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)

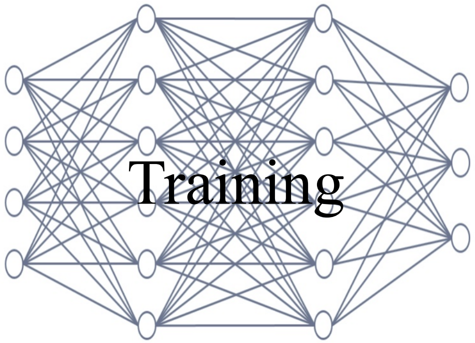
INFORMS Annual Meeting 2025 Job Market Showcase

Optimization Under Uncertainty

ML model training:

Training hyperparameters → Training → Accuracy

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



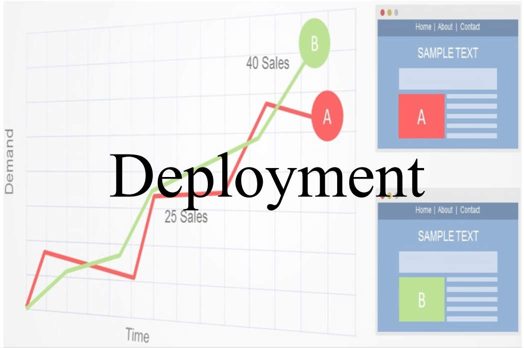
Optimization Under Uncertainty

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:

non-analytical &
no gradient info

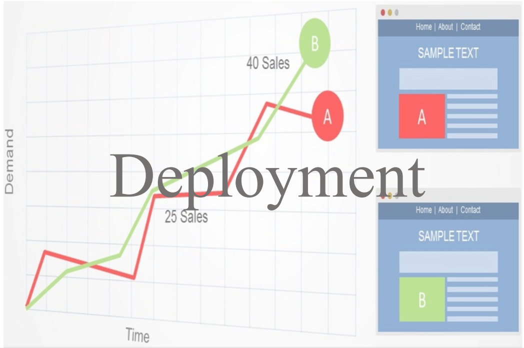
Input x ⟶  ⟶ Performance metric $f(x)$

ML model training:

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

⟶ Accuracy

Adaptive experimentation:

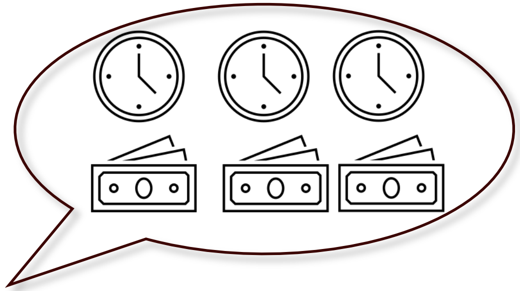
Decision/design variables (e.g., layout, pricing level) ⟶ 

⟶ Revenue

Black-Box Optimization

expensive-to-evaluate

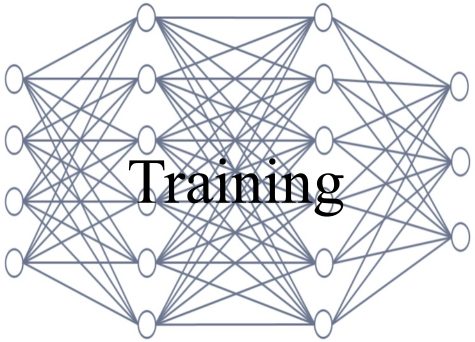
Input x ⟶  ⟶ Performance metric $f(x)$



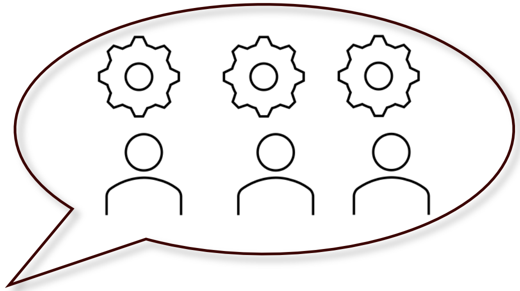
Training time

Compute credits

ML model training:

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

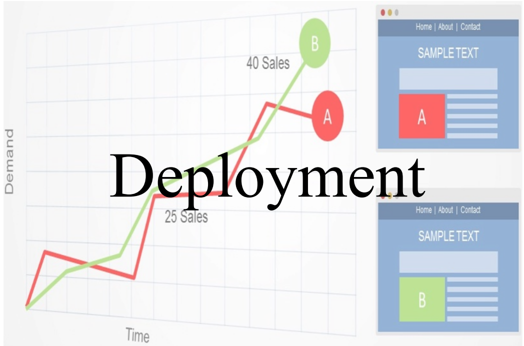
⟶ Accuracy



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 $x_1, \ldots, x_T$ to maximize the expected best observed value

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

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

$f \sim$ Stochastic Process

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

Black-box function

Bayesian Optimization

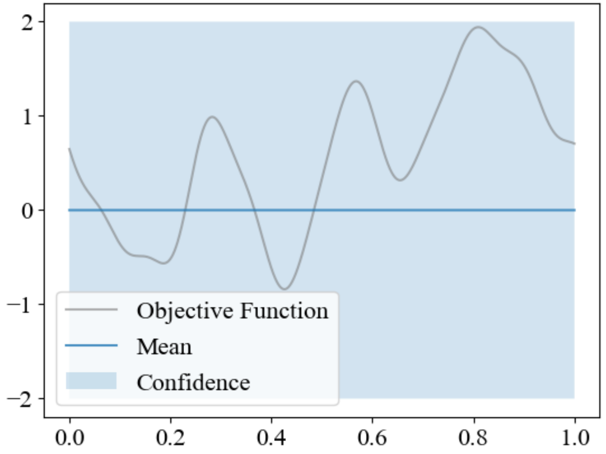
Time 0

$f \sim$Stochastic Process

x →  → $f(x)$

Black-box function

Model belief



Probabilistic model

(e.g., Gaussian process)

Bayesian Optimization

Time t

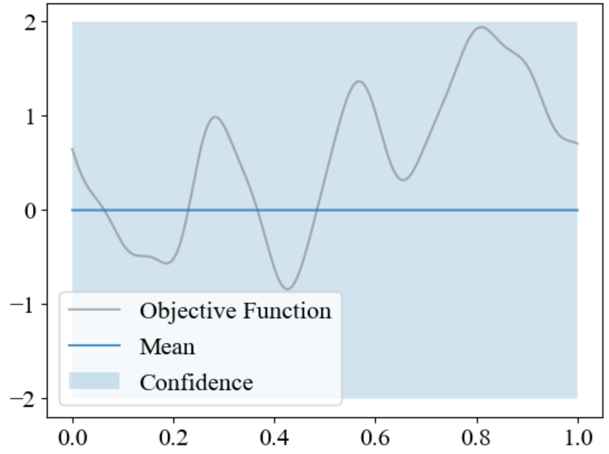
$x_1, \dots, x_t \longrightarrow$

Black-box function

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

$f \sim$ Stochastic Process

Model belief



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Time t

$f \sim$ Stochastic Process

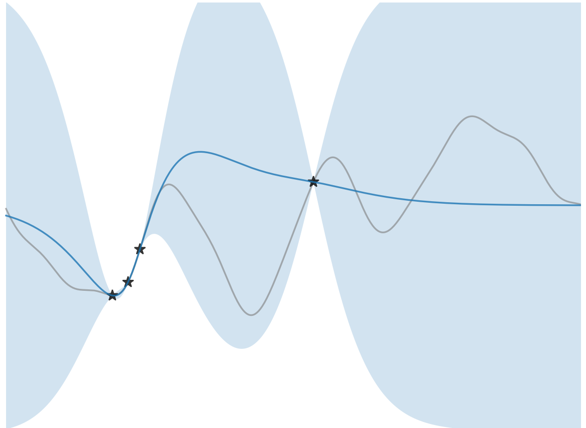
$x_1, \dots, x_t \longrightarrow$

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

Black-box function

Update belief

(Bayes' rule)



