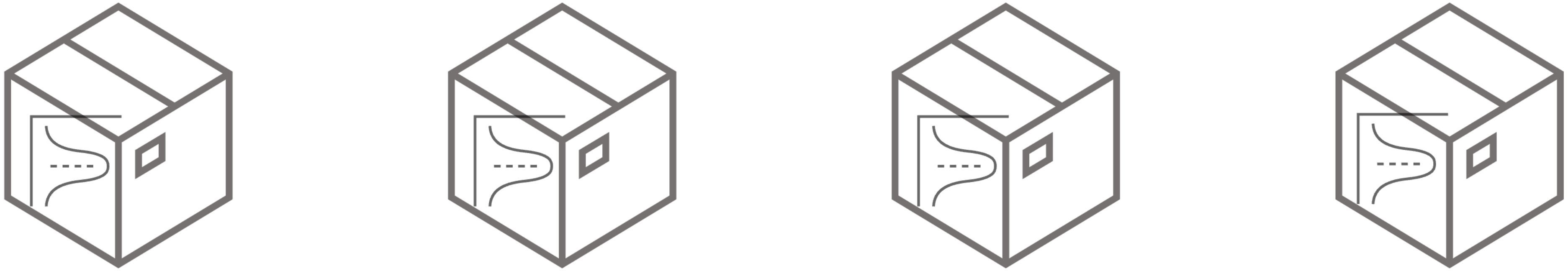
Features in Markovian bandits

New design principle:
Gittins index

Optimal in related sequential decision problems



Pandora's Box



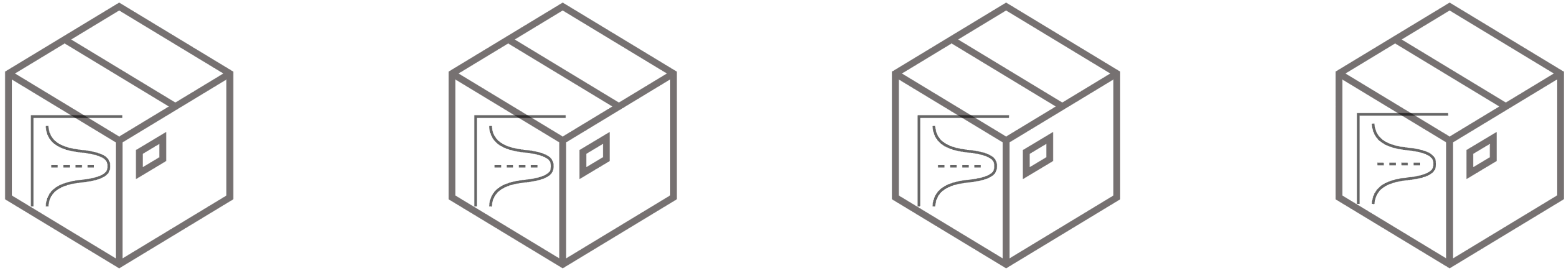
High-level goal: Choose box $x_1, \ldots, x_T$ to open to maximize the expected utility

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

Flexible stopping time

Pandora's Box

$t = 0$



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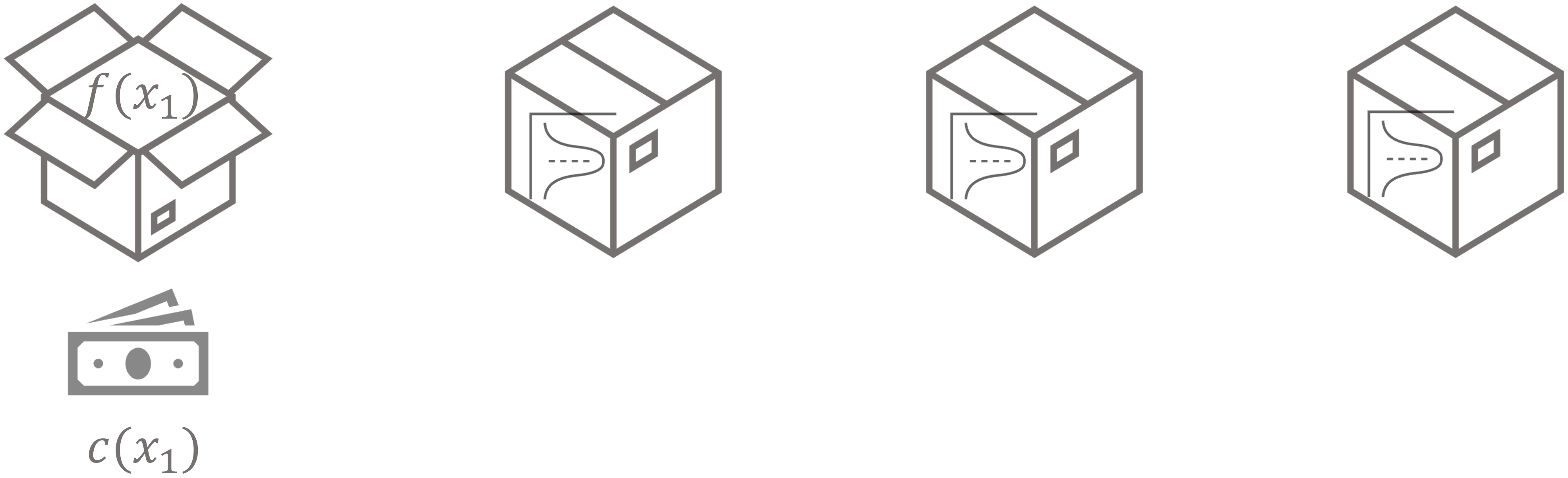
$$\mathbb{E} \max_{t=1,2,\ldots,T} f(x_t) - \mathbb{E} \sum_{t=1}^{T} c(x_t)$$

Pandora’s Box

$t = 1$

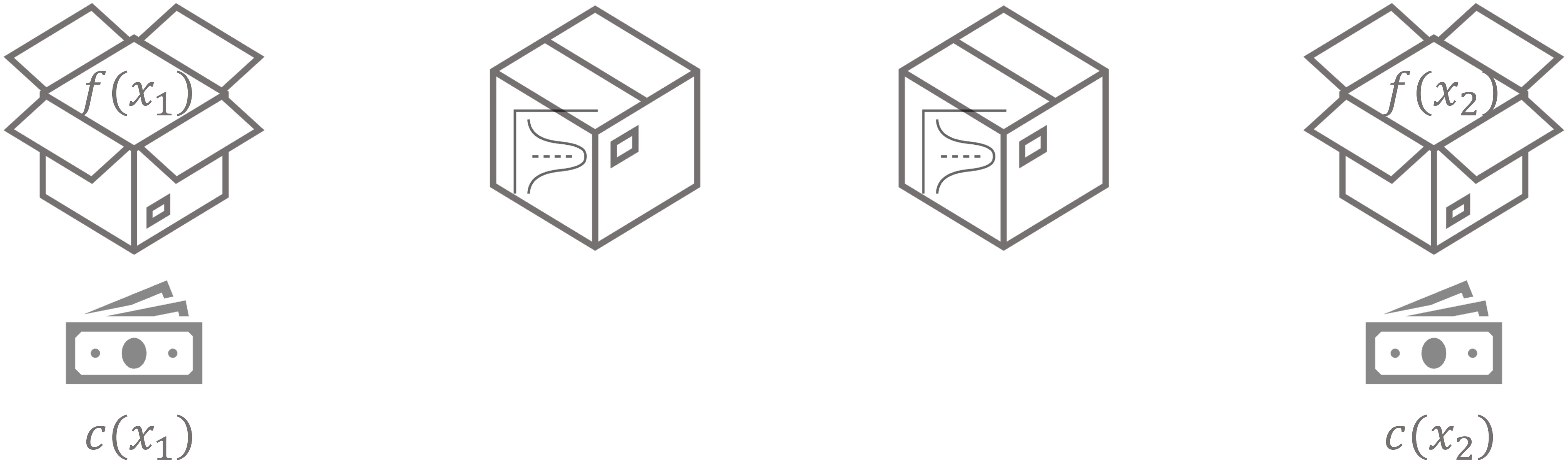


High-level goal: Choose box $x_1, \ldots, x_T$ to open to maximize the expected utility

