Cost-Aware Bayesian Optimization with Adaptive Stopping via Gittins Indices

Qian Xie 谢倩 (Cornell ORIE)

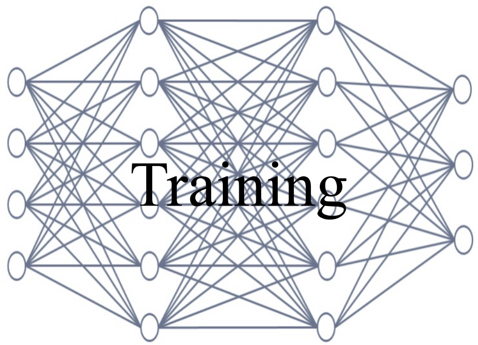
Joint work with Linda Cai (UC Berkeley), Raul Astudillo (MBZUAI), Theodore Brown (UCL), Peter Frazier, Alexander Terenin, Ziv Scully (Cornell), Yu Yu and Li Jin (SJTU)

INFORMS Annual Meeting 2025 Job Market Showcase

Optimization Under Uncertainty

ML model training:

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



⟶ Accuracy

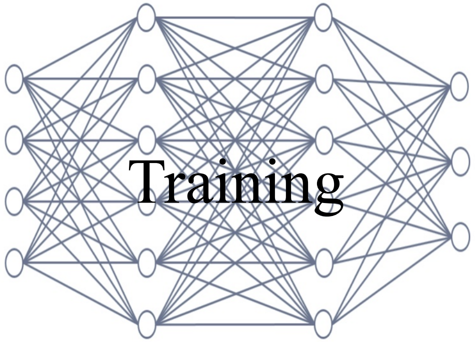
Optimization Under Uncertainty

Black-box optimization:

non-analytical & no gradient info

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

ML model training:

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

$\longrightarrow$ Accuracy

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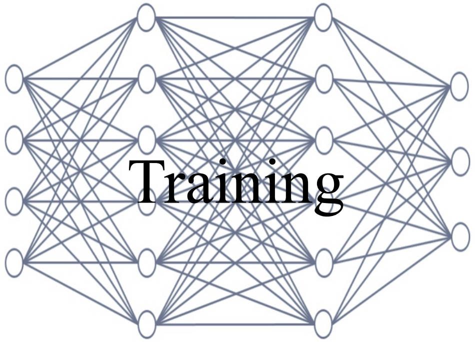
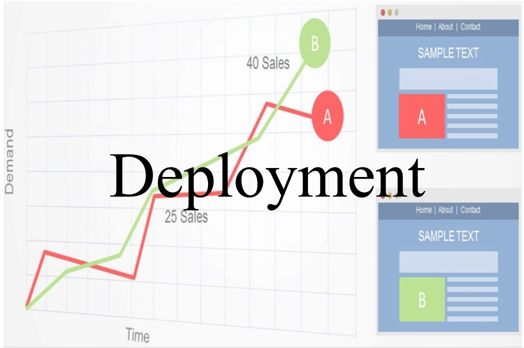
Training hyperparameters (e.g., learning rate, # layers) ⟶  Training ⟶ Accuracy

Adaptive experimentation:

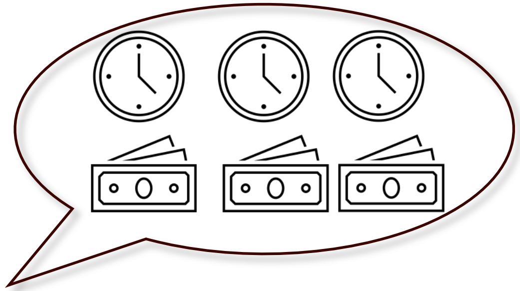
Decision/design variables (e.g., layout, pricing level) ⟶ 

Deployment ⟶ Revenue

Black-Box Optimization

expensive-to-evaluate

Input x ⟶ ⟶ Performance metric $f(x)$

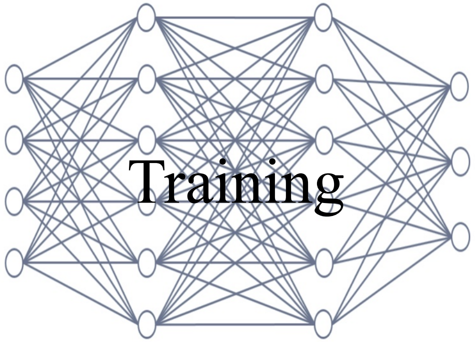


Training time

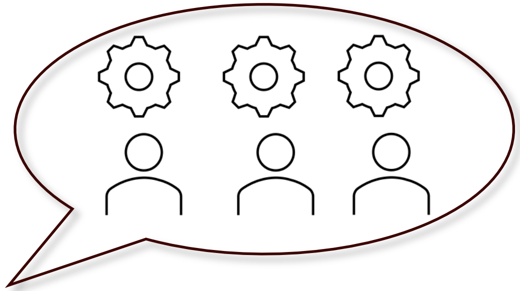
Compute credits

ML model training:

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



⟶ Accuracy

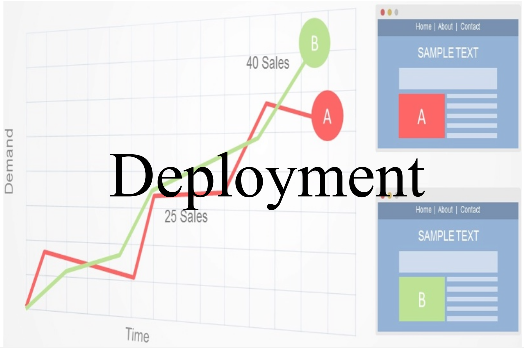


Operational cost

User experience

Adaptive experimentation:

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



⟶ Revenue

Black-Box Optimization

expensive-to-evaluate

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

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

Data-Driven Black-Box Optimization

Input x $\longrightarrow$

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

expensive-to-evaluate

adaptively

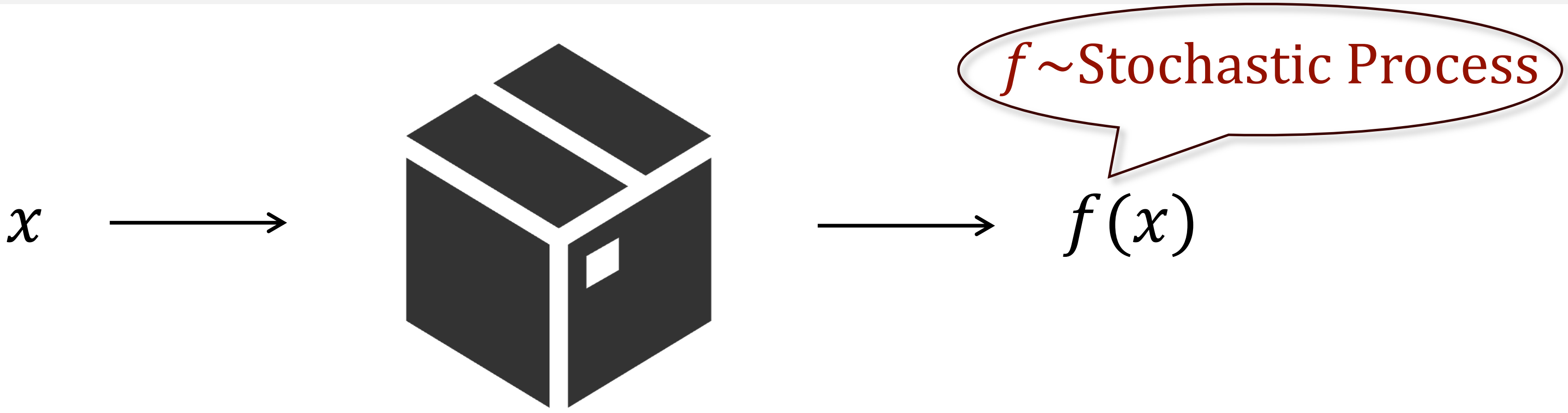
High-level goal: Choose $x_1, \dots, x_T$ to maximize the expected best observed value

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

Fewer #evaluations

Efficient framework: Bayesian optimization

Bayesian Optimization



Black-box function

Bayesian Optimization

Time 0

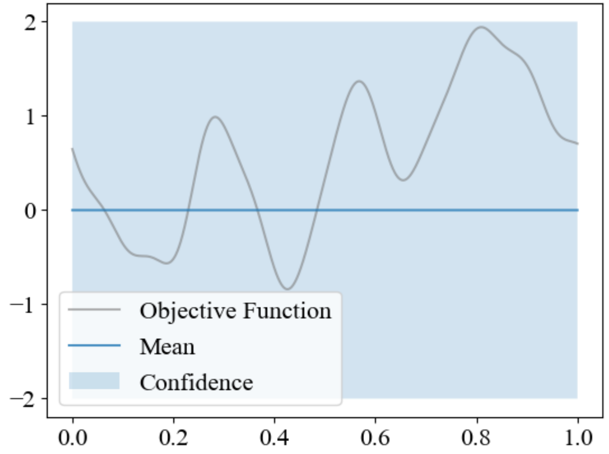
x $\longrightarrow$

$\longrightarrow$ $f(x)$

$f \sim$Stochastic Process

Black-box function

Model belief



Probabilistic model

(e.g., Gaussian process)

Bayesian Optimization

Time t

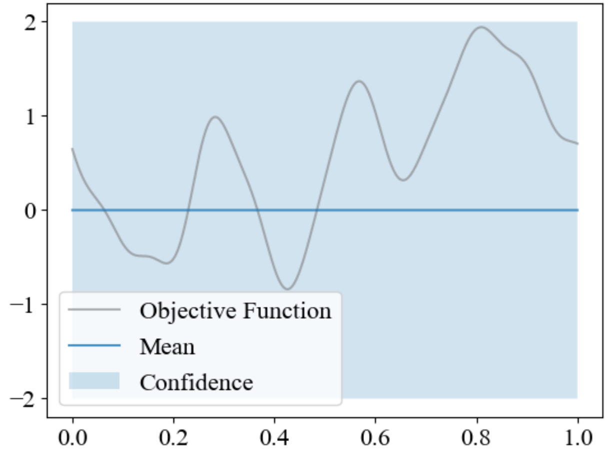
$x_1, \ldots, x_t$ →

Black-box function

→ $f(x_1), \ldots, f(x_t)$

$f \sim$ Stochastic Process

Model belief



Probabilistic model
(e.g., Gaussian process)