Probabilistic model

(e.g., Gaussian process)

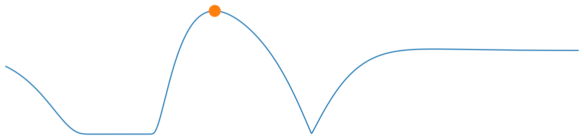
Bayesian Optimization

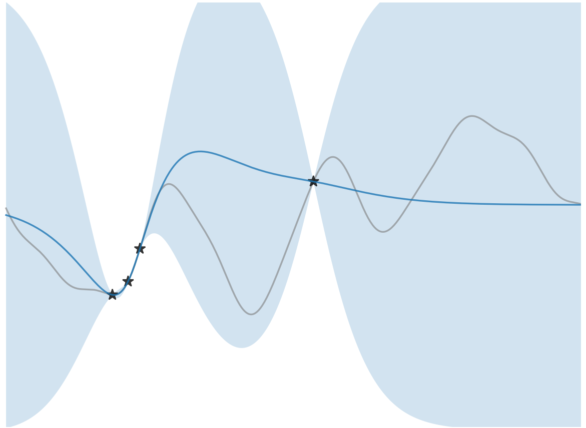
Time t

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

Black-box function

Update belief
(Bayes' rule)





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

scoring (worth of each point

Probabilistic model
(e.g., Gaussian process)

Bayesian Optimization

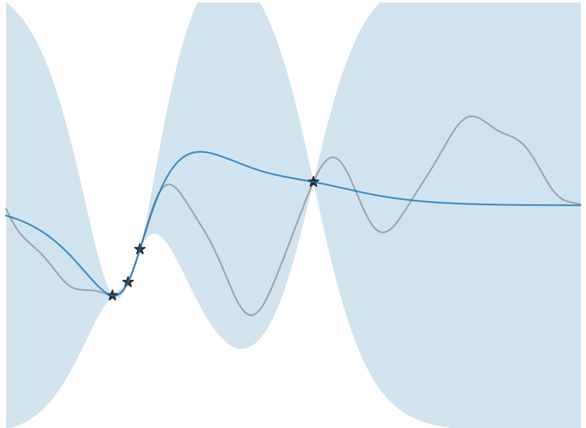
Time t

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

Black-box function

Acquire next input
(gradient-based optimization)

Update belief
(Bayes' rule)



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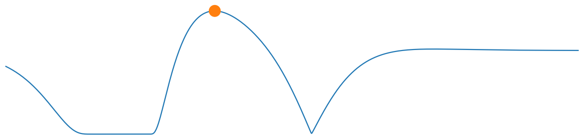


Acquisition function
(e.g., EI, UCB, TS)

scoring (worth of each point

Bayesian Optimization

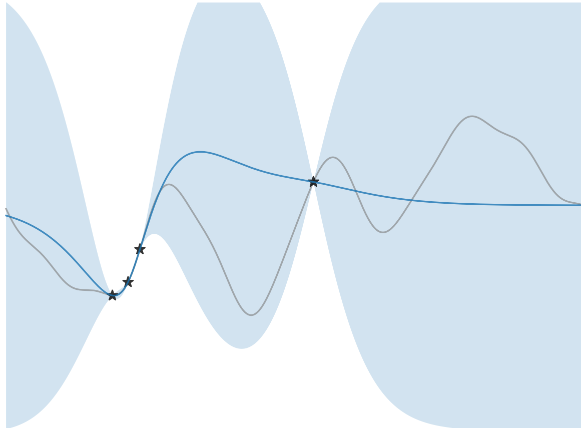
Time $t+1$

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

Black-box function

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

Update belief
(Bayes' rule)



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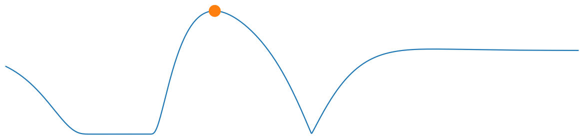

Acquisition function
(e.g., EI, UCB, TS)

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Acquire next input
(gradient-based optimization)

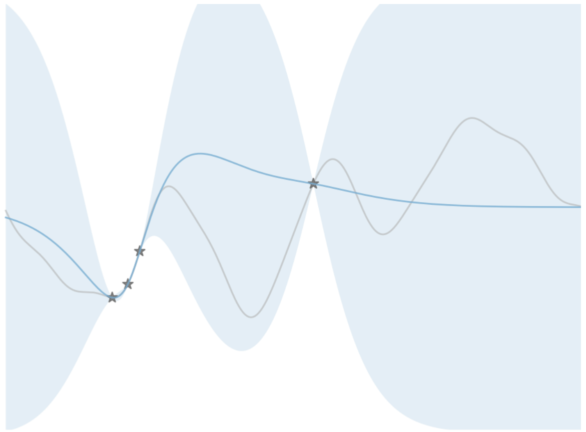
Bayesian Optimization

x →  → $f(x)$

Black-box function

Acquire next input (gradient-based optimization)

Update belief (Bayes' rule)



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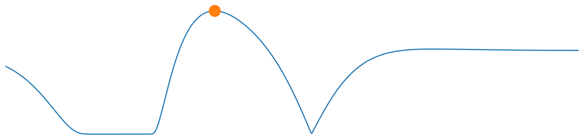

My focus

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

scoring (worth of each point

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
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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

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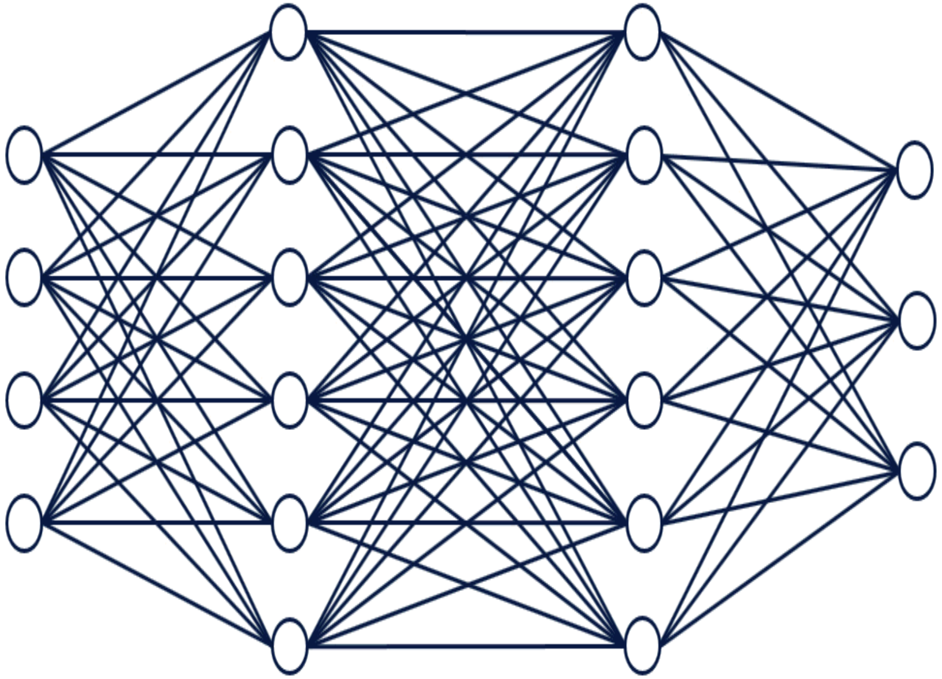
Under-explored Side Info and Flexibility