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

Pandora's Box

$t = 2$

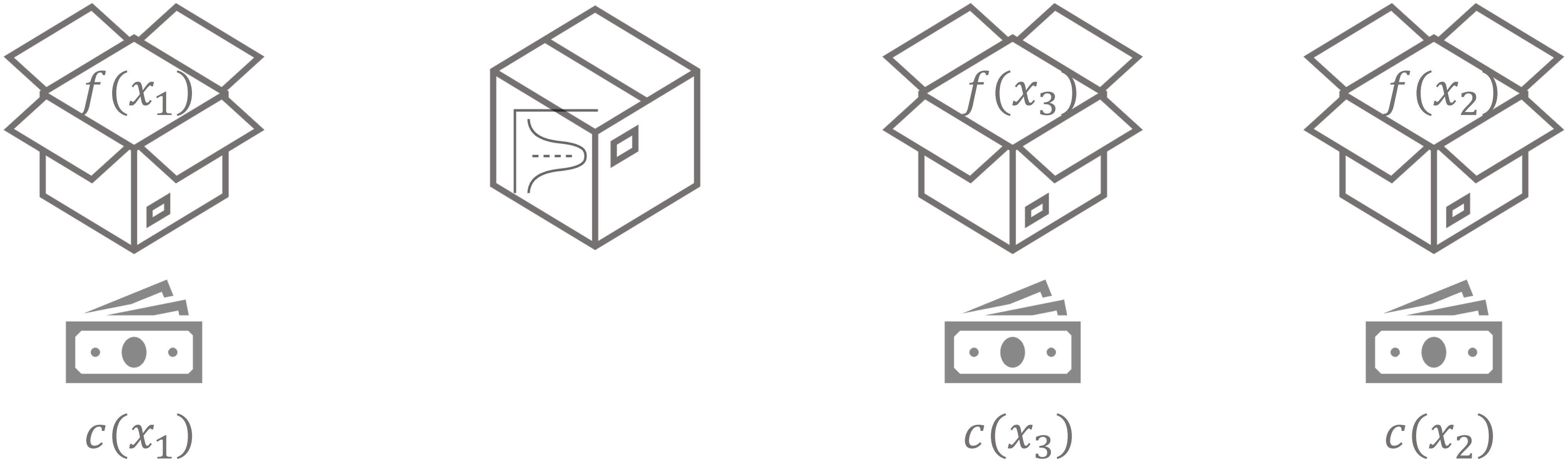


High-level goal: Choose box $x_1, \ldots, x_T$ to open to maximize the expected utility

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

Pandora's Box

$t = 3$

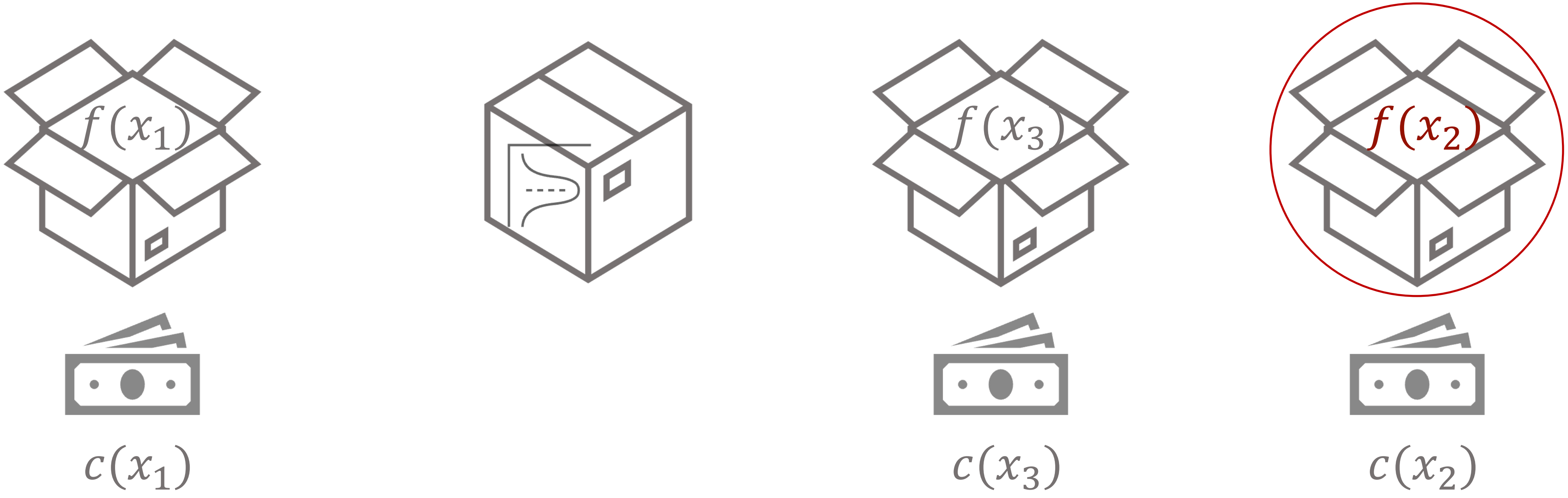


High-level goal: Choose box $x_1, \ldots, x_T$ to open to maximize the expected utility

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

Pandora's Box

$t = T$, stop

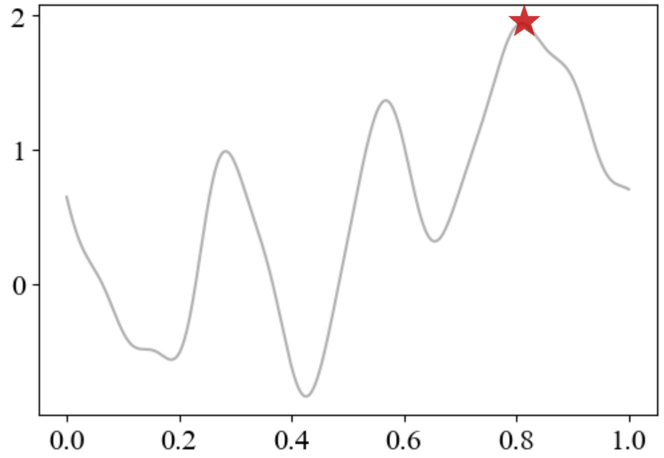


High-level goal: Choose box $x_1, \dots, x_T$ to open to maximize the expected utility