Bayesian Optimization

Time t

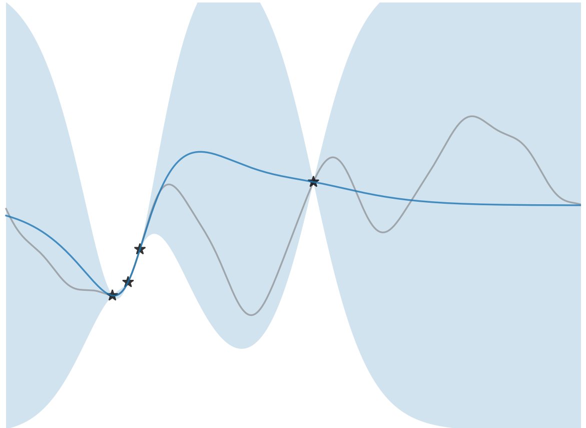
$x_1, \ldots, x_t \longrightarrow$

Black-box function

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

$f \sim$Stochastic Process

Update belief
(Bayes' rule)



Probabilistic model
(e.g., Gaussian process)

Bayesian Optimization

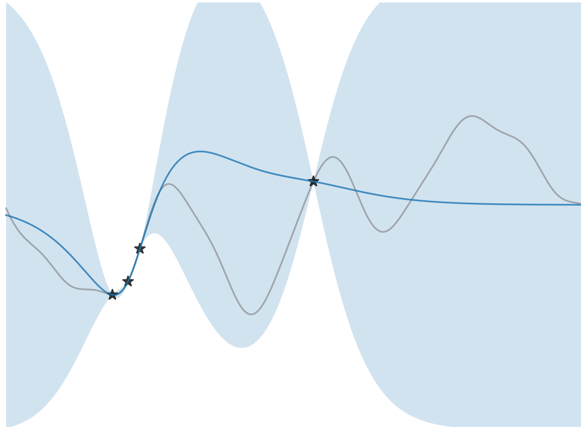
Time t

$x_1, \ldots, x_t$

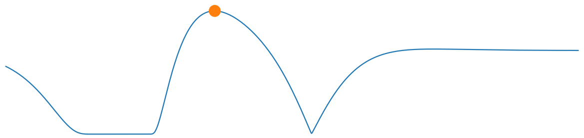
Black-box function

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

Update belief
(Bayes' rule)



Probabilistic model
(e.g., Gaussian process)



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

scoring (worth
of each point

Bayesian Optimization

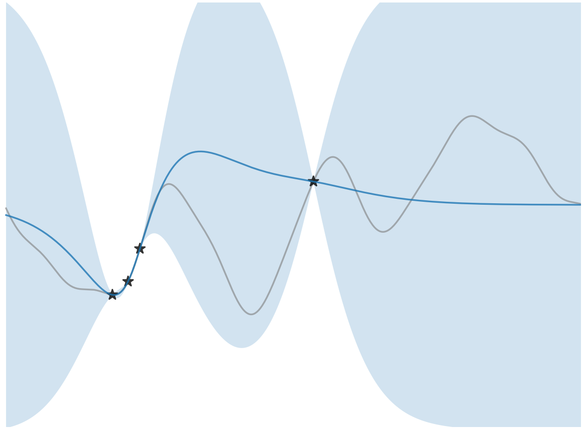
Time t

$x_1, \ldots, x_t \longrightarrow$

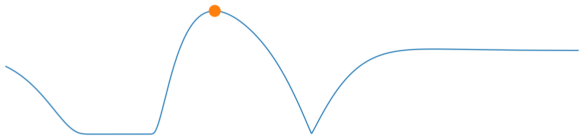
Black-box function

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

Update belief
(Bayes' rule)



Probabilistic model
(e.g., Gaussian process)



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

scoring (worth of each point

Acquire next data
(gradient-based optimization)

Bayesian Optimization

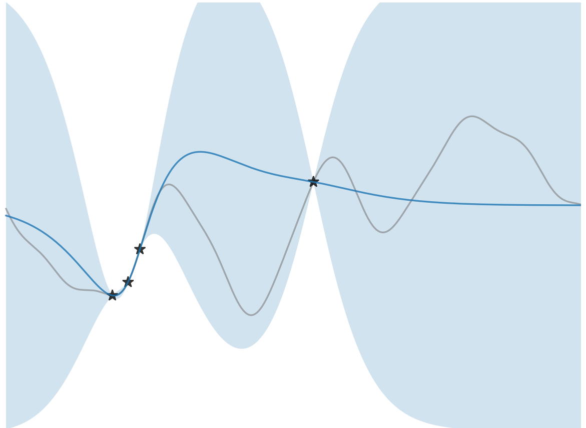
Time $t+1$

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

Black-box function

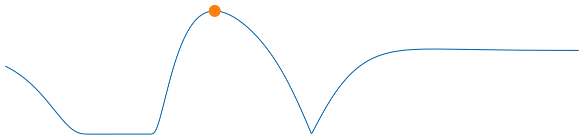
$\longrightarrow f(x_1), \ldots, f(x_{t+1})$

Update belief
(Bayes' rule)



Probabilistic model
(e.g., Gaussian process)

scoring (worth of each point



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

Acquire next data
(gradient-based optimization)

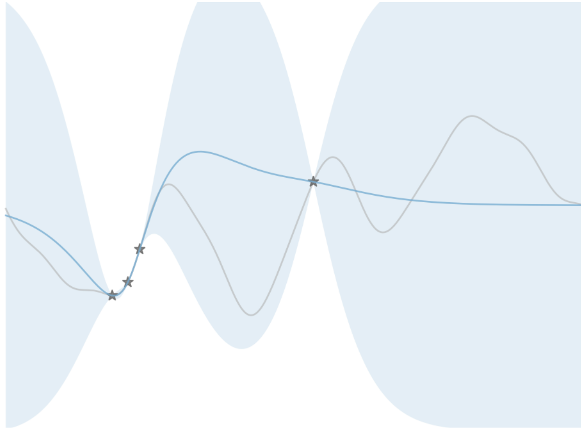
Bayesian Optimization

$x \longrightarrow$

Black-box function

$\longrightarrow f(x)$

Update belief
(Bayes' rule)



Probabilistic model
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scoring (worth
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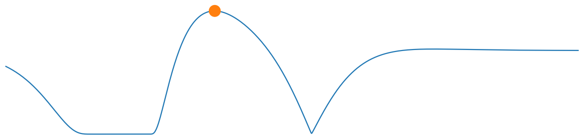

Acquisition function
(e.g., UCB, TS)

My focus

Acquire next data
(gradient-based
optimization)

Existing Design Principles

- Improvement-based
- Entropy-based
- Confidence bounds (UCB/LCB)
- Thompson sampling

New Design Principle: Gittins Index

- Improvement-based
- Entropy-based
- Confidence bounds (UCB/LCB)
- Thompson sampling (TS)
- Gittins Index

New Design Principle: Gittins Index

- Improvement-based
- Entropy-based
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? Why another principle?

Our Contribution: Gittins Index Principle

- Improvement-based
- Entropy-based
- Confidence bounds (UCB/LCB)
- Thompson sampling
- Gittins Index

? Why another principle?

1. Naturally handles practical considerations
2. Performs competitively on benchmarks
3. Comes with theoretical guarantees

Our Contribution: Gittins Index Principle

- Improvement-based
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- Confidence bounds (UCB/LCB)
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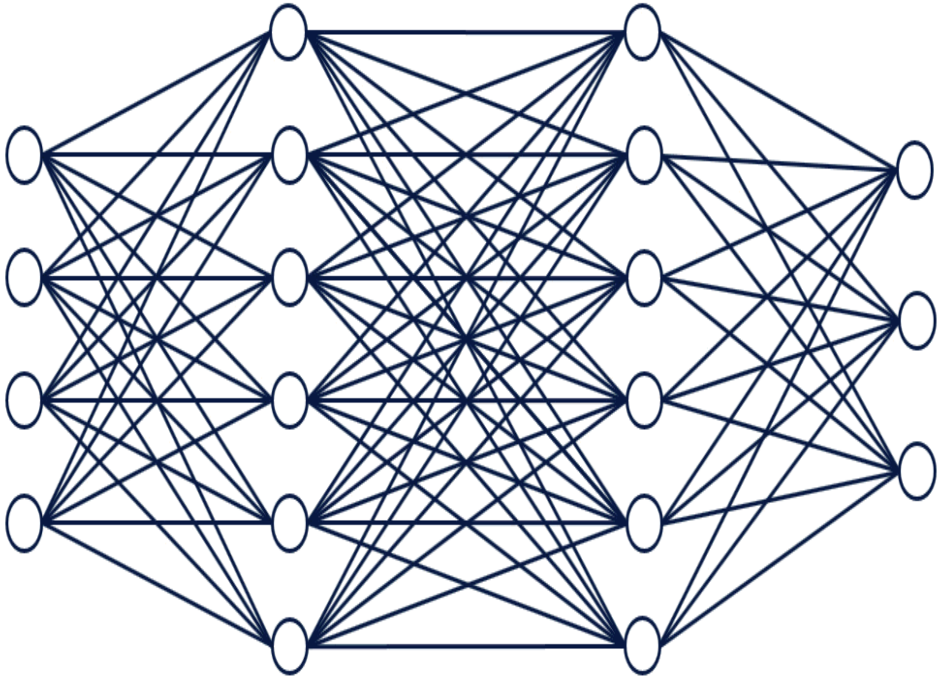
1. Naturally handles practical considerations
2. Performs competitively on benchmarks
3. Comes with theoretical guarantees