Varying evaluation costs

Smart stopping time

Observable multi-stage feedback

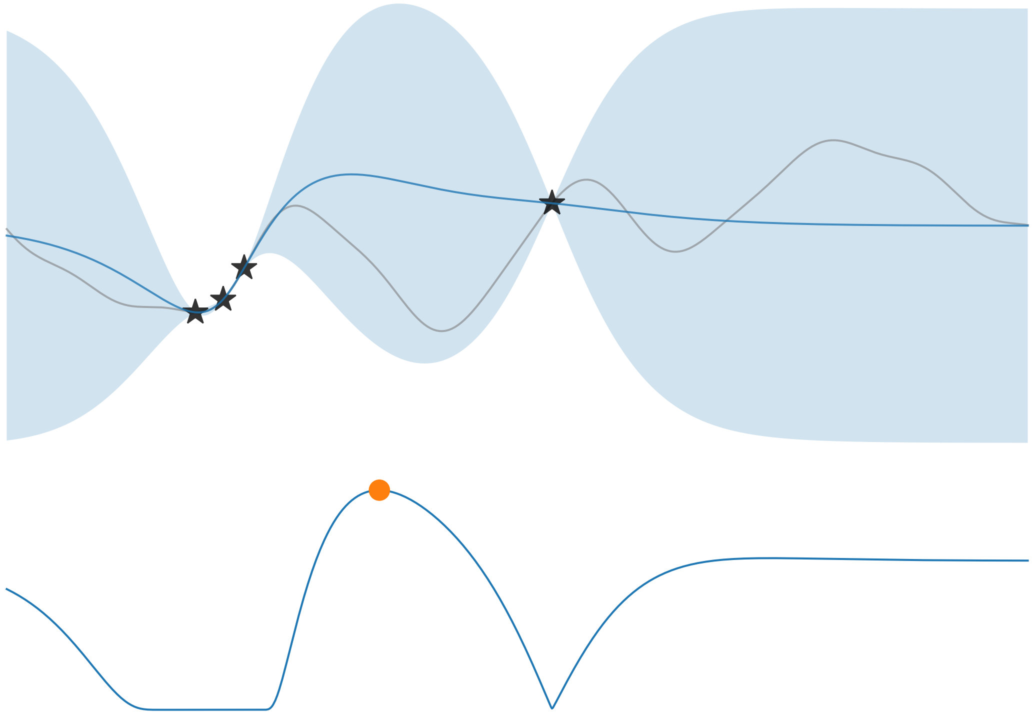


How does existing principle incorporate them?

Varying evaluation costs

Smart stopping time

Observable multi-stage feedback



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

How does existing principle incorporate them?

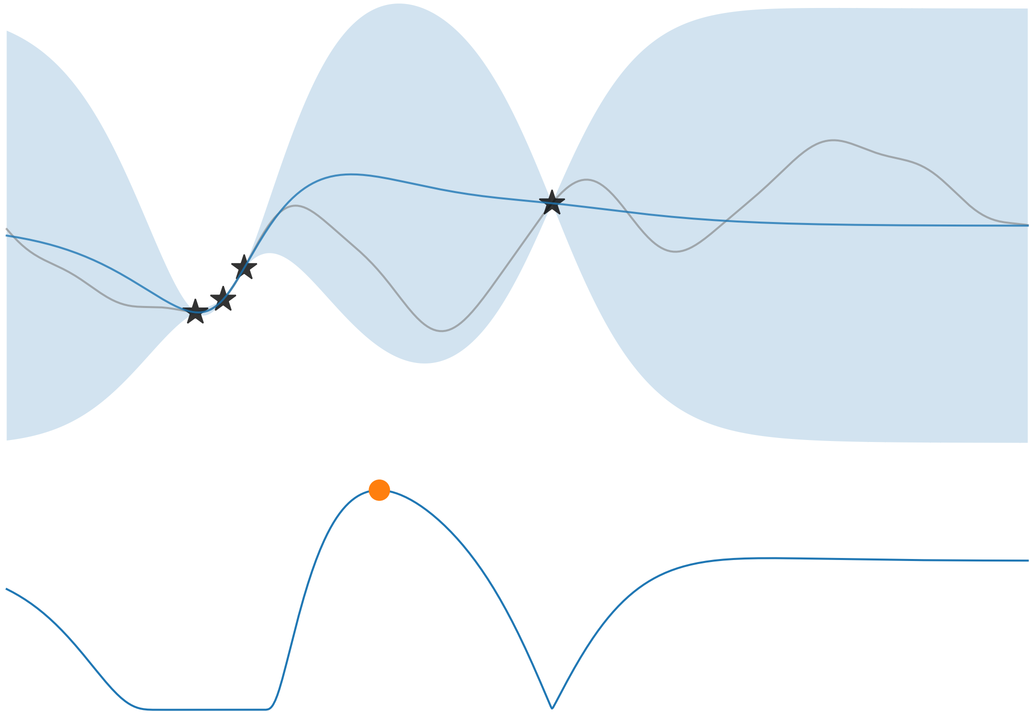
Varying evaluation costs

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

Why divide?