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

Bayesian Optimization

$f(x)$



Continuous

Correlated

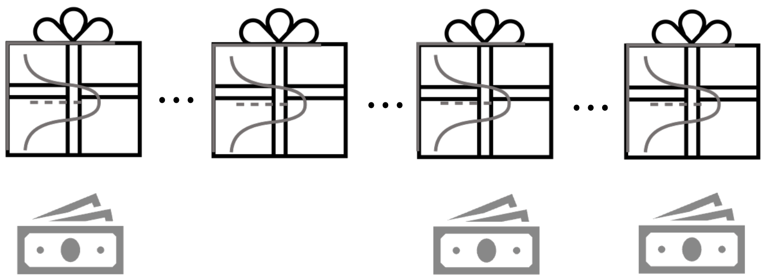
Fixed-iteration

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

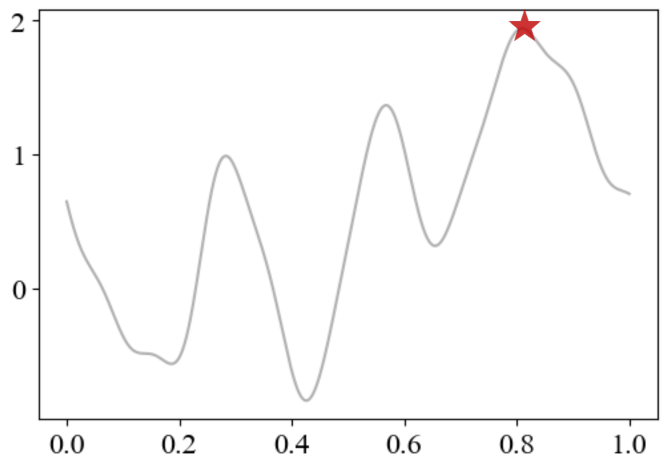
Expected utility

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

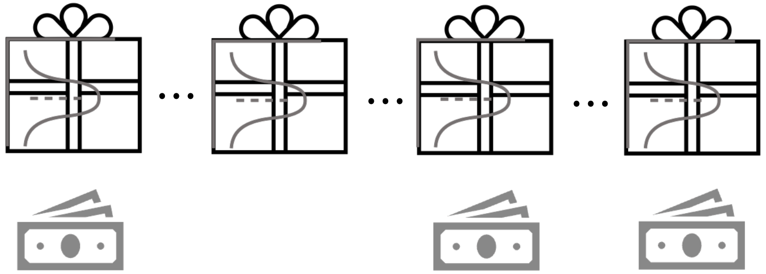
Fixed-iteration

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

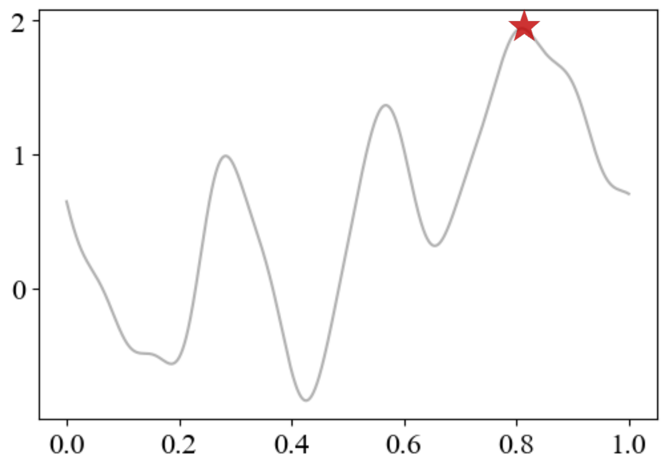
Expected utility

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

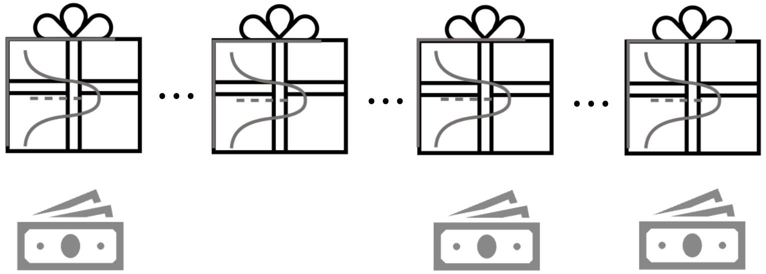
Fixed-iteration

Expected regret

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

Pandora's Box

[Weitzman'79]



$f(x)$

$c(x)$

Discrete

Independent

Flexible-stopping

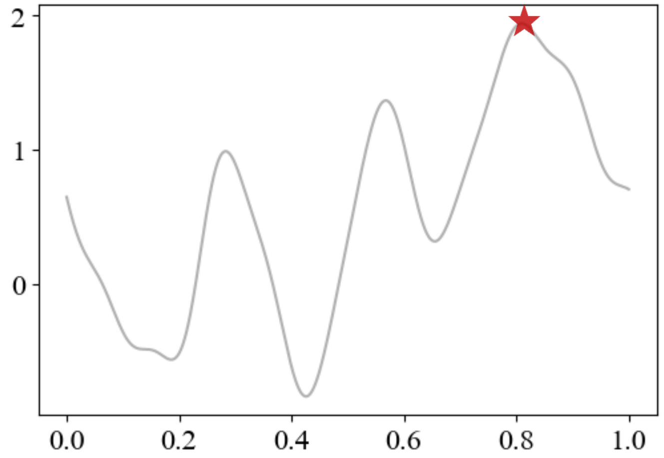
Expected utility

cumulative cost

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

Bayesian Optimization

$f(x)$



Continuous

Correlated

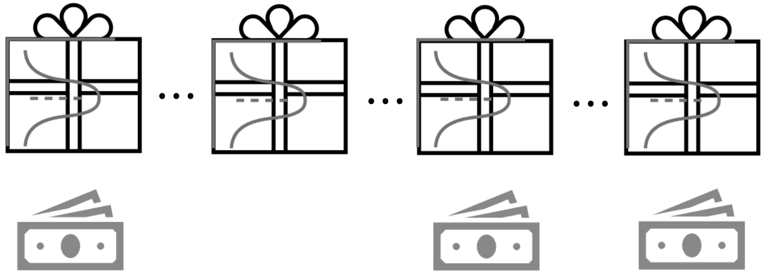
Fixed-iteration

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

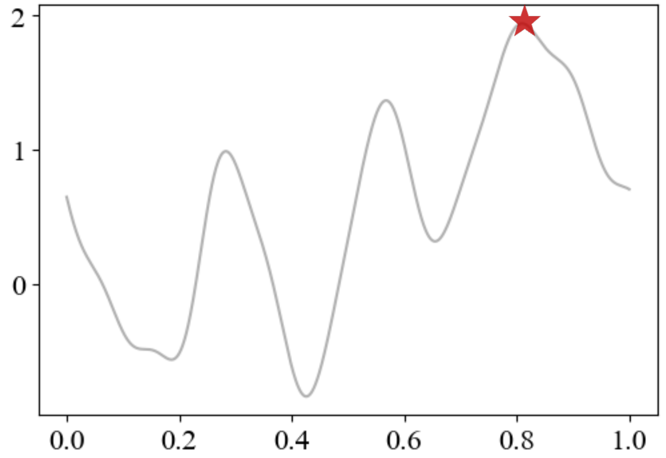
Expected cost-adjusted regret

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

cumulative cost

Bayesian Optimization

$f(x)$



Continuous

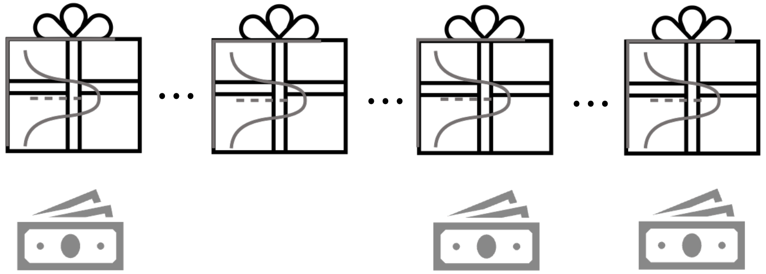
Correlated

Fixed-budget / Flexible-stopping

Expected (cost-adjusted) regret

Pandora's Box

[Weitzman'79]



$f(x)$

$c(x)$

Discrete

Independent

Flexible-stopping

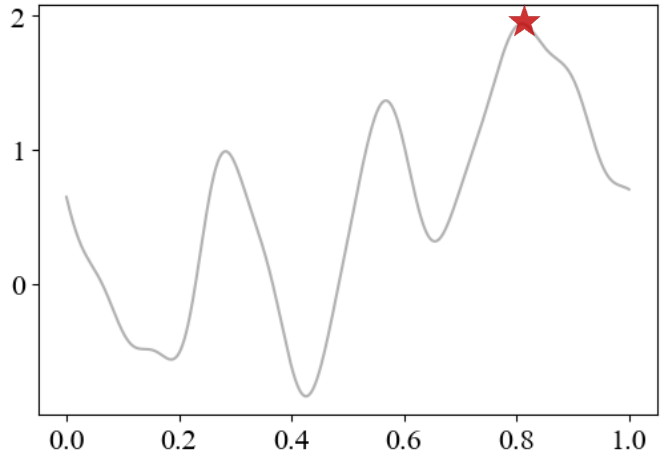
Expected cost-adjusted regret

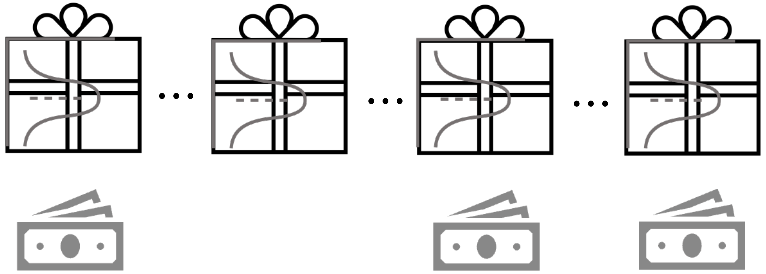
Bayesian Optimization

Pandora's Box

[Weitzman'79]