Under-explored Practical Considerations

Varying evaluation costs

Smart stopping time

Observable multi-stage feedback



Under-explored Practical Considerations

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

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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

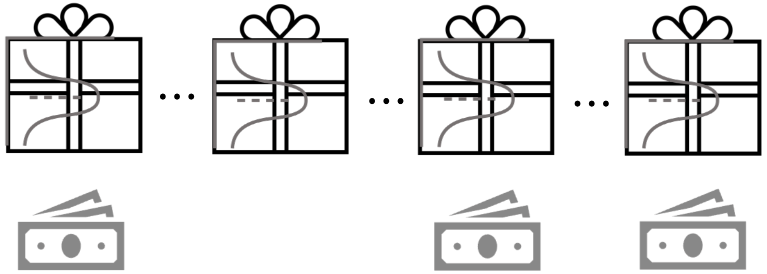
Features in Pandora's box

Observable multi-stage feedback

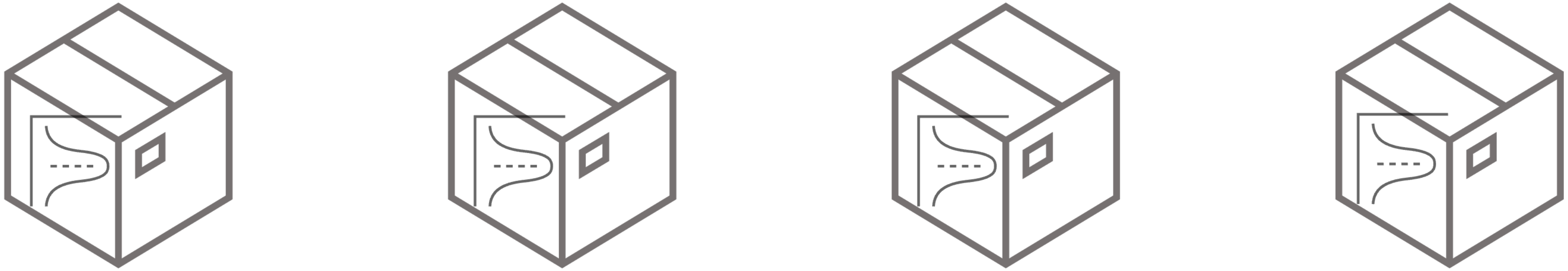
Features in Markovian bandits

New design principle:
Gittins index

Optimal in related sequential decision problems



Pandora's Box



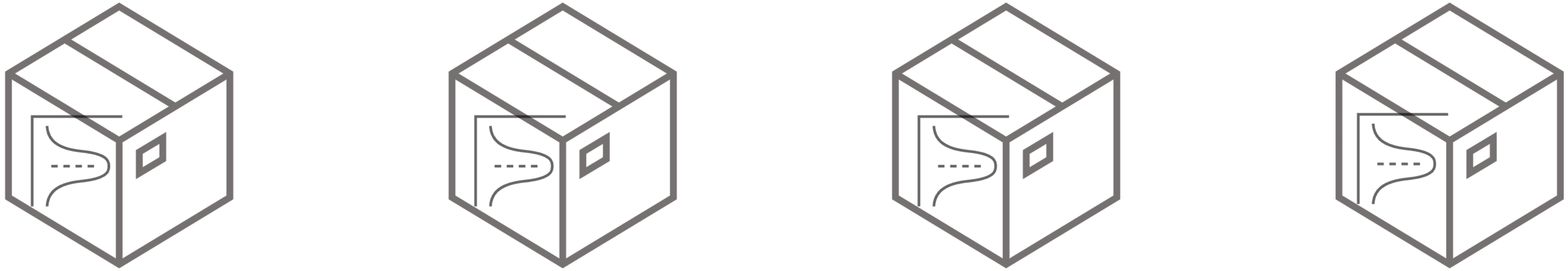
High-level goal: Choose $x_1, \dots, x_T$ to maximize the expected utility

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

Flexible stopping time

Pandora's Box

$t = 0$



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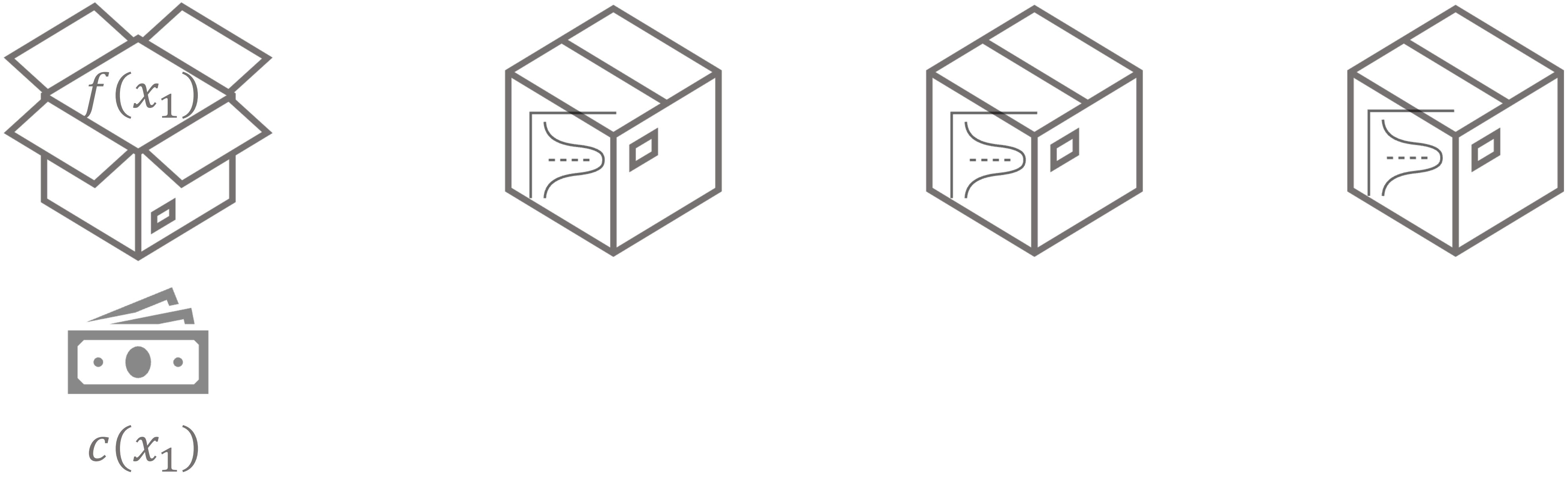
Pandora's Box