Smart stopping time

Observable multi-stage feedback



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

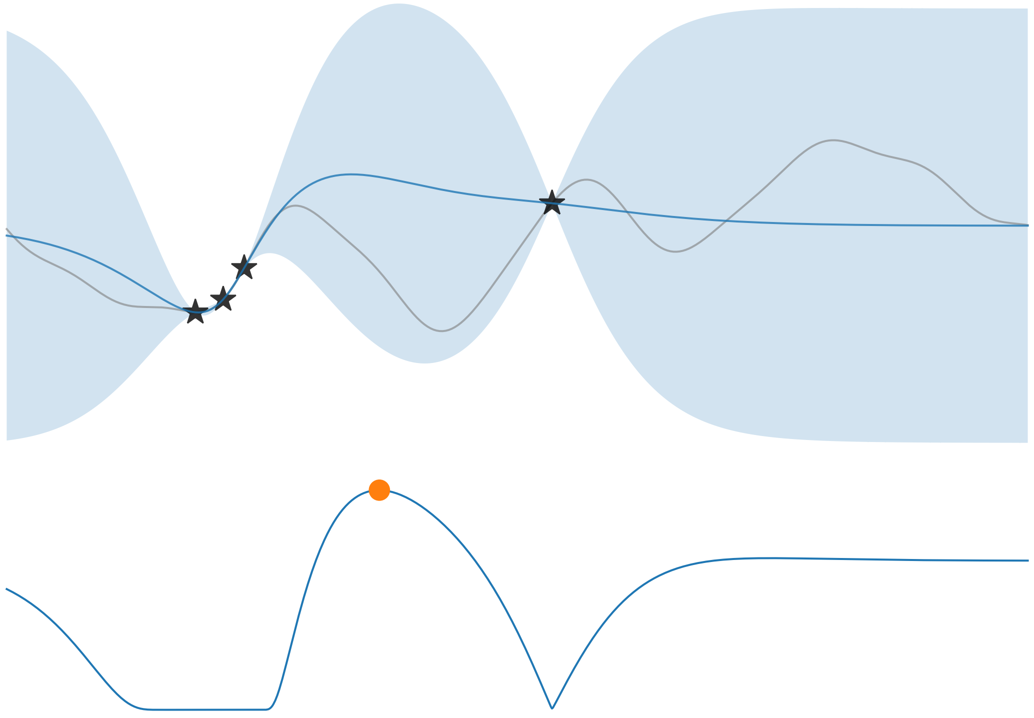
Why divide?

Smart stopping time

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

Which threshold?

Observable multi-stage feedback



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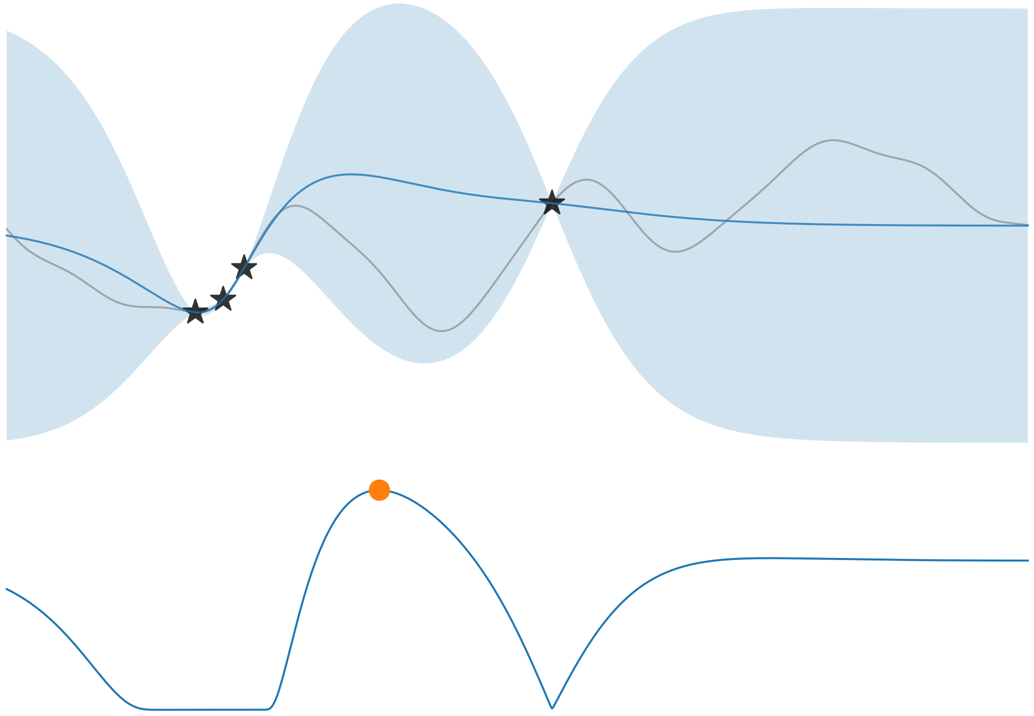

Expected improvement $\mathrm{EI}(x)$

Under-explored Side Info and Flexibility

Varying evaluation costs

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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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Smart stopping time

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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:
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Optimal in related sequential decision problems

What is Pandora’s Box?

Varying evaluation costs

Features in Pandora’s box

Smart stopping time

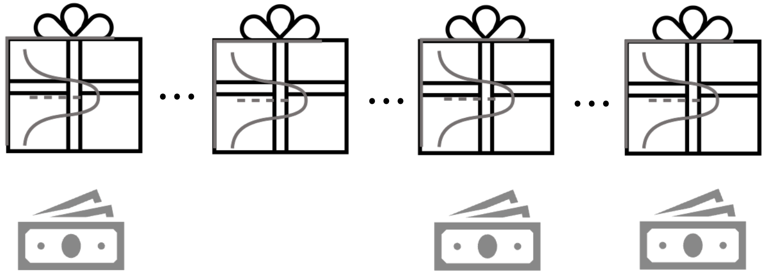
Features in Pandora’s box

Observable multi-stage feedback

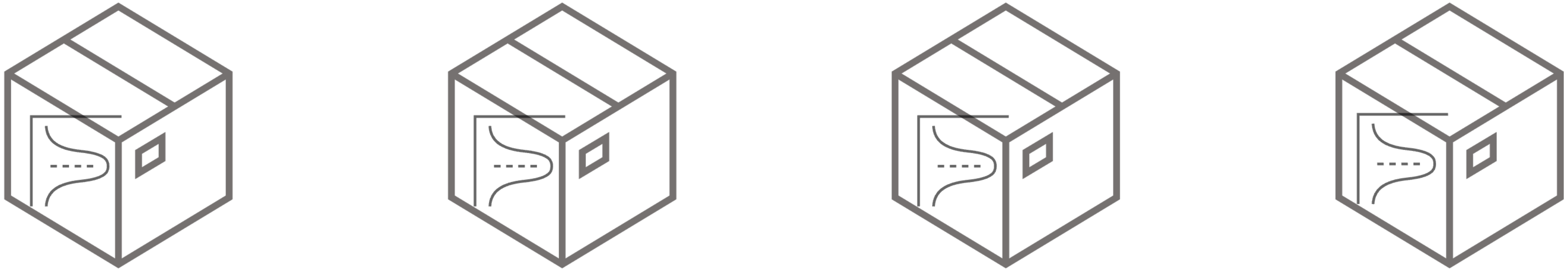
Features in Markovian bandits

New design principle:
Gittins index

Optimal in related sequential decision problems



Pandora's Box



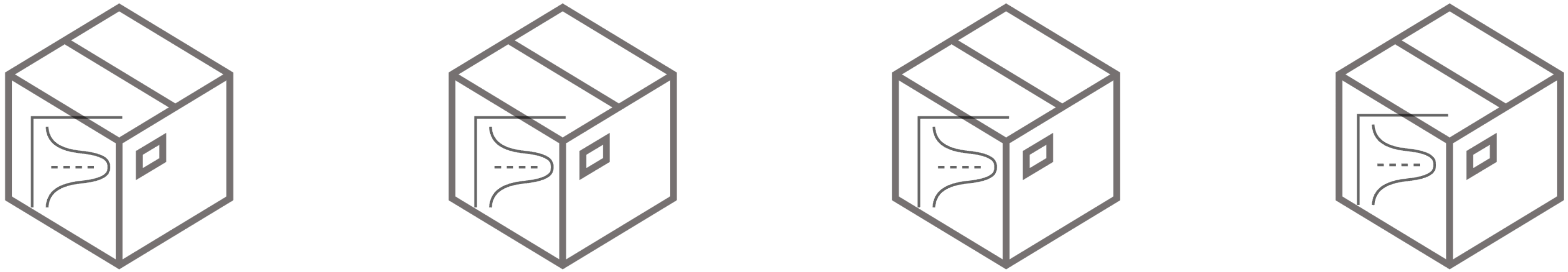
High-level goal: Choose box $x_1, \dots, x_T$ to open to maximize the expected utility