$f(x)$





$f(x)$

$c(x)$

Continuous

Correlated

Fixed-budget / Flexible-stopping

Expected (cost-adjusted) regret

Discrete

Independent

Flexible-stopping

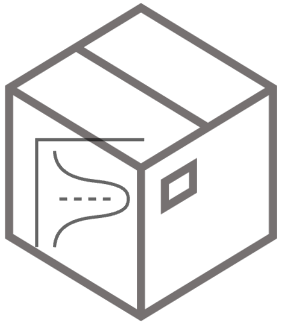
Expected cost-adjusted regret

Optimal policy: Gittins index

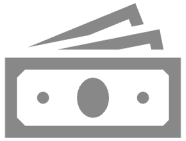
Optimal Policy: Gittins Index

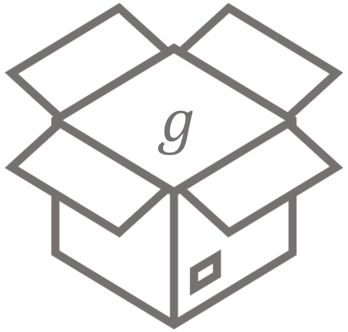
Step 1: Assign each box a Gittins index (higher is better)

$f(x)$



$c(x)$





$\downarrow$

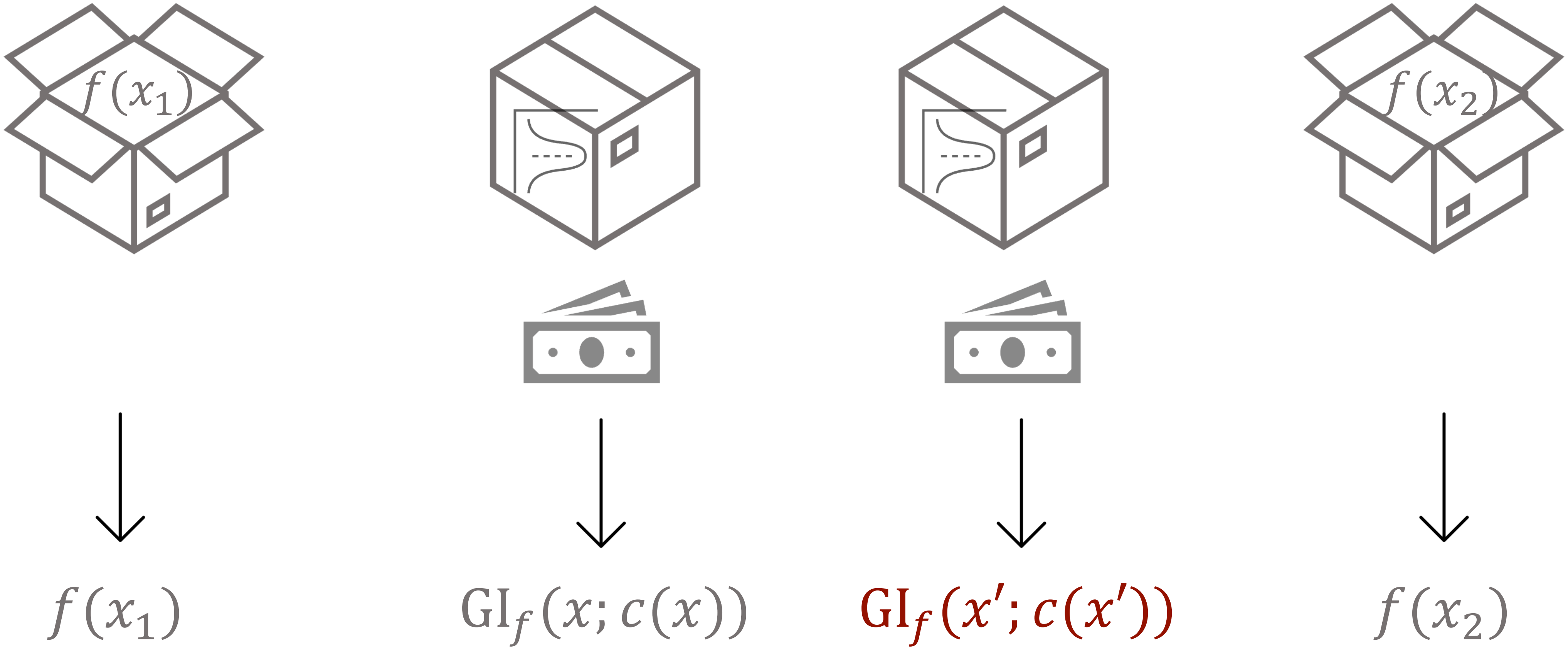
$\mathrm{GI}_f(x; c(x))$

$\downarrow$

g

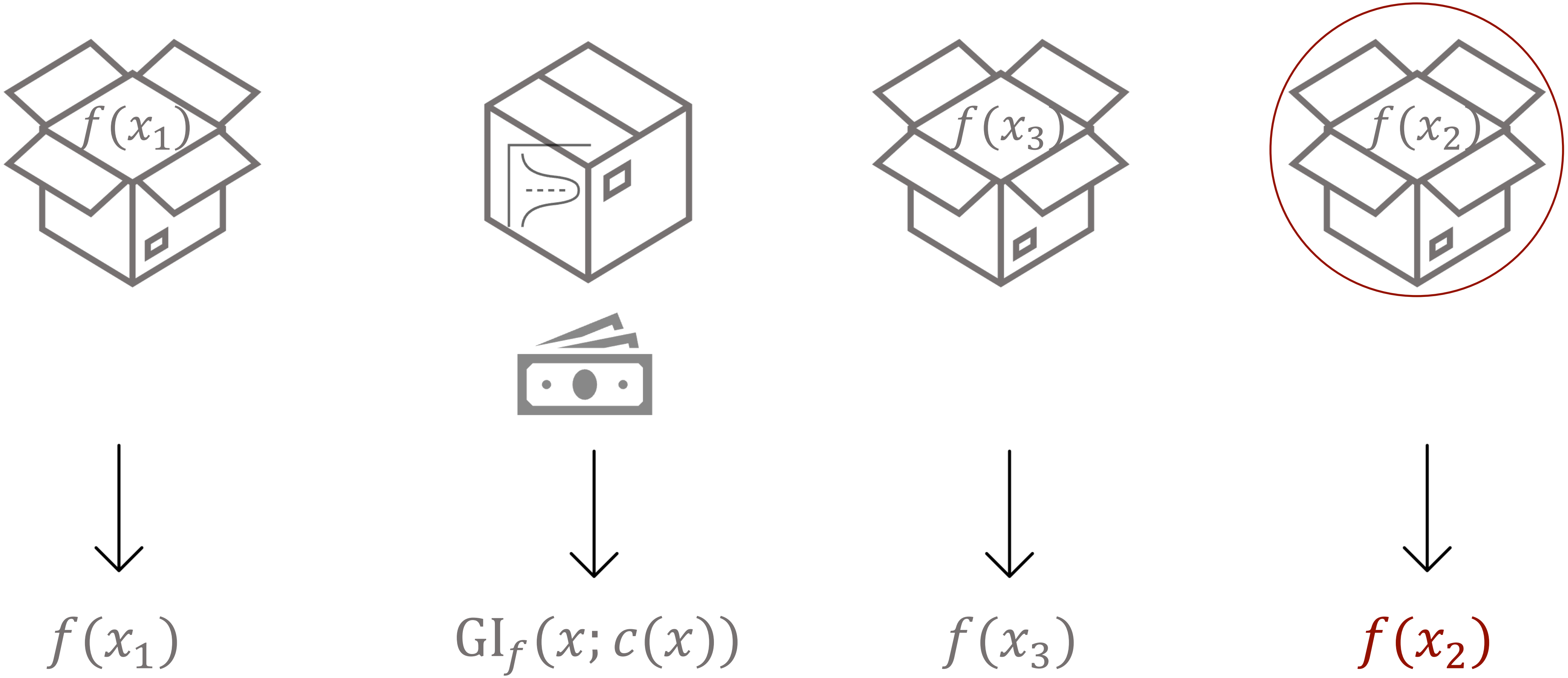
Optimal Policy: Gittins Index

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



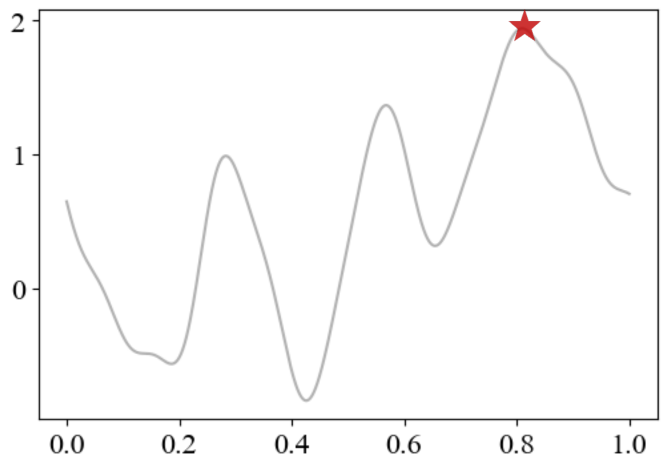
Optimal Policy: Gittins Index