$t = 1$

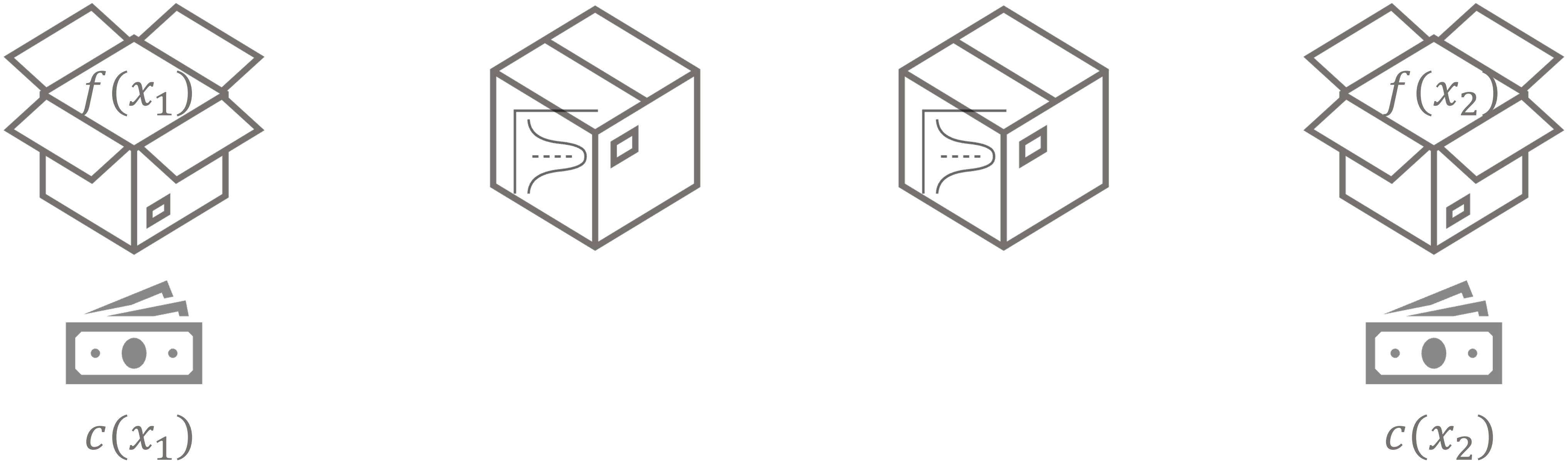


High-level goal: Choose $x_1, \dots, x_T$ to maximize the expected utility

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

Pandora's Box

$t = 2$

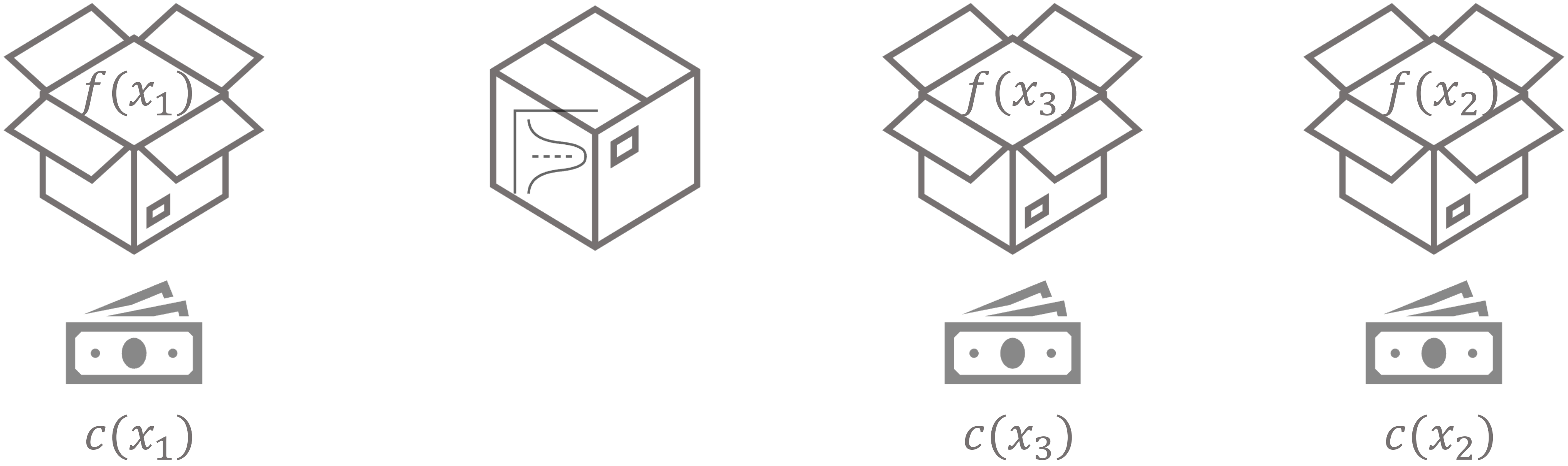


High-level goal: Choose $x_1, \ldots, x_T$ to maximize the expected utility

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

Pandora's Box

$t = 3$

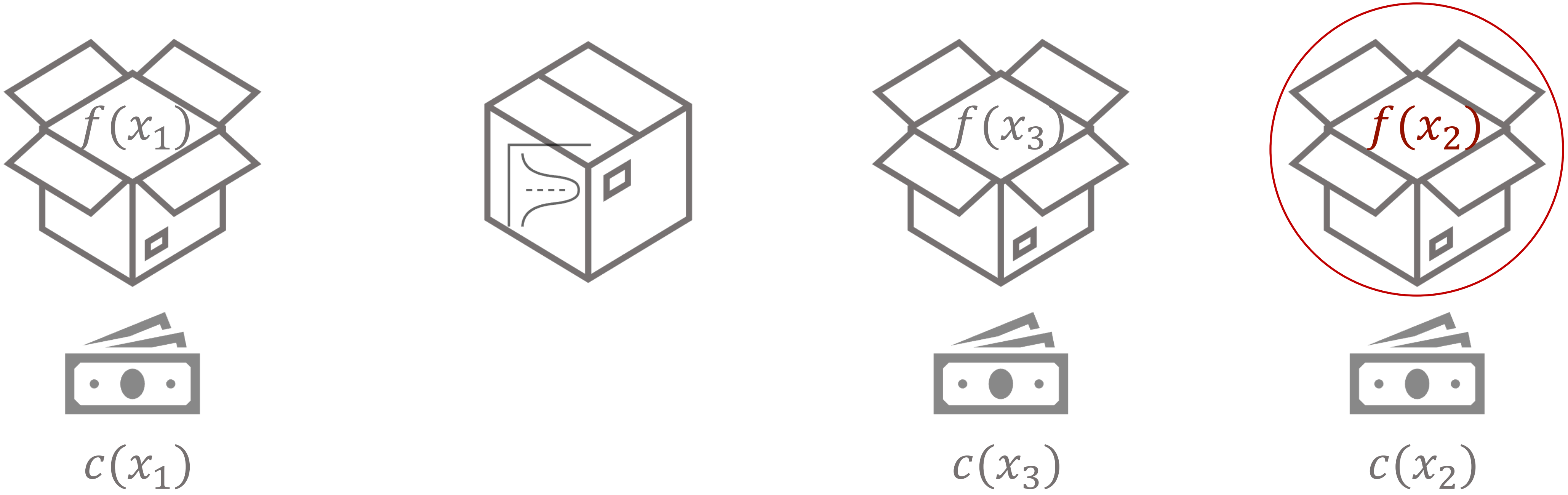


High-level goal: Choose $x_1, \ldots, x_T$ to maximize the expected utility

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

Pandora's Box

$t = T$, stop

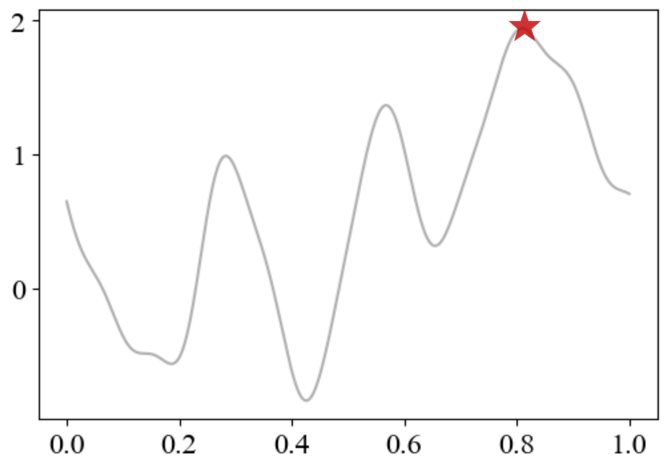


High-level goal: Choose $x_1, \ldots, x_T$ to maximize the expected utility

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

Bayesian Optimization

$f(x)$



Continuous

Correlated

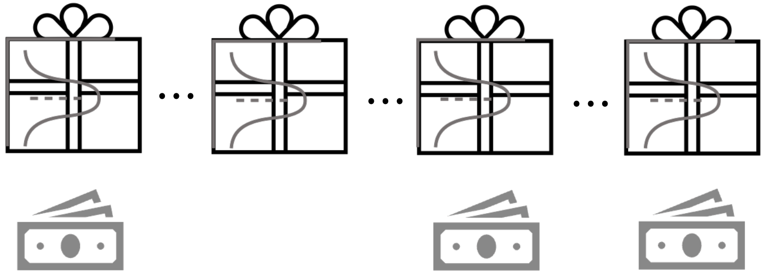
Fixed-iteration

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

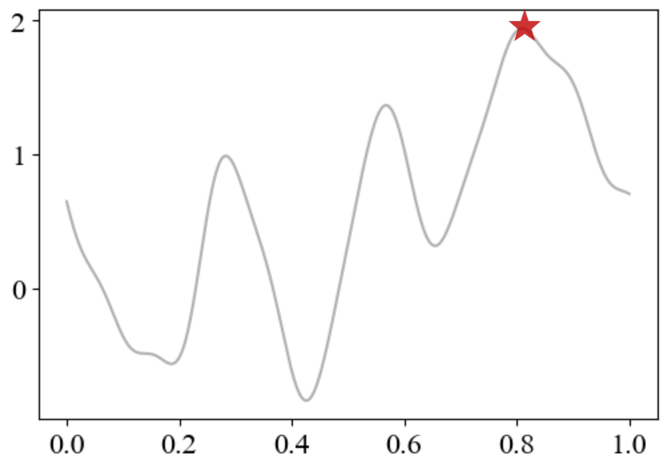
Flexible-stopping

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

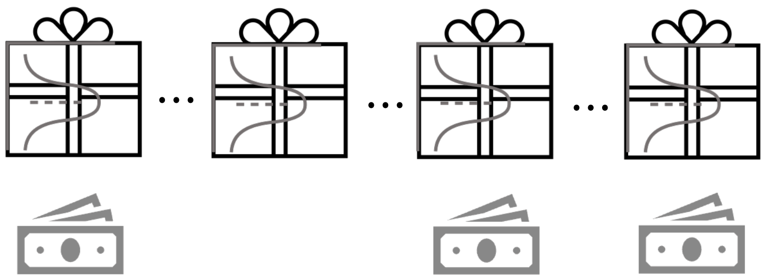
Fixed-iteration

Expected best-observed value

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

Pandora's Box

[Weitzman'79]



$f(x)$

$c(x)$

Discrete

Independent

Flexible-stopping

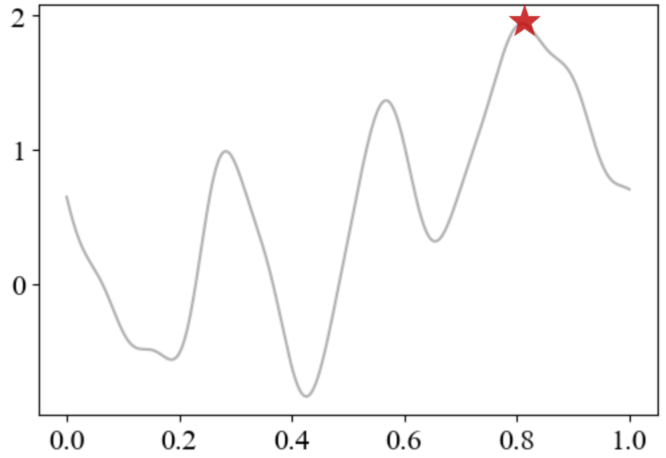
Expected utility

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

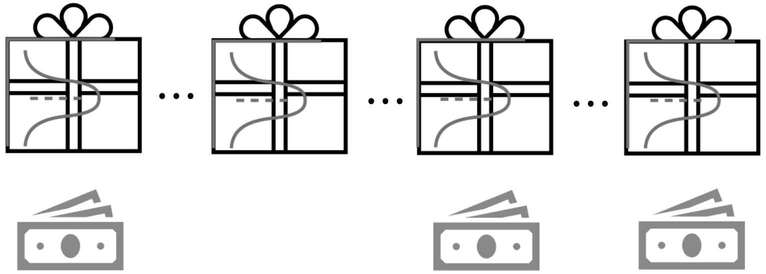
Fixed-iteration

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 utility

cumulative cost

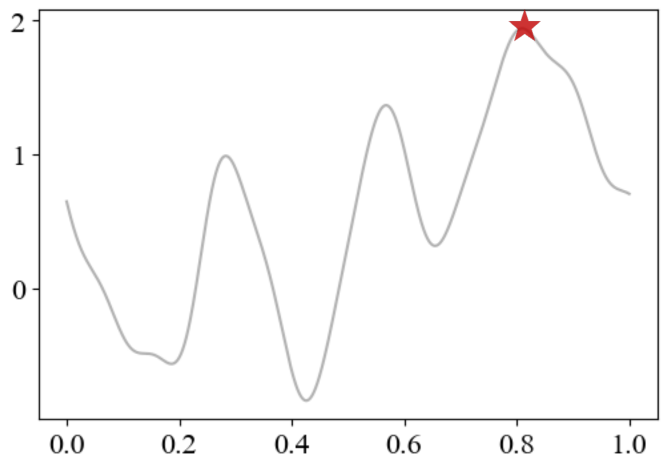
$$\mathbb{E} \max_{t=1,2,\ldots,T} f(x_t) - \mathbb{E} \sum_{t=1}^{T} c(x_t)$$