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

Flexible stopping time

Pandora's Box

$t = 0$



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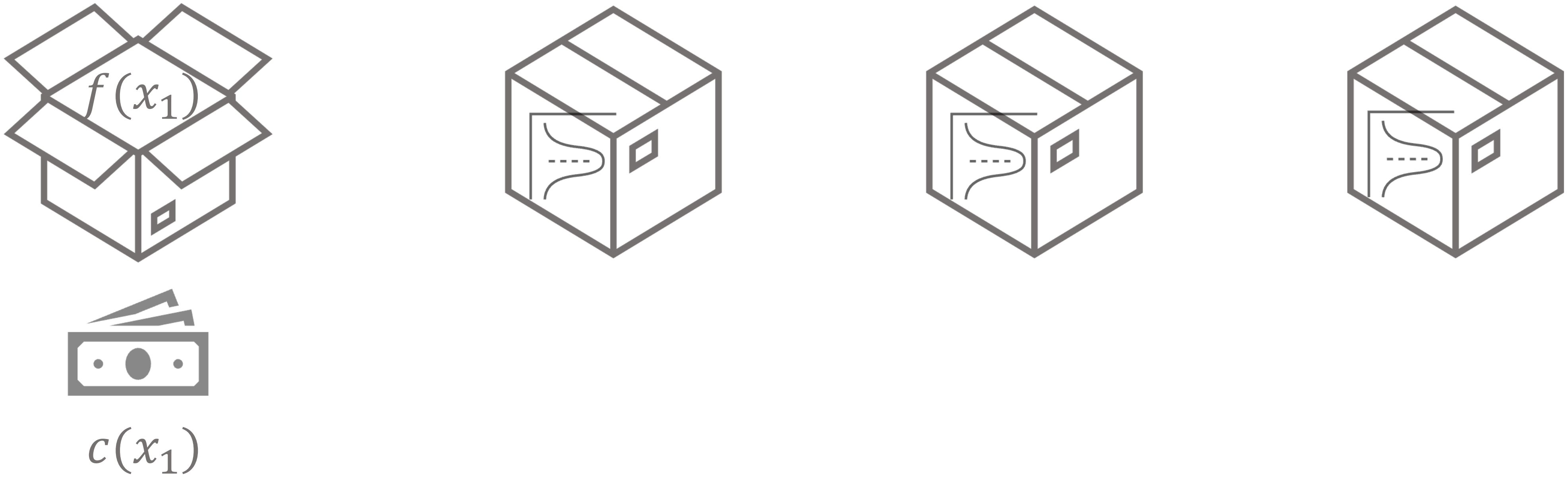
Pandora’s Box

$t = 1$

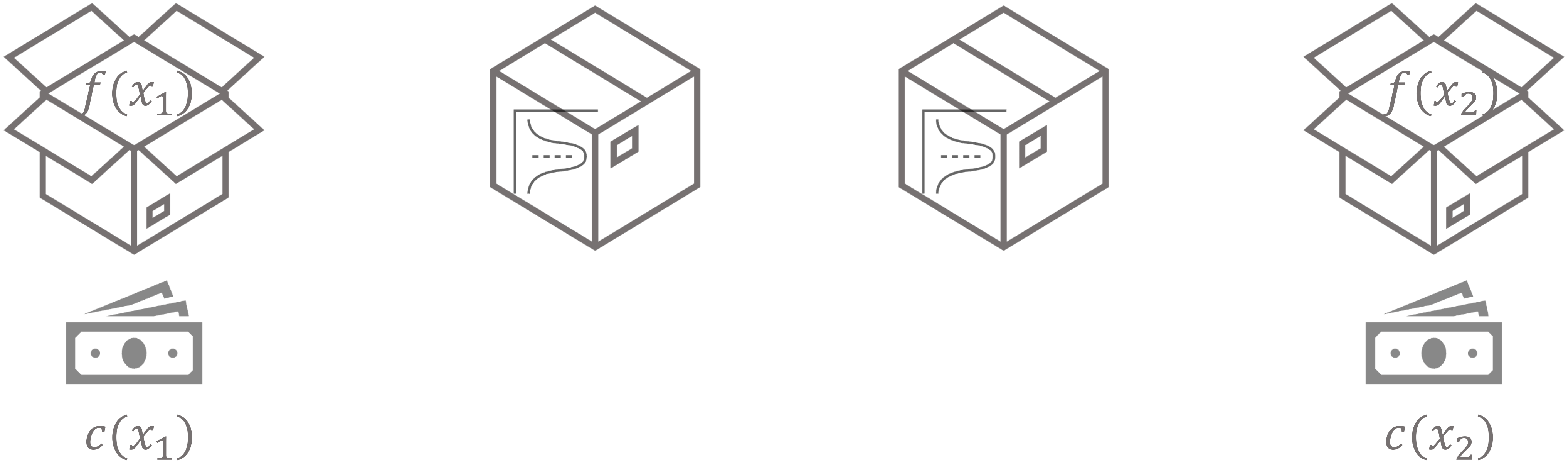


High-level goal: Choose box $x_1, \ldots, x_T$ to open to maximize the expected utility

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

Pandora's Box

$t = 2$

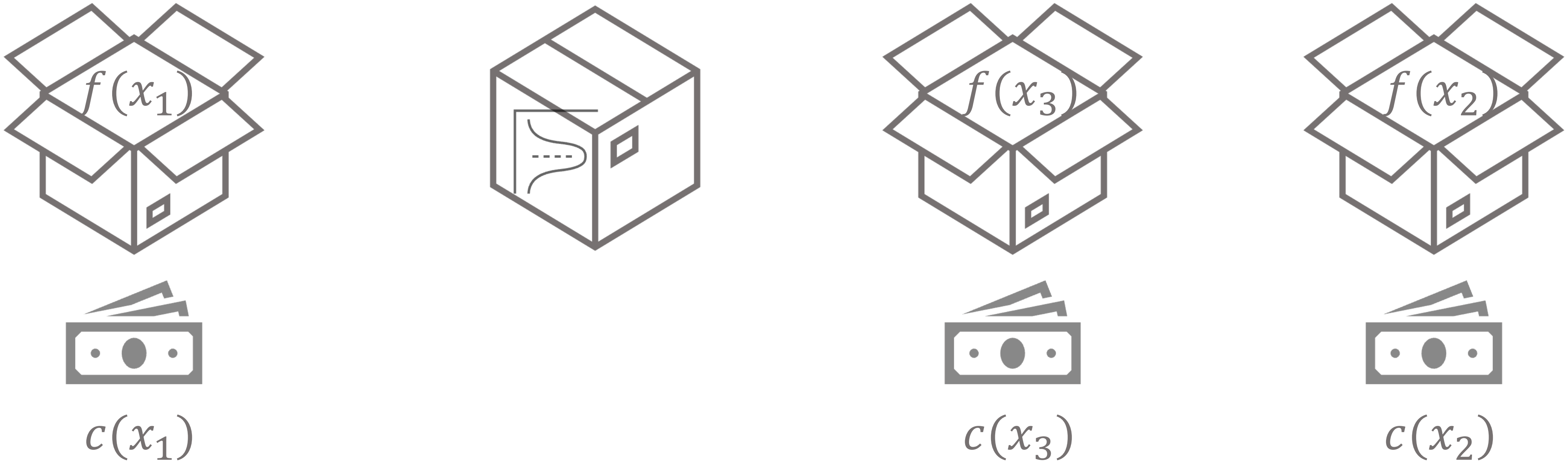


High-level goal: Choose box $x_1, \ldots, x_T$ to open to maximize the expected utility