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



Bayesian Optimization

$f(x)$



Continuous

Correlated

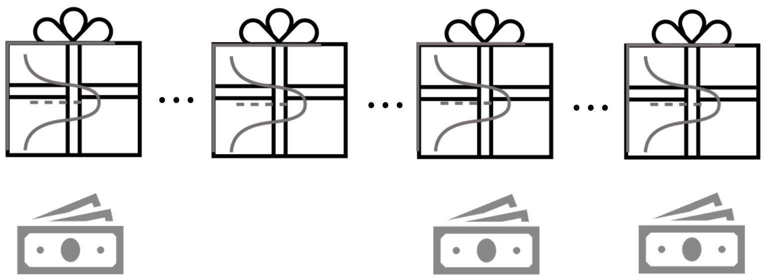
Fixed-budget / Flexible-stopping

Expected (cost-adjusted) regret

Is Gittins index good?

Pandora's Box

[Weitzman'79]



$f(x)$

$c(x)$

Discrete

Independent

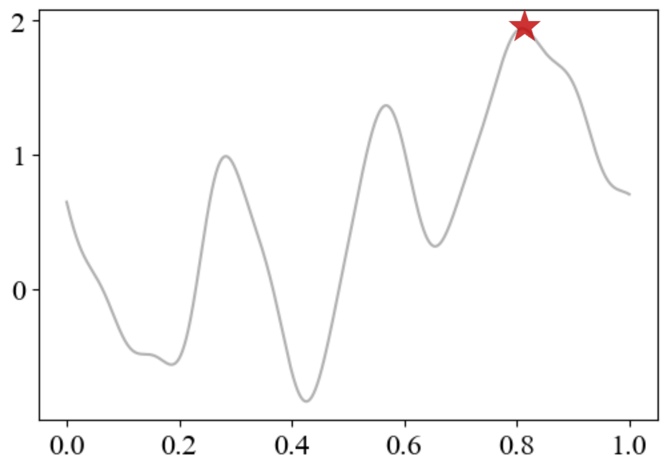
Flexible-stopping

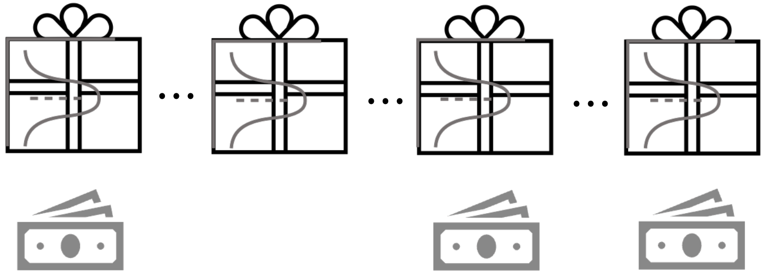
Expected cost-adjusted regret

Gittins index is optimal

Bayesian Optimization	Pandora's Box
	[Weitzman'79]

$f(x)$





$f(x)$

$c(x)$

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
empirically	

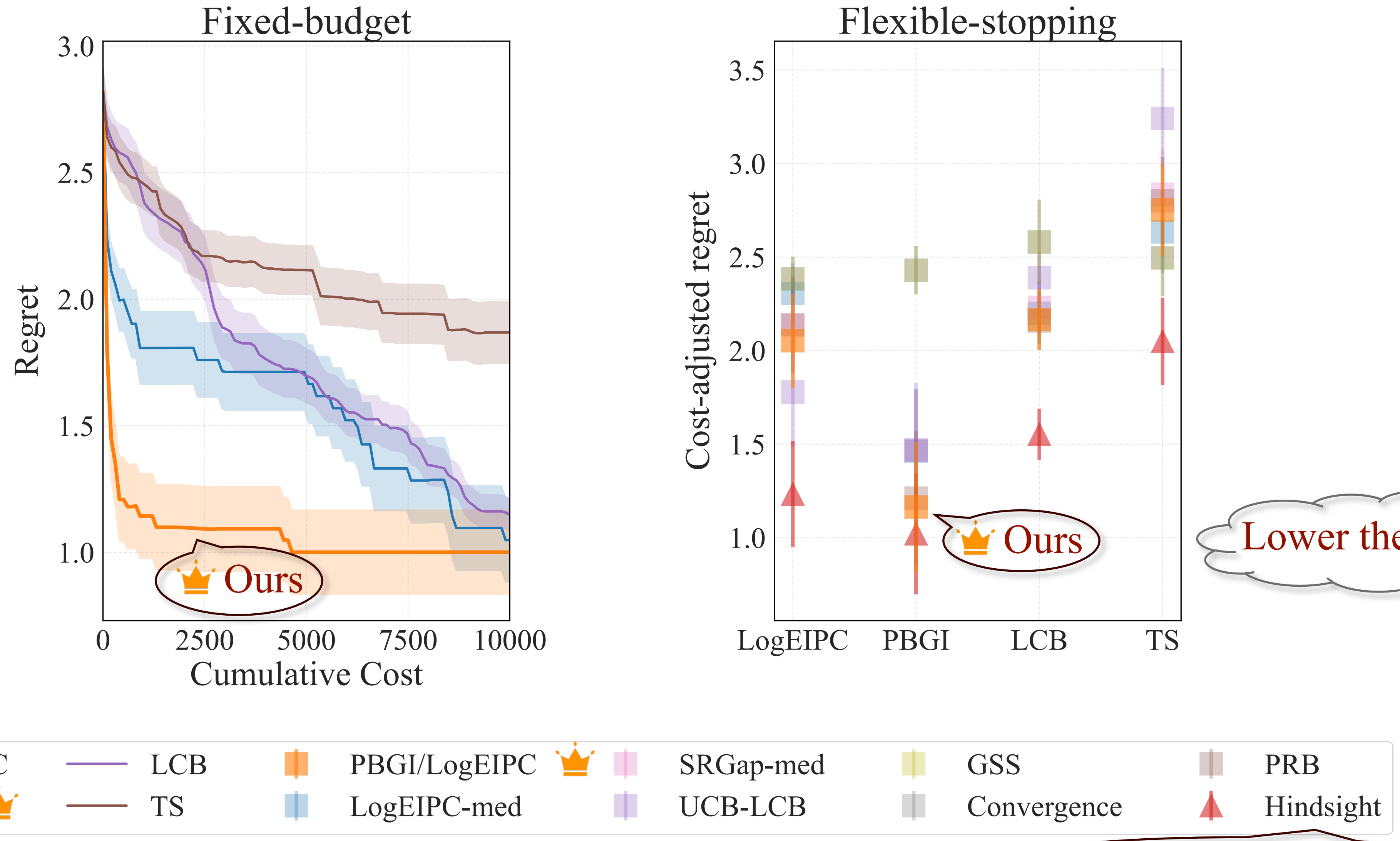
Our Contribution: Gittins Index Principle

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

? Why another principle?