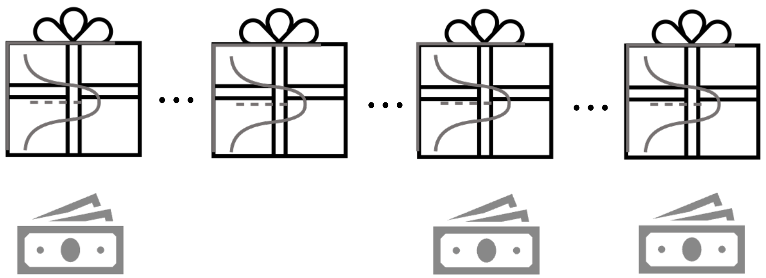
Bayesian Optimization

Pandora's Box

[Weitzman'79]

$f(x)$





$f(x)$

$c(x)$

Bayesian Optimization	Pandora's Box
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

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

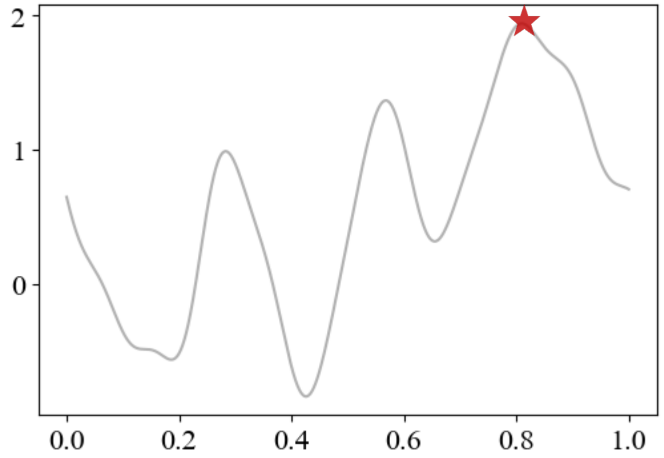
cumulative cost

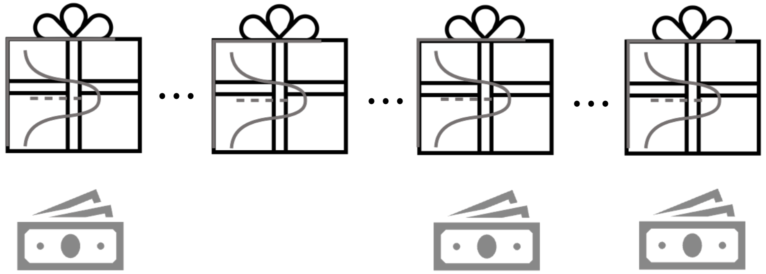
Bayesian Optimization

Pandora's Box

[Weitzman'79]

$f(x)$



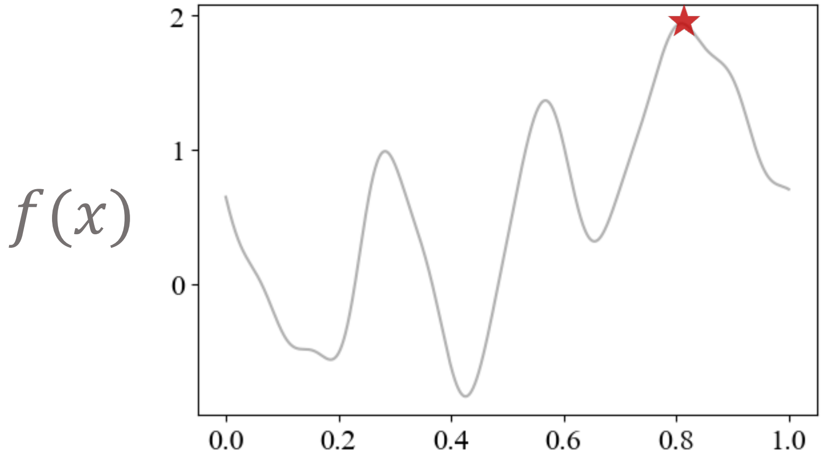


$f(x)$

$c(x)$

Continuous	Discrete
Correlated	Independent
Fixed-budget / Flexible-stopping	Flexible-stopping
Expected (cost-adjusted) regret	Expected cost-adjusted regret

Bayesian Optimization



Continuous

Correlated

Fixed-budget / Flexible-stopping

Expected (cost-adjusted) regret

Pandora's Box

[Weitzman'79]

Discrete

Independent

Flexible-stopping

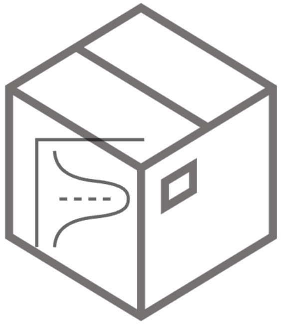
Expected cost-adjusted regret

Optimal policy: Gittins index

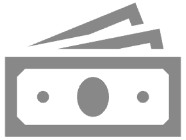
Optimal Policy: Gittins Index

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

$f(x)$

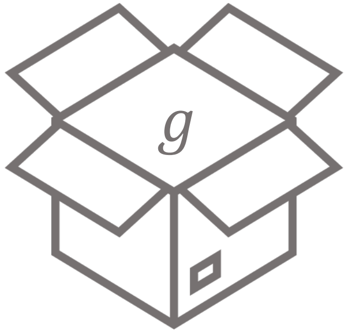


$c(x)$



$\downarrow$

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

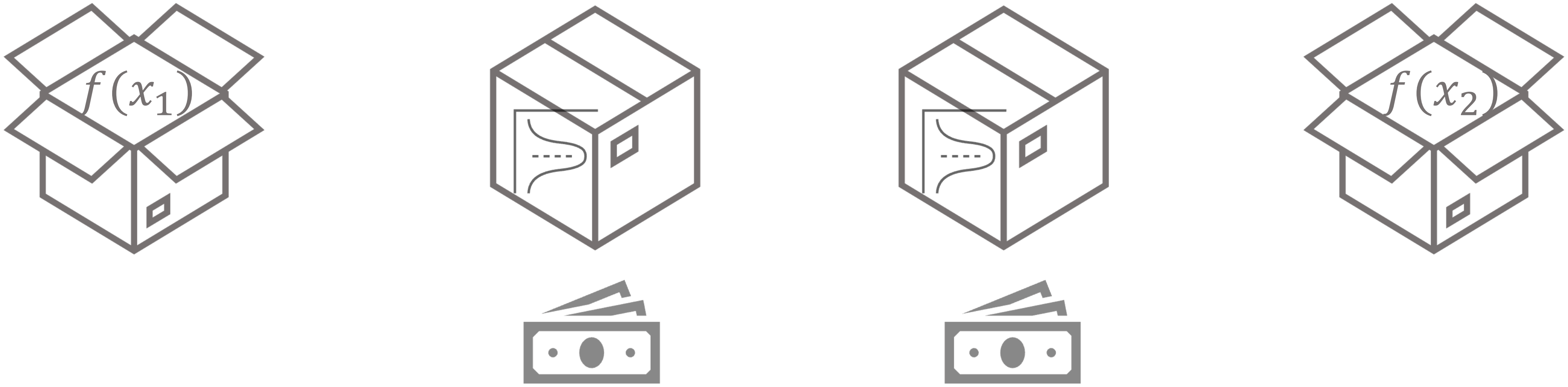


$\downarrow$

g

Optimal Policy: Gittins Index

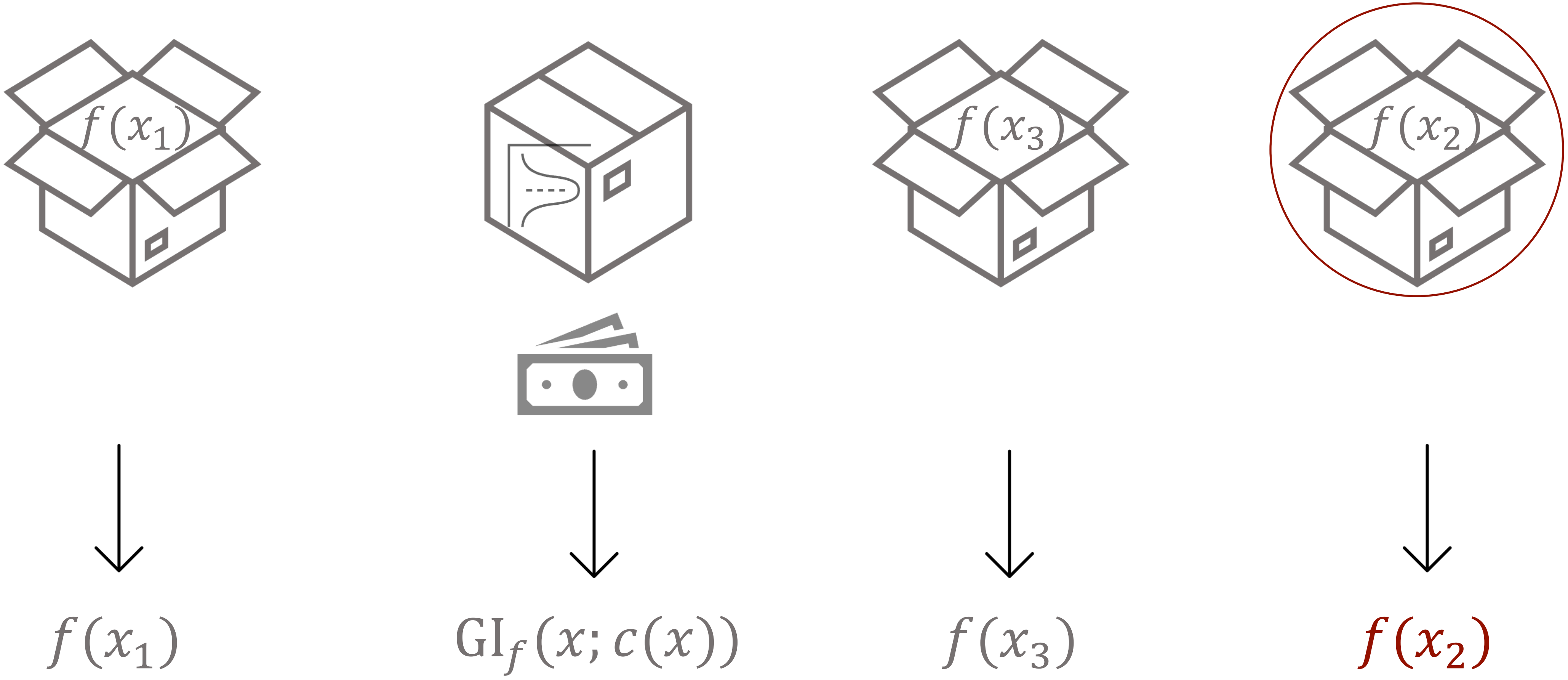
Step 2: Open the box with highest index if it is closed