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

Pandora's Box

$t = 3$

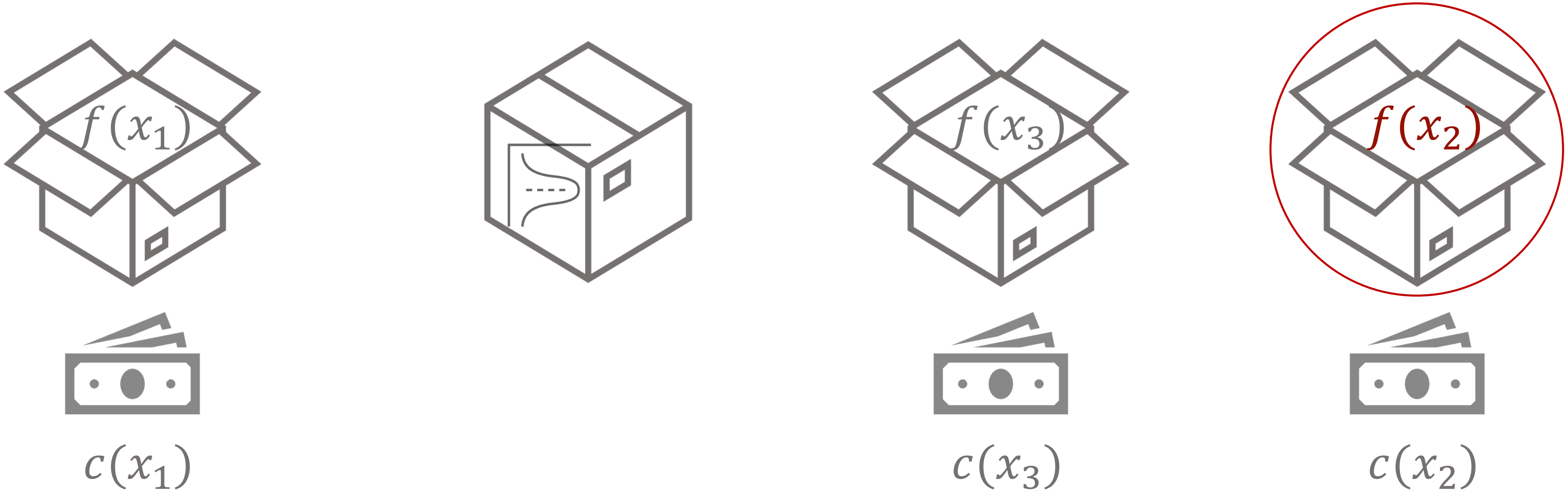


High-level goal: Choose box $x_1, \dots, x_T$ to open to maximize the expected utility

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

Pandora's Box

$t = T$, stop

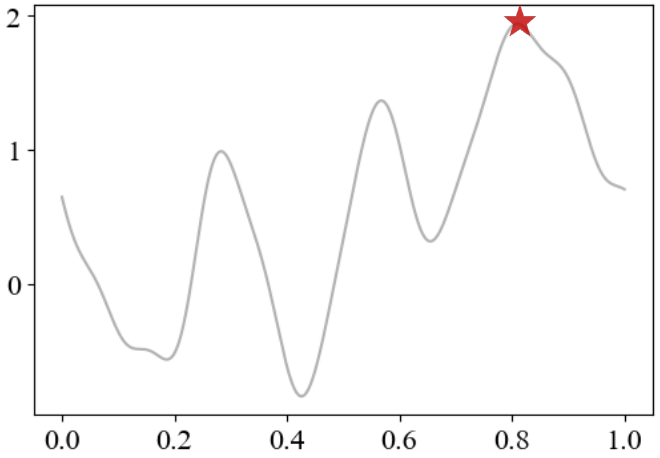


High-level goal: Choose box $x_1, \ldots, x_T$ to open to maximize the expected utility

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

Bayesian Optimization

$f(x)$



Continuous

Correlated

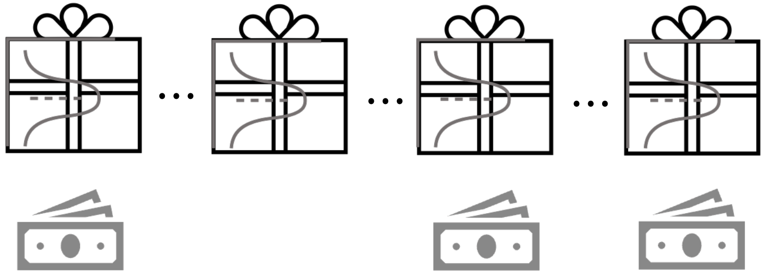
Fixed-iteration

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

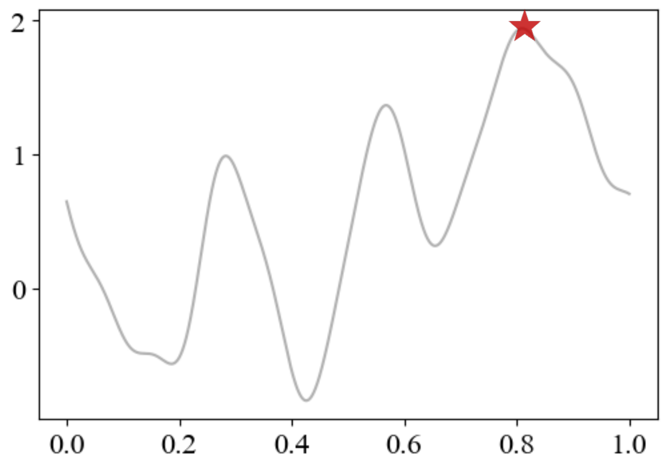
Expected utility

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

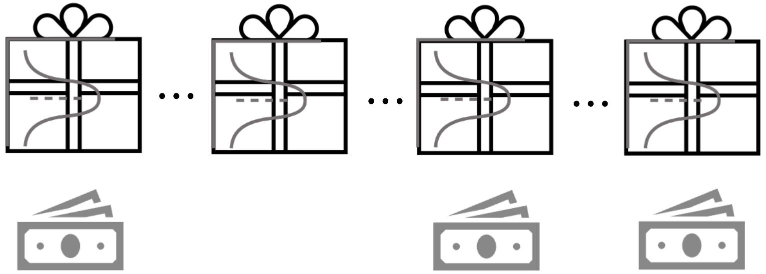
Fixed-iteration

Expected best-observed value

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

Pandora's Box

[Weitzman'79]