1. Naturally incorporates side info and practical flexibility
2. Performs competitively on benchmarks
3. Comes with theoretical guarantees

Gittins Index vs Baselines on AutoML Benchmark

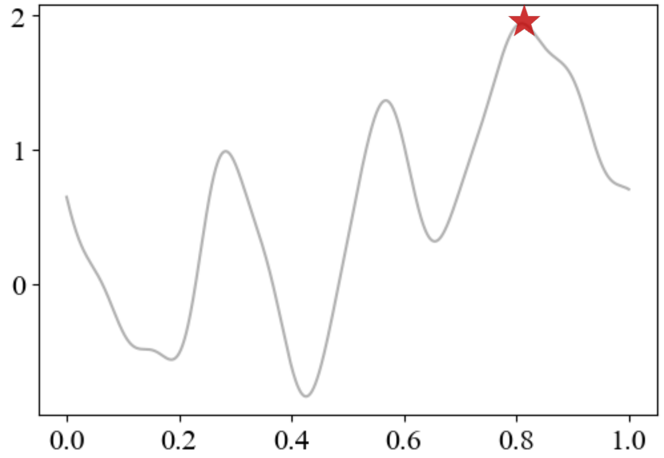


Lower the better

Bound on achievable performance

Bayesian Optimization

$f(x)$



Continuous

Correlated

Fixed-budget / Flexible-stopping

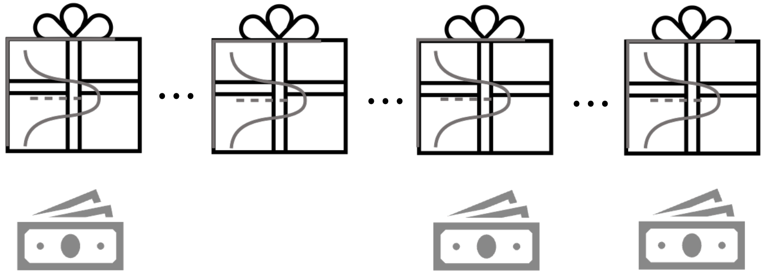
Expected (cost-adjusted) regret

Is Gittins index good?

theoretically

Pandora's Box

[Weitzman'79]



$f(x)$

$c(x)$

Discrete

Independent

Flexible-stopping

Expected cost-adjusted regret

Gittins index is optimal

Our Contribution: Gittins Index Principle

- Improvement-based (e.g., LogEIPC)
- Entropy-based
- Confidence bounds
- Thompson sampling
- Gittins Index

? Why another principle?

1. Naturally incorporates side info and practical flexibility
2. Performs competitively on benchmarks
3. Comes with theoretical guarantees

Theoretical Guarantee and Empirical Validation

Theorem (No worse than stopping-immediately)

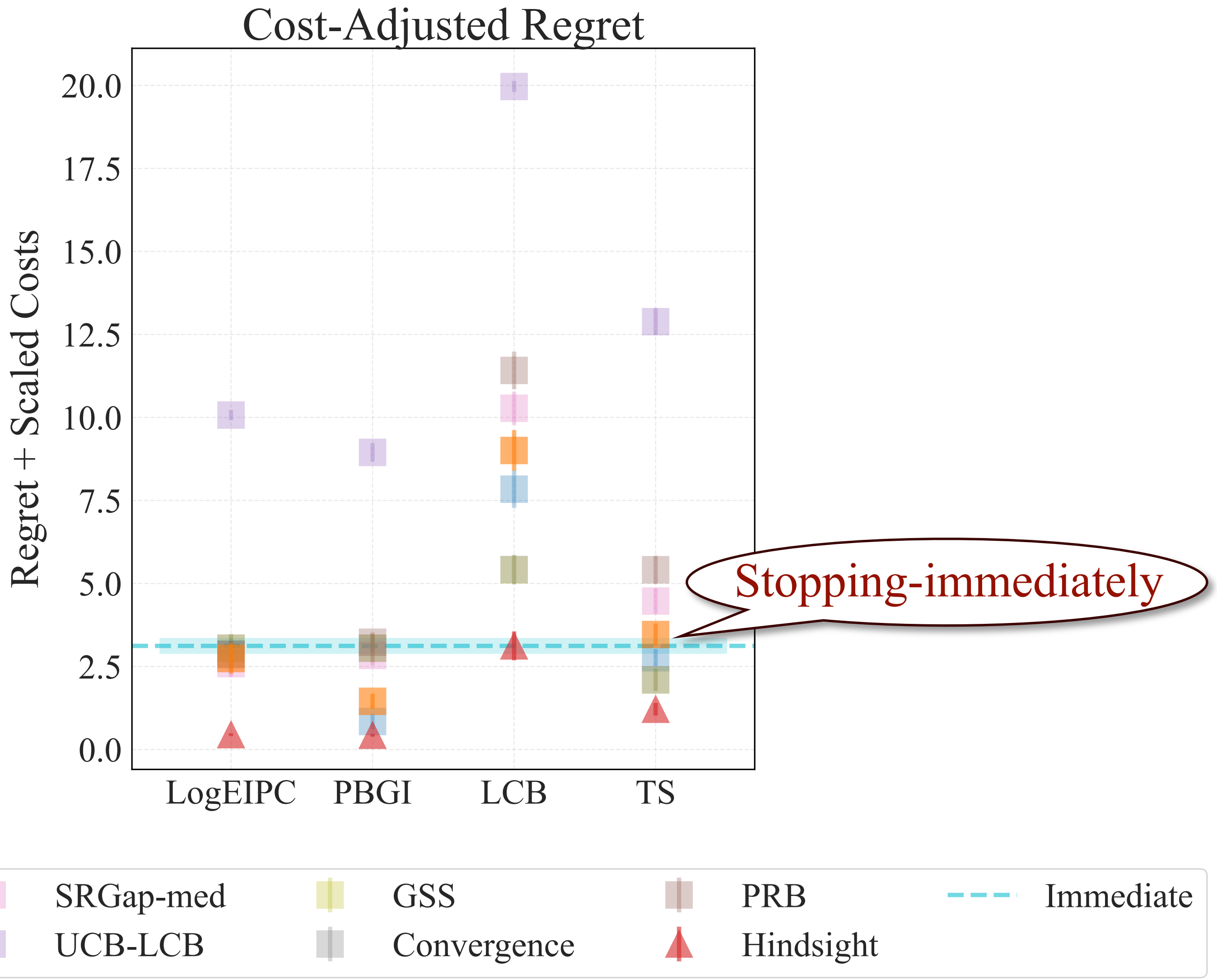
$$\mathbb{E}[R(\text{ours}; \text{PBGI})] \le R[\text{stopping immediately}]$$

or LogEIPC

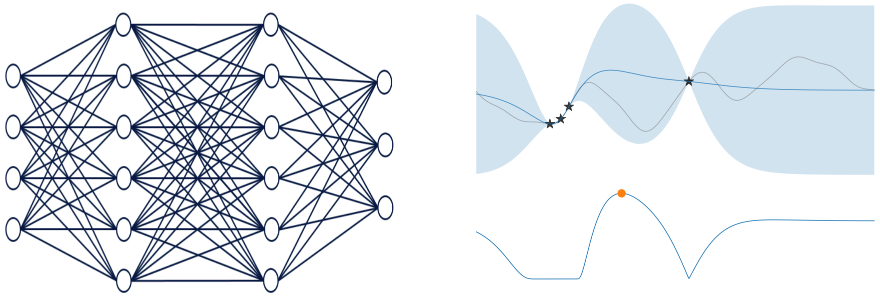
cost-adjusted regret

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.