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

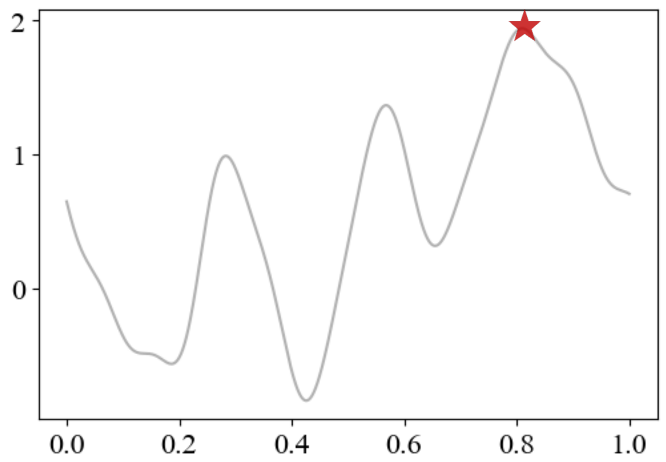
Optimal Policy: Gittins Index

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



Bayesian Optimization

$f(x)$



Continuous

Correlated

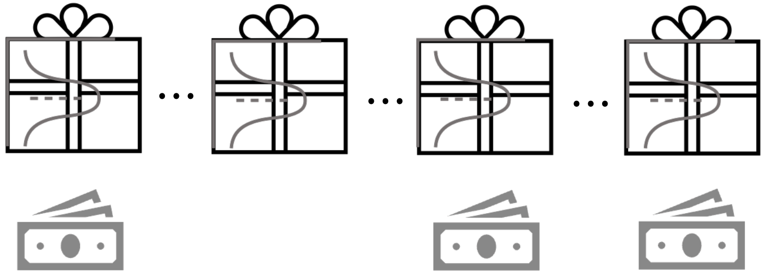
Fixed-budget / Flexible-stopping

Expected (cost-adjusted) regret

Is Gittins index good?

Pandora's Box

[Weitzman'79]



$f(x)$

$c(x)$

Discrete

Independent

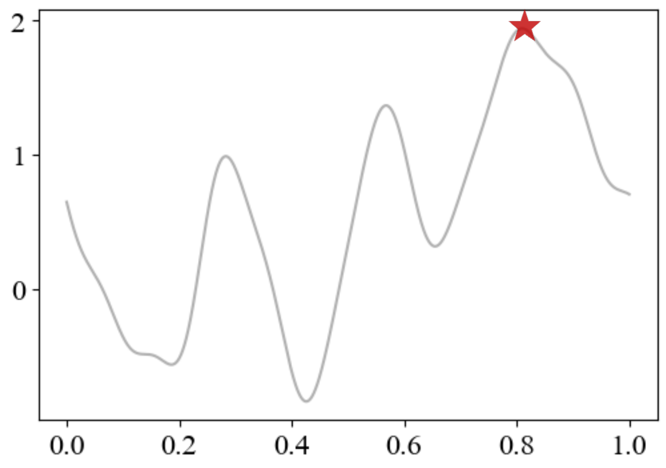
Flexible-stopping

Expected cost-adjusted regret

Gittins index is optimal

Bayesian Optimization

$f(x)$



Continuous

Correlated

Fixed-budget / Flexible-stopping

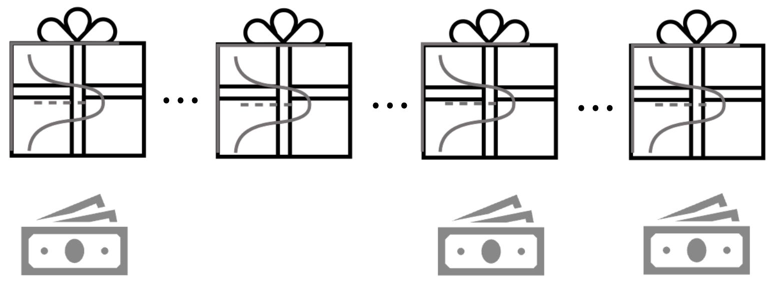
Expected (cost-adjusted) regret

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

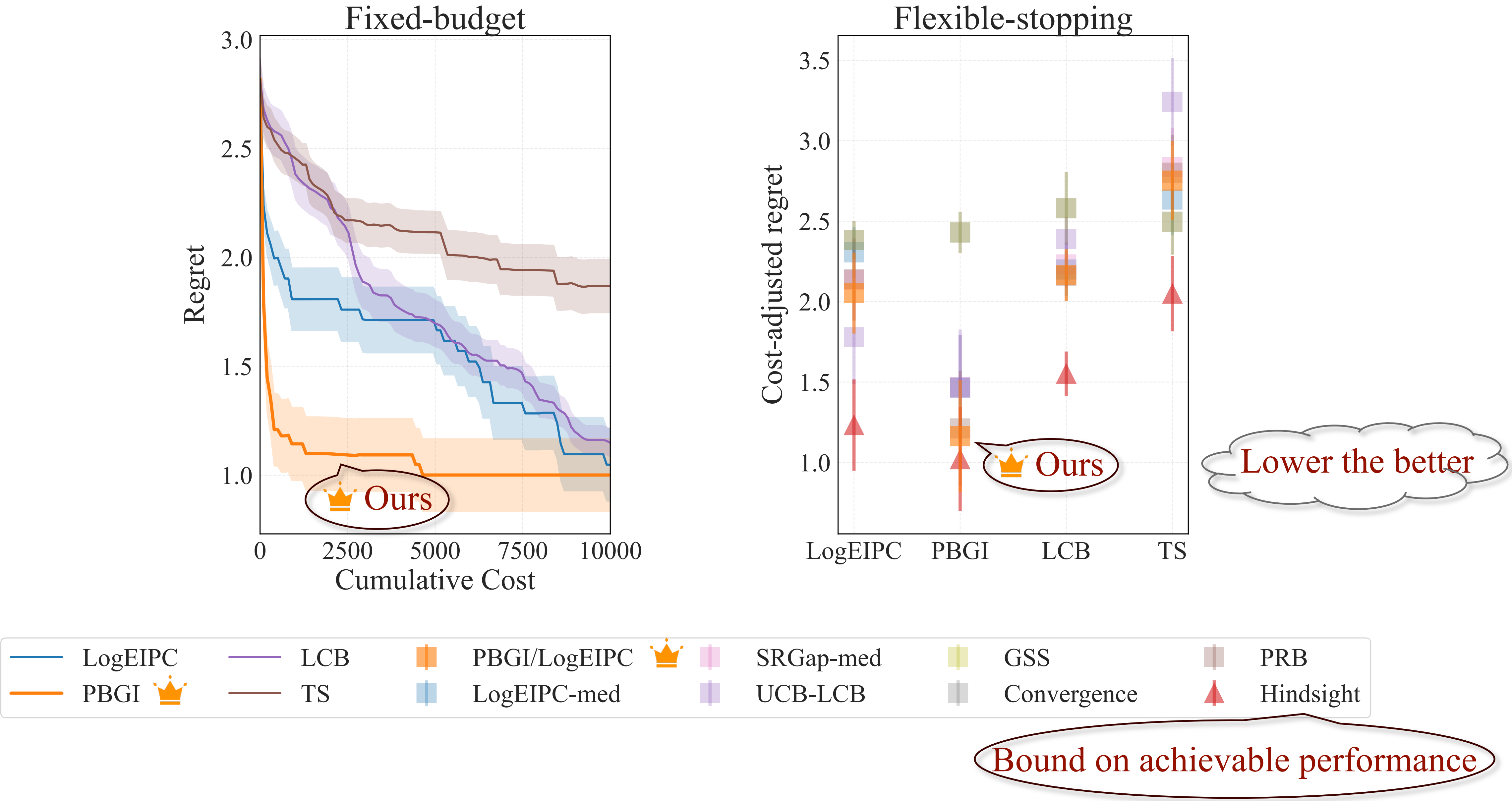
Our Contribution: Gittins Index Principle

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

? Why another principle?