$f(x)$

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Expected utility

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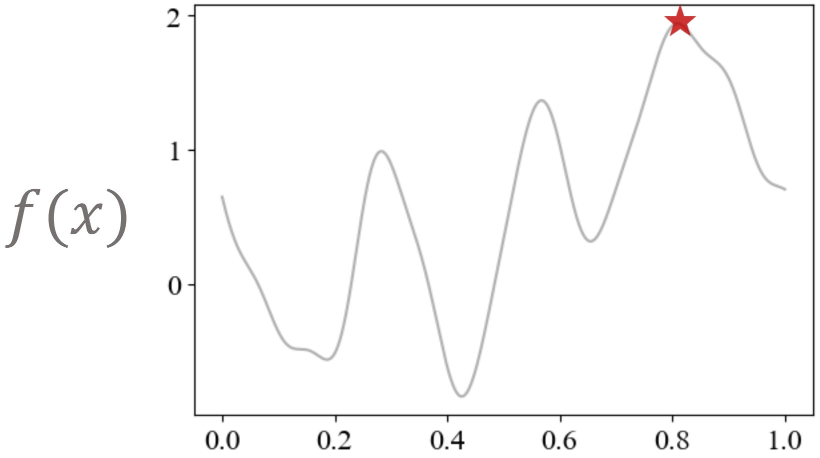
Bayesian Optimization



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]

Discrete

Independent

Flexible-stopping

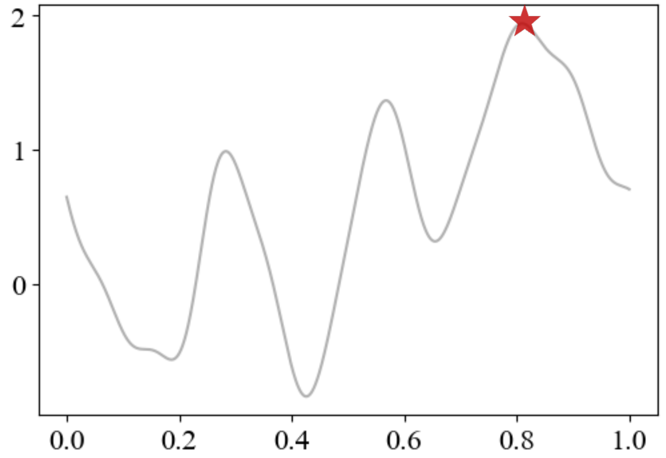
Expected utility

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

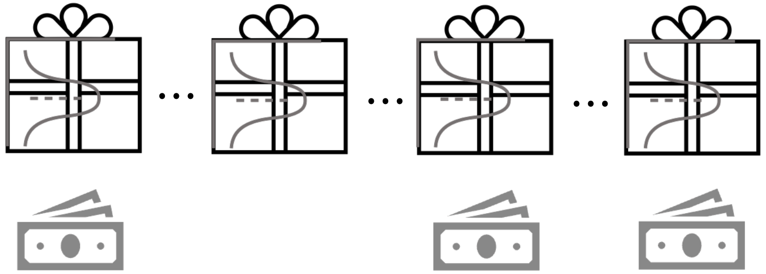
Fixed-iteration

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

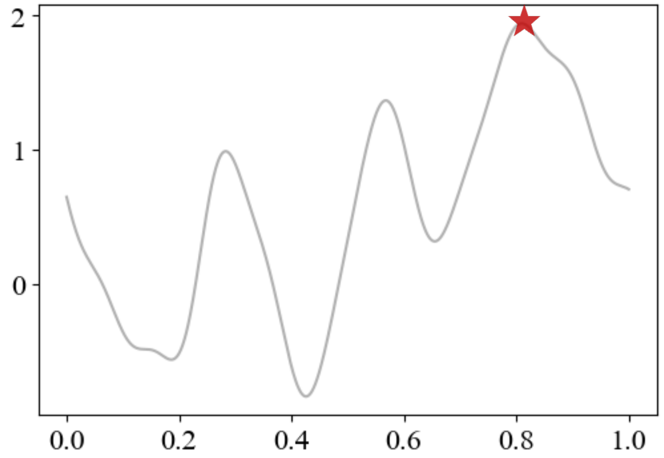
Expected cost-adjusted regret

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

cumulative cost

Bayesian Optimization

$f(x)$



Continuous

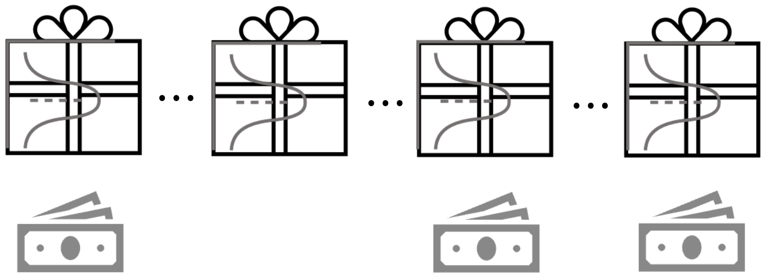
Correlated

Fixed-budget / Flexible-stopping

Expected (cost-adjusted) regret

Pandora's Box

[Weitzman'79]



$f(x)$

$c(x)$

Discrete

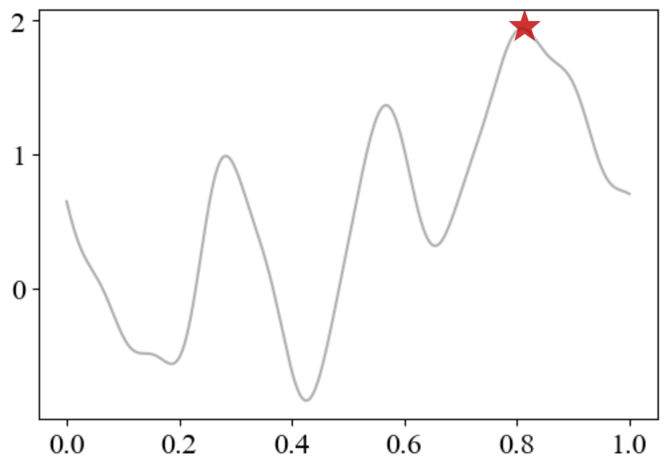
Independent

Flexible-stopping

Expected cost-adjusted regret

Bayesian Optimization

$f(x)$



Continuous

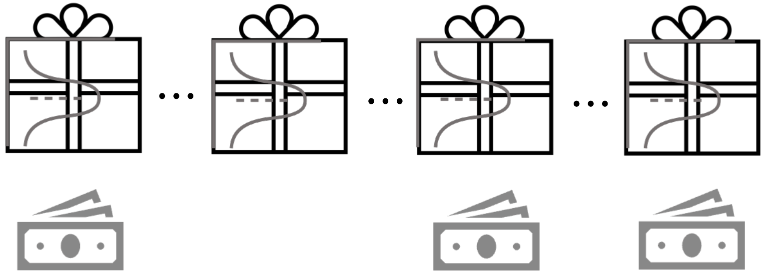
Correlated

Fixed-budget / Flexible-stopping

Expected (cost-adjusted) regret

Pandora's Box

[Weitzman'79]