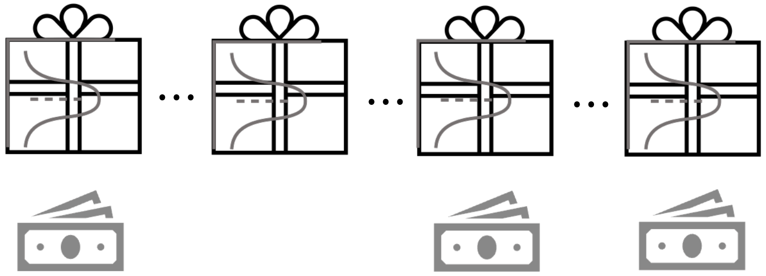
Studied problem



Varying evaluation costs

Adaptive stopping time

Key idea



Link to Pandora's Box problem
& Gittins index theory

Impact

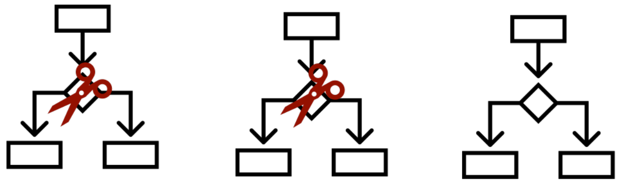
Meta

BoTorch Ax

Competitive empirical performance & interests from practitioners

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

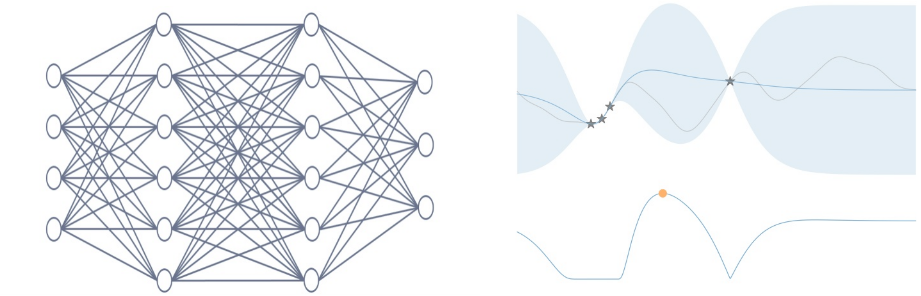
Ongoing work



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

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

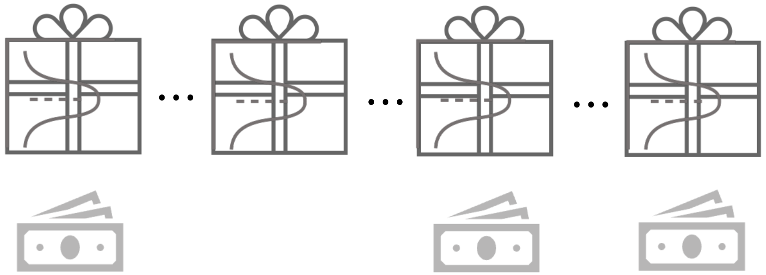
Studied problem



Varying evaluation costs

Adaptive stopping time

Key idea



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Ongoing work

ChatGPT Gemini

deepseek Claude

LLM-driven black-box optimization

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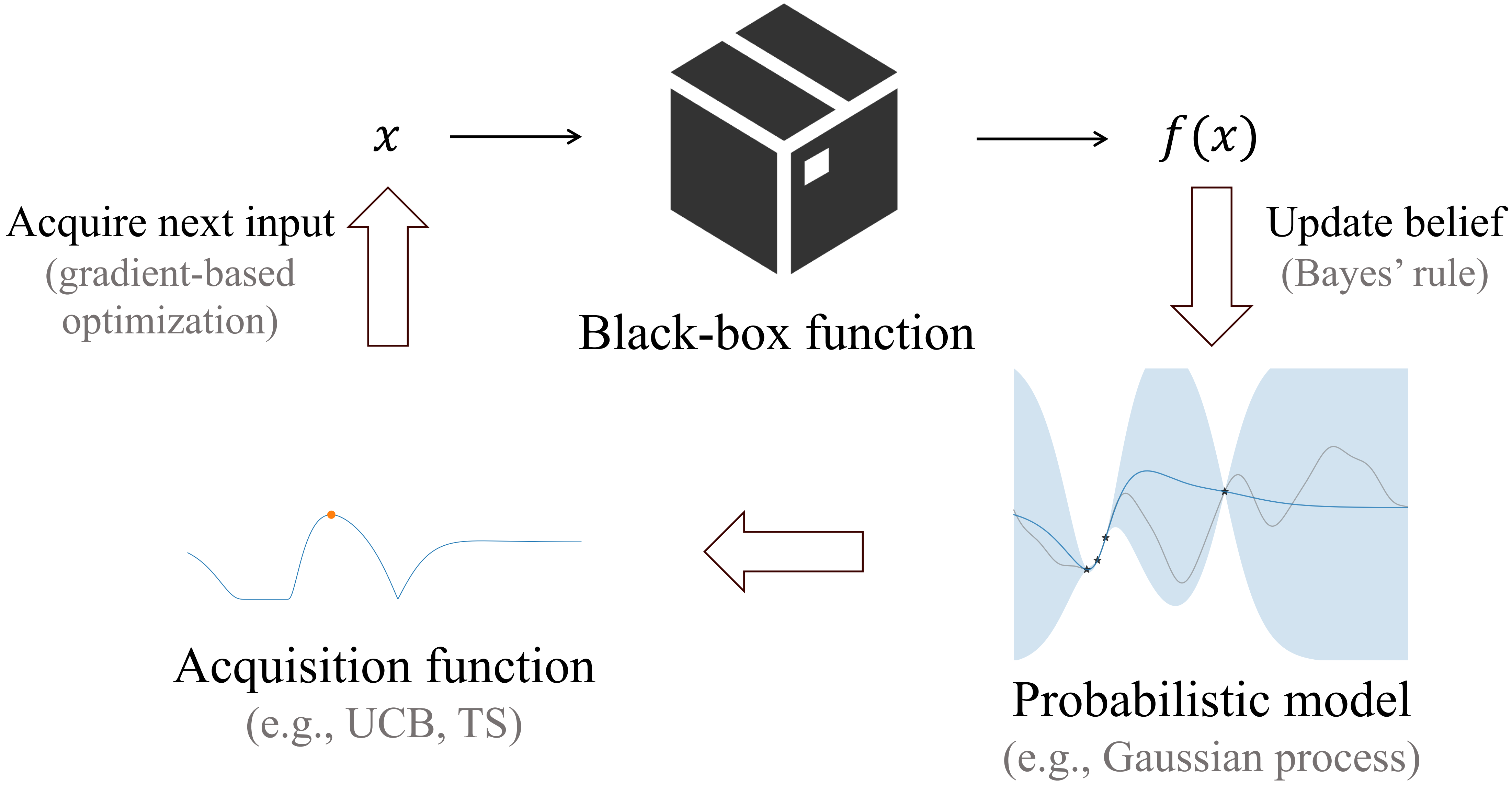
Recap: Bayesian Optimization