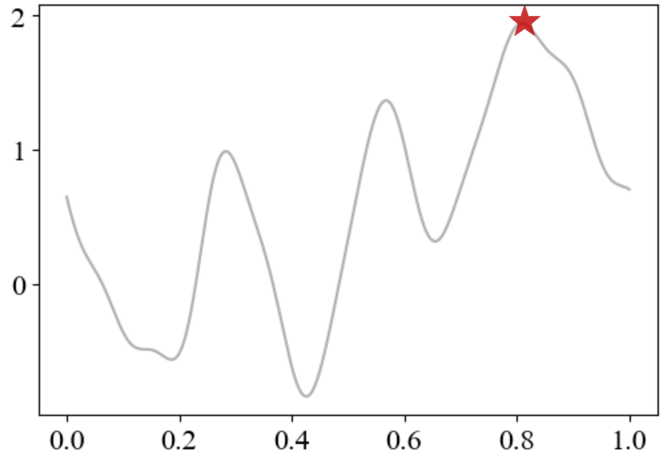
1. Naturally handles practical considerations
2. Performs competitively on benchmarks
3. Comes with theoretical guarantees

Gittins Index vs Baselines on AutoML Benchmark



Bayesian Optimization

$f(x)$



Continuous

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Fixed-budget / Flexible-stopping

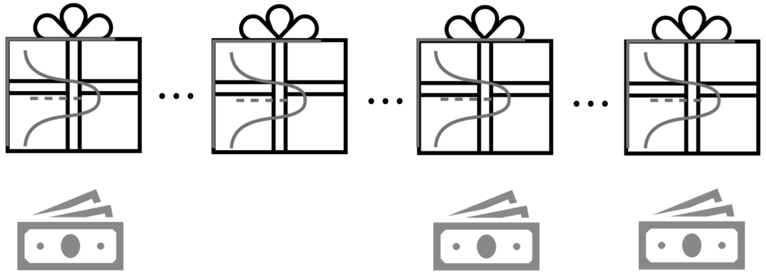
Expected (cost-adjusted) regret

Is Gittins index good?

theoretically

Pandora's Box

[Weitzman'79]



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Theoretical Guarantee and Empirical Validation

Theorem (No worse than stopping-immediately)

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

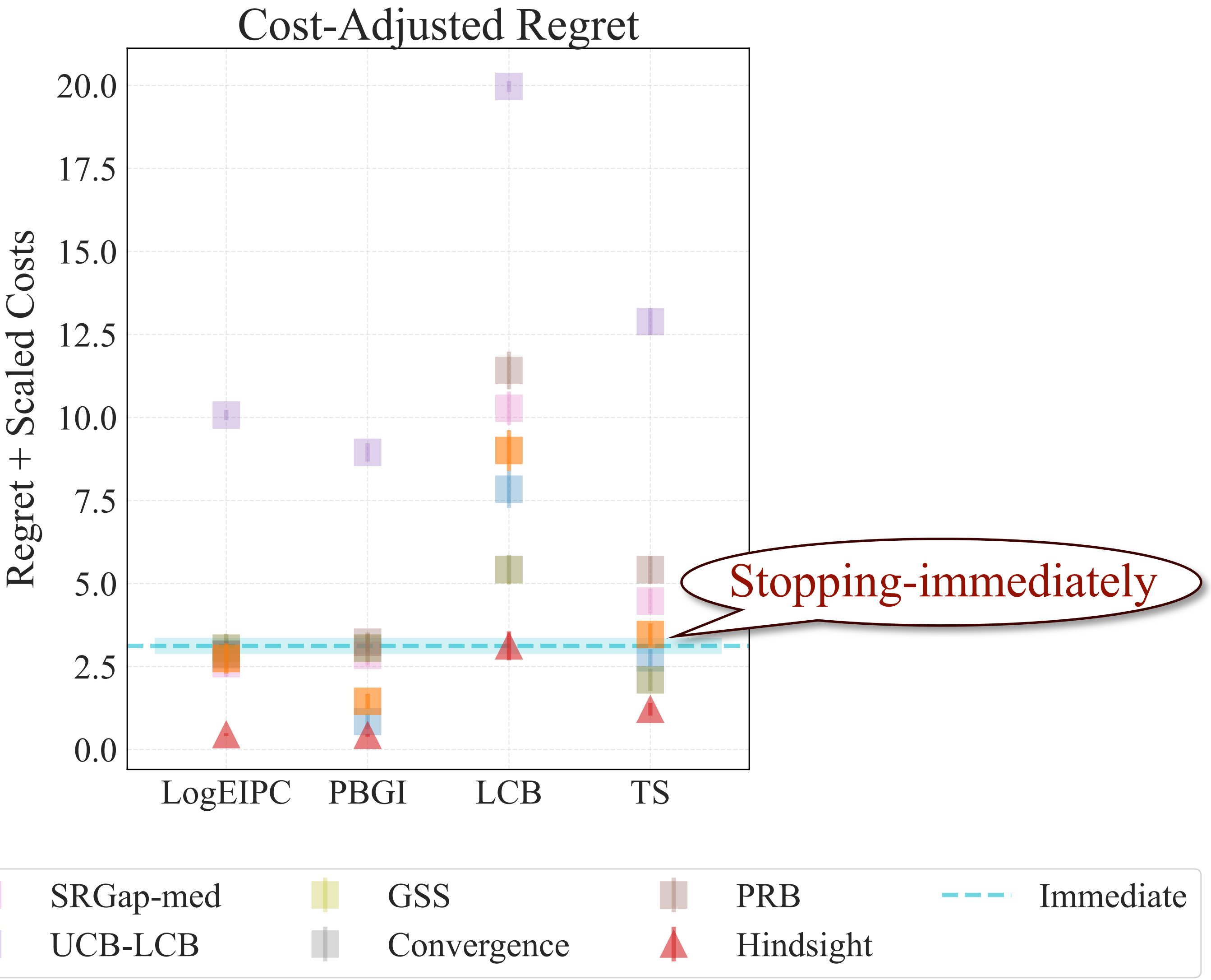
or LogEIPC

cost-adjusted regret

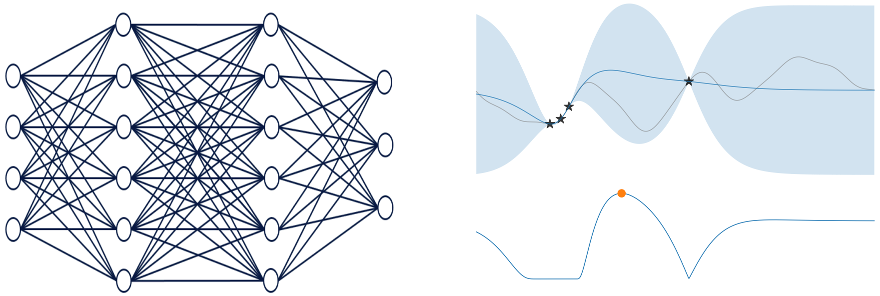
Implication:

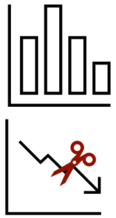
- Matches the best achievable performance in the worst case (evaluations are all very costly).

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



Studied problem

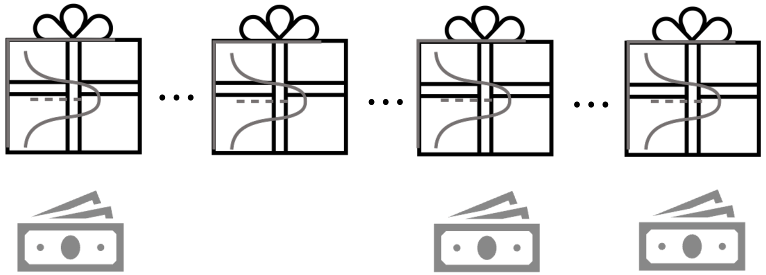




Varying evaluation costs

Adaptive stopping time

Key idea



Link to Pandora's Box problem
& Gittins index theory

Impact

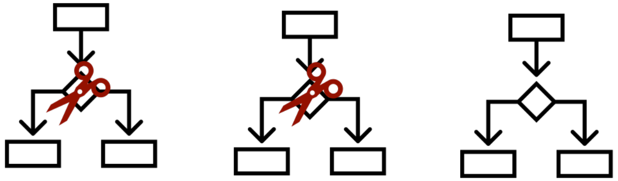
Meta

BoTorch Ax

Competitive empirical performance &
interests from practitioners

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

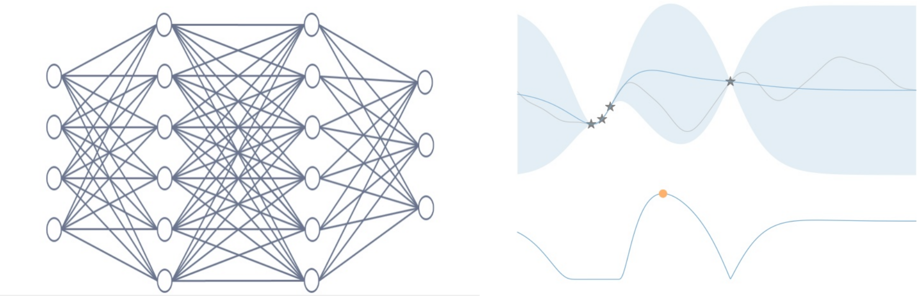
Ongoing work



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

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

Studied problem



Varying evaluation costs

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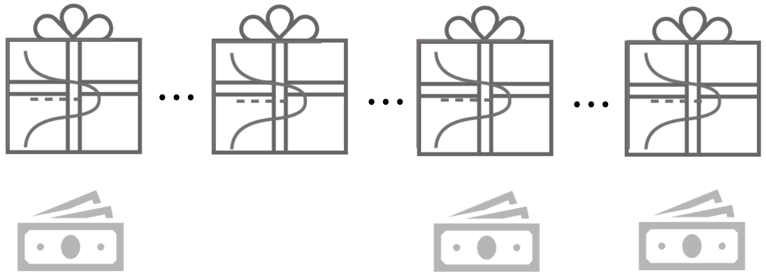

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Ongoing work

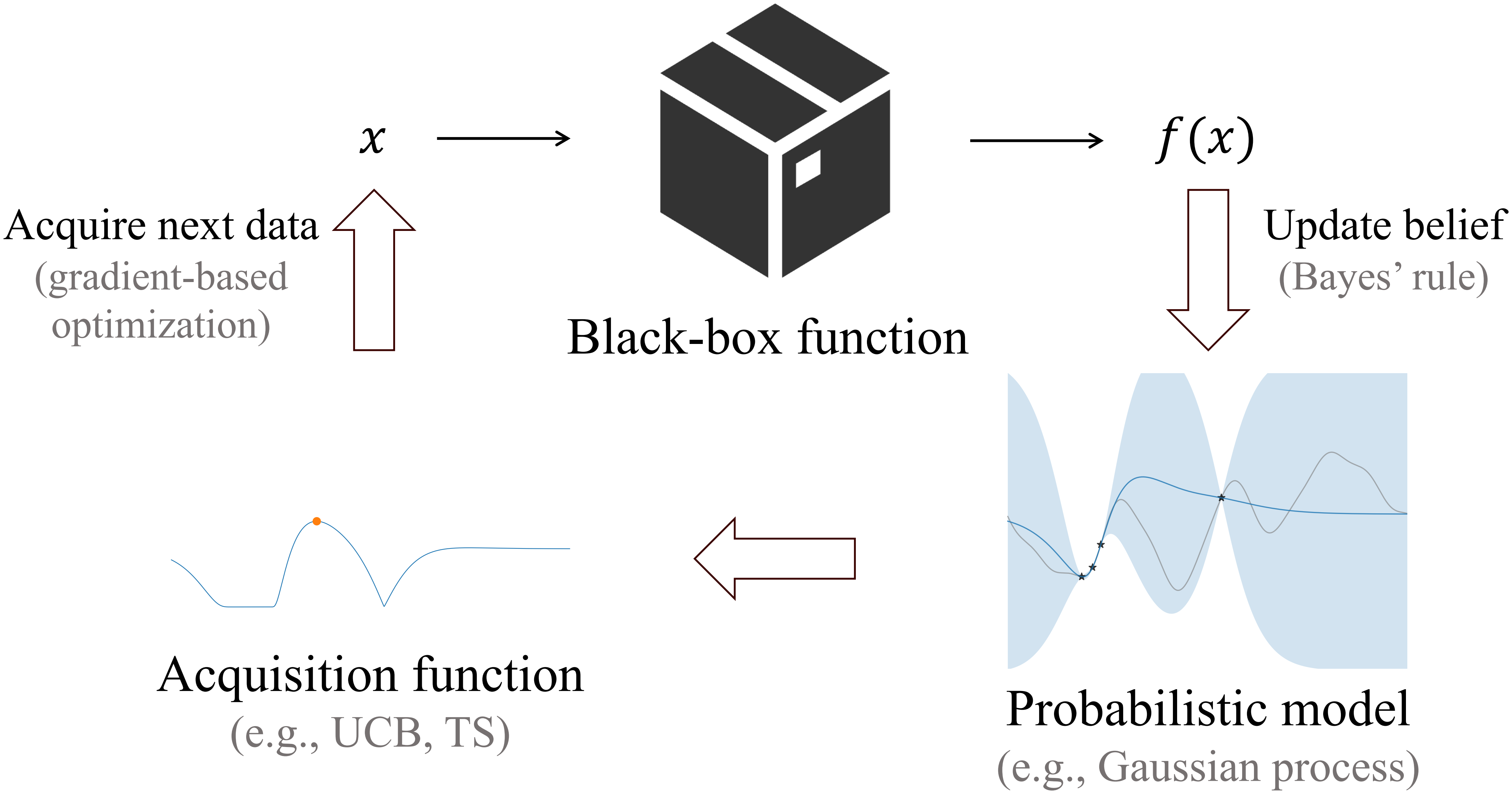
ChatGPT Gemini

deepseek Claude

LLM-driven black-box optimization

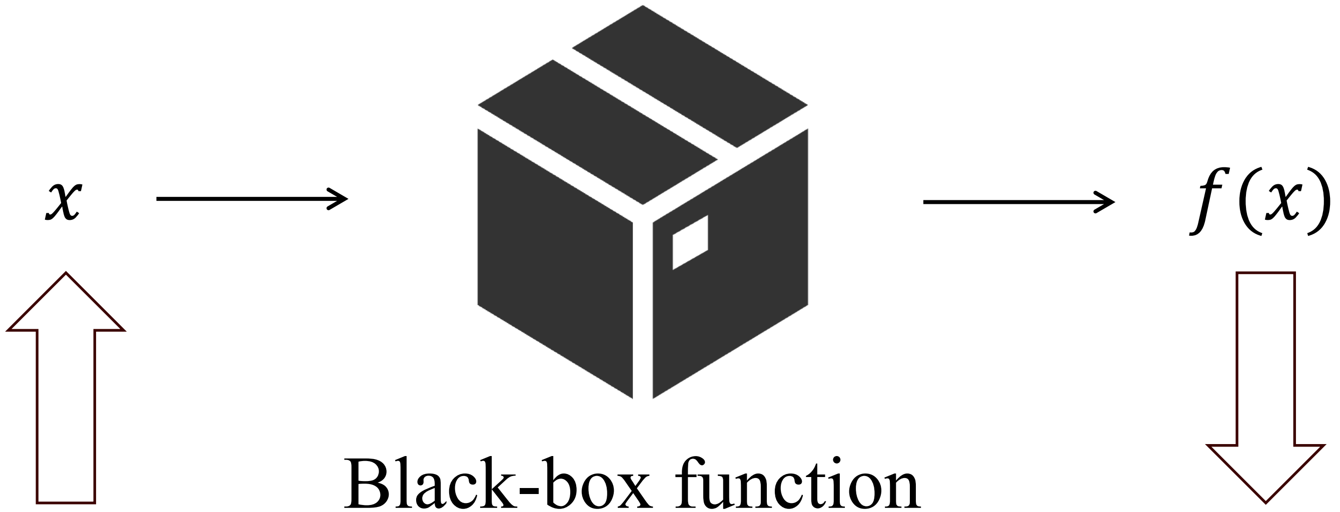
"Cost-aware Stopping for Bayesian Optimization." Under review.

Recap: Bayesian Optimization



Ongoing: LLM-Driven Black-Box Optimization

Acquire next data
(LLM proposal)



Black-box function

Update belief
(feedback-augmented context)

Acquisition function
(e.g., Softmax sampling)

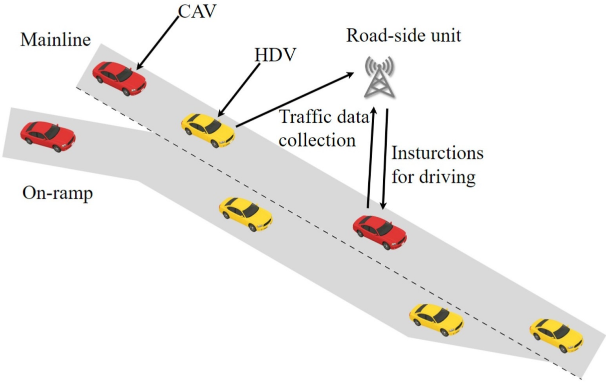
Probabilistic model
(e.g., autoregressive model)

Ongoing: LLM-Driven RL Training Optimization

Mixed-autonomy traffic control:

(e.g., Transformer config)

x ⟶



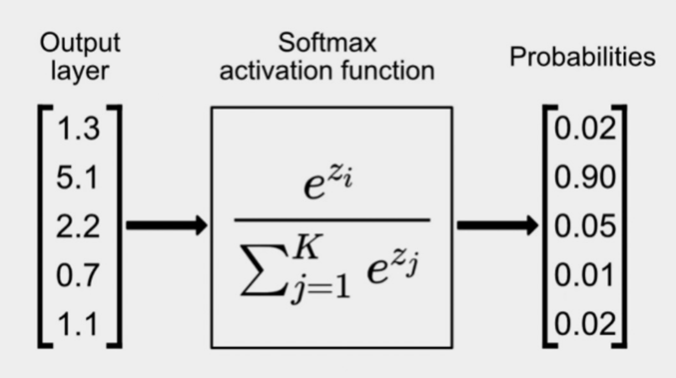
⟶ $f(x)$

(e.g., average speed)

Acquire next data
(LLM proposal)

Update belief
(feedback-augmented context)

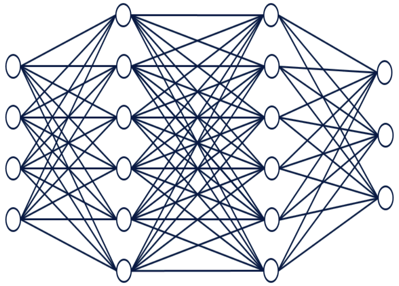
Black-box function
(RL training & evaluation)

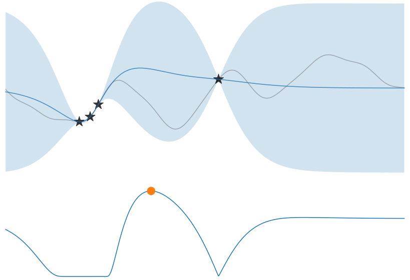


Acquisition function
(e.g., Softmax sampling)

Probabilistic model
(large language model)

Studied problem





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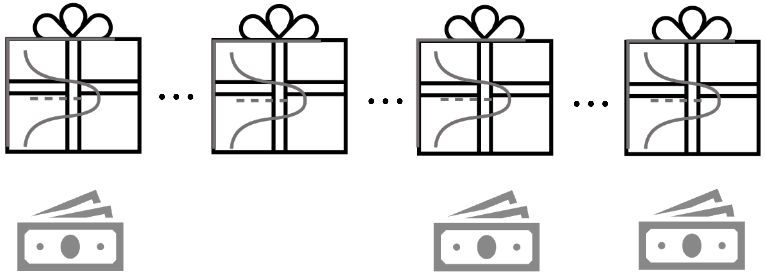
Adaptive stopping time

Key idea



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