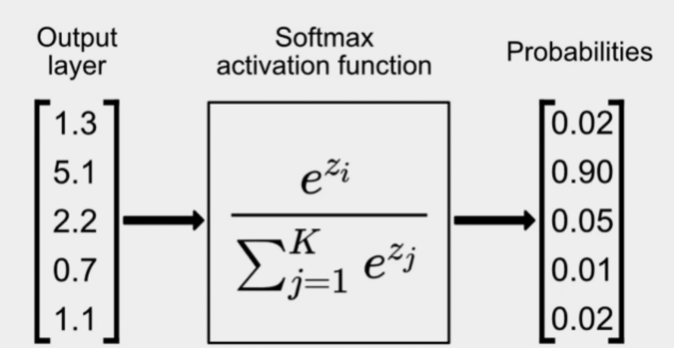
Ongoing: LLM-Driven Black-Box Optimization

x →  → $f(x)$

Acquire next input
(LLM proposal)

Black-box function

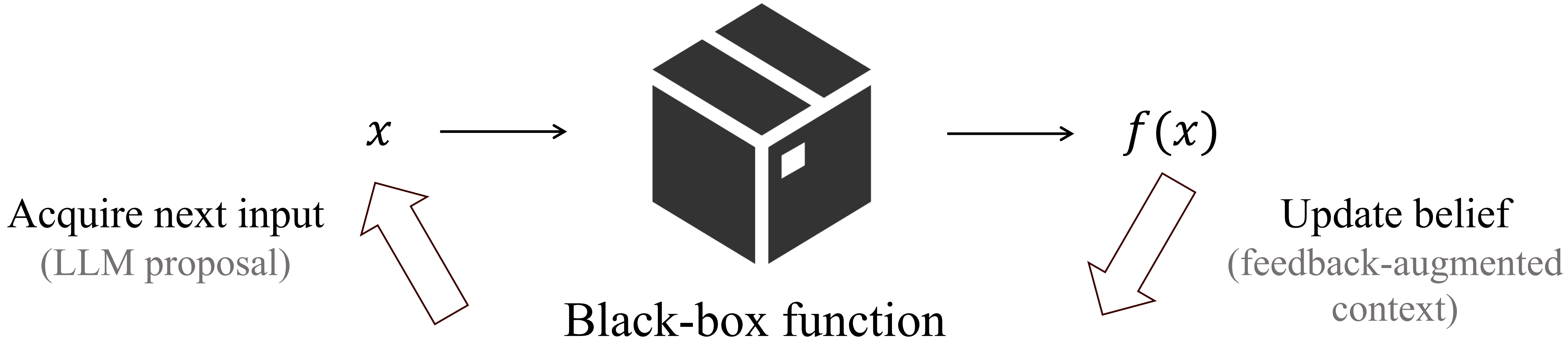
Update belief
(feedback-augmented context)



Acquisition function
(e.g., Softmax sampling)

Probabilistic model
(e.g., autoregressive model)

Ongoing: LLM-Driven Black-Box Optimization



ChatGPT Gemini

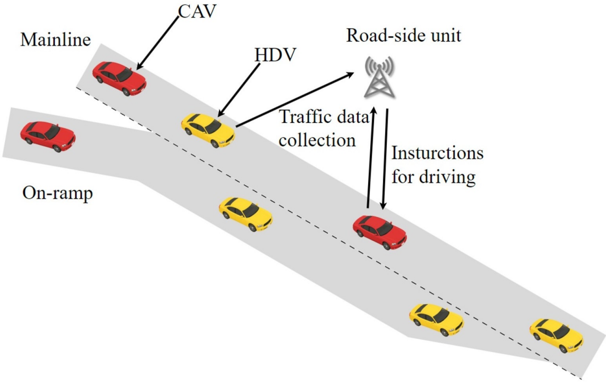
deepseek Claude

Large language model

Ongoing: LLM-Driven Black-Box Optimization

Mixed-autonomy traffic control:

(e.g., Transformer config)
RL state representation



Average speed

Acquire next input
(LLM proposal)

Update belief
(feedback-augmented context)

Black-box function
(RL training & evaluation)

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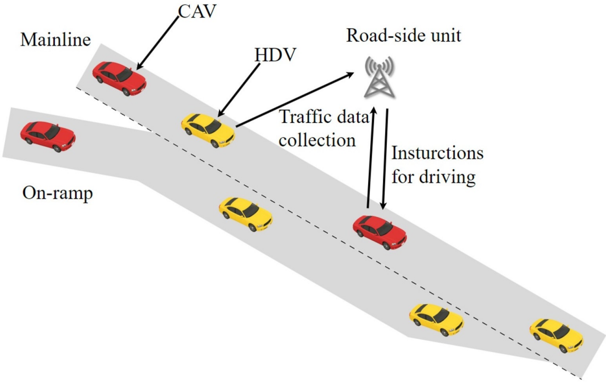
Large language model

Ongoing: LLM-Driven Black-Box Optimization

Mixed-autonomy traffic control:

(e.g., Transformer config)
RL state representation



Average speed

Acquire next input
(LLM proposal)

Update belief
(feedback-augmented context)

Black-box function
(RL training & evaluation)

Can side info help?

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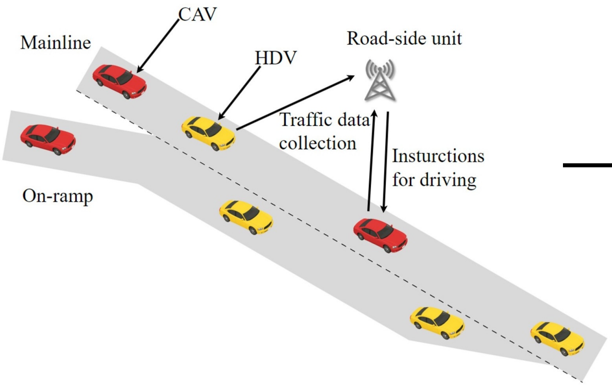
Large language model

Our LLM-Driven Method: Incorporate Side Info

Mixed-autonomy traffic control:

(e.g., Transformer config)
RL state representation



Average speed

Acquire next input
(LLM proposal)

Update belief
(feedback-augmented context)

Black-box function
(RL training & evaluation)

performance metric + representation quality

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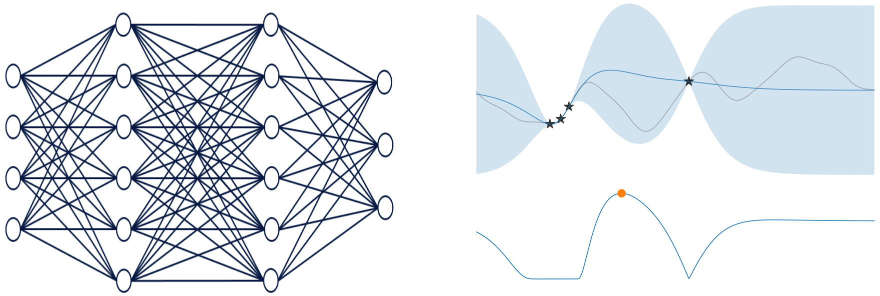
Large language model

Studied problem



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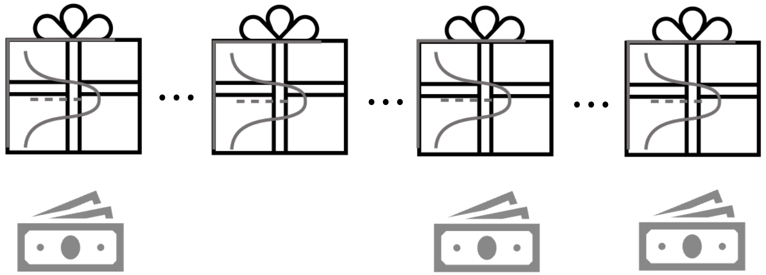
Adaptive stopping time

Key idea



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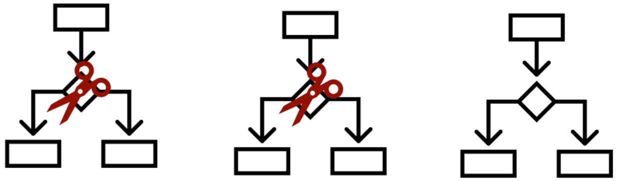

Black-box optimization w/ side info

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