$f(x)$

$c(x)$

Discrete

Independent

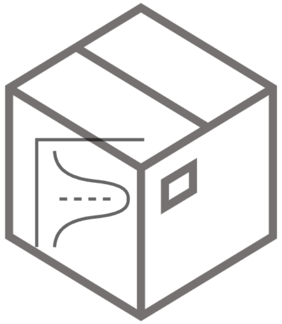
Flexible-stopping

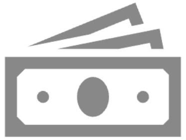
Expected cost-adjusted regret

Optimal policy: Gittins index

Optimal Policy: Gittins Index

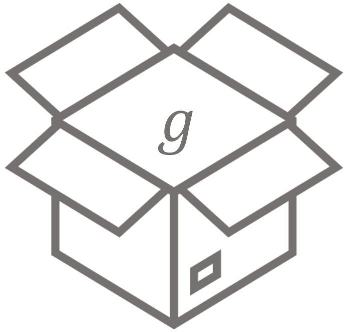
Step 1: Assign each box a Gittins index (higher is better)

$f(x)$ 

$c(x)$ 

$\downarrow$

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

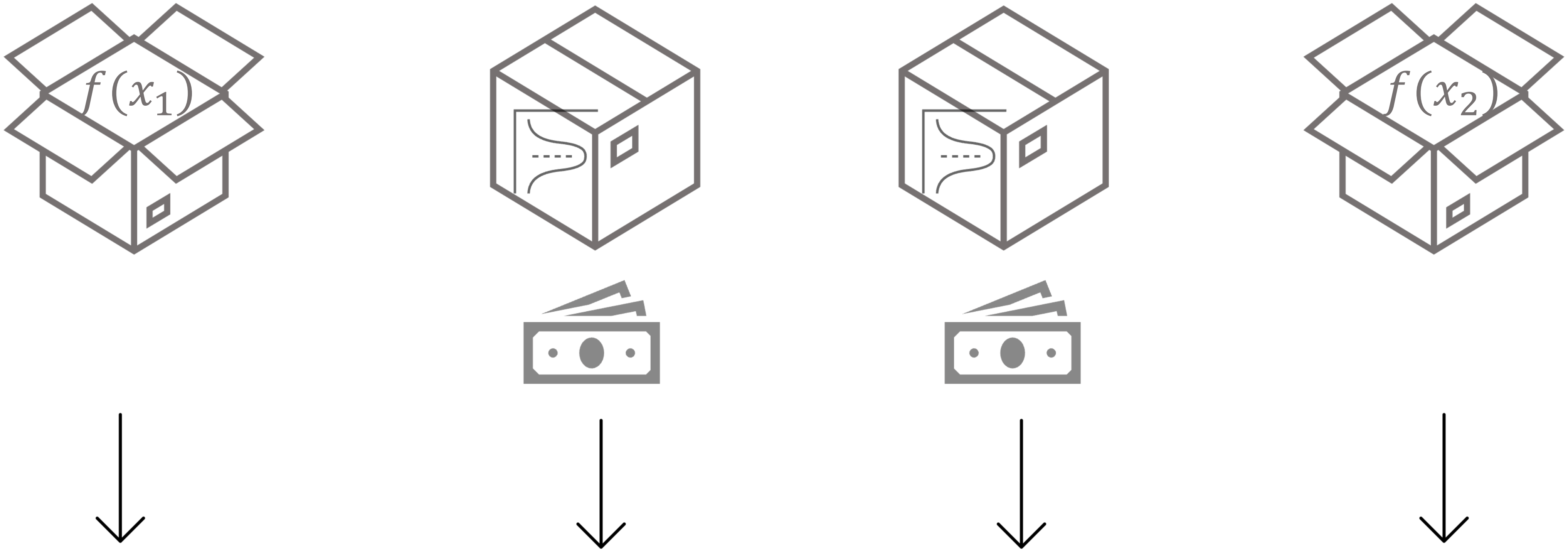


$\downarrow$

g

Optimal Policy: Gittins Index

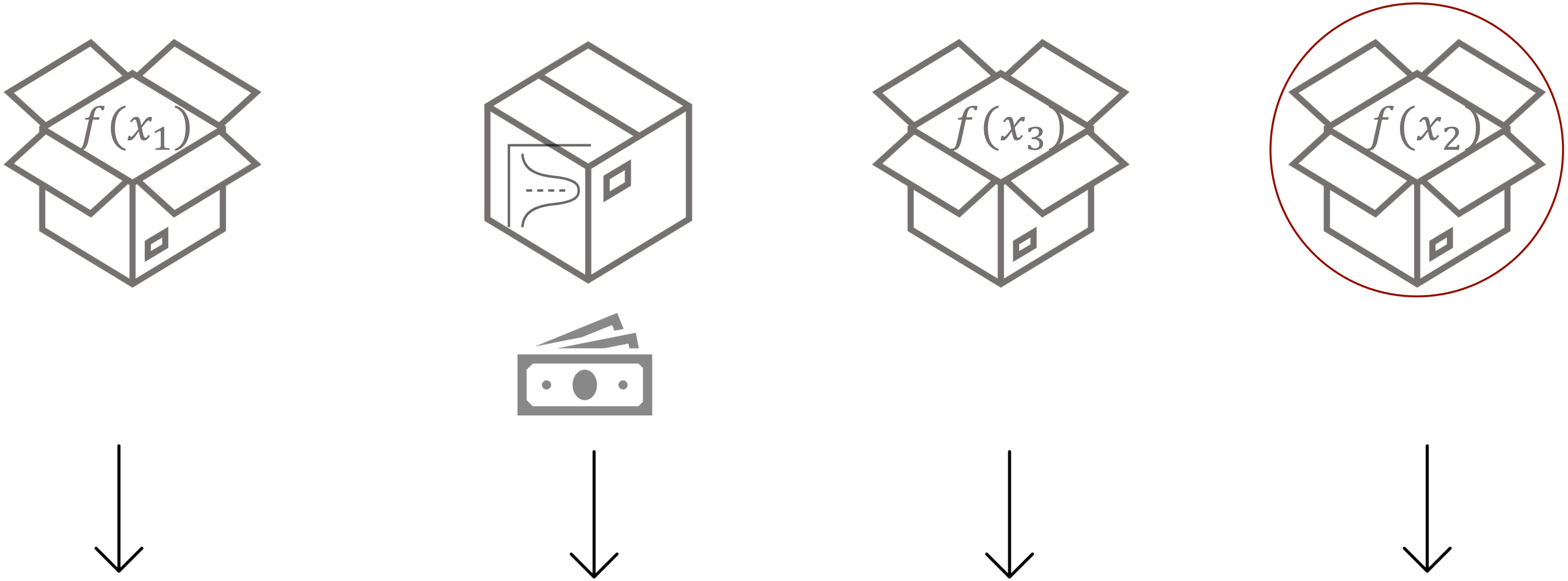
Step 2: Open the box with highest index if it is closed



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

Optimal Policy: Gittins Index

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



$f(x_1)$ $\quad$ $\mathrm{GI}_f(x; c(x))$ $\quad$ $f(x_3)$ $\quad$ $f(x_2)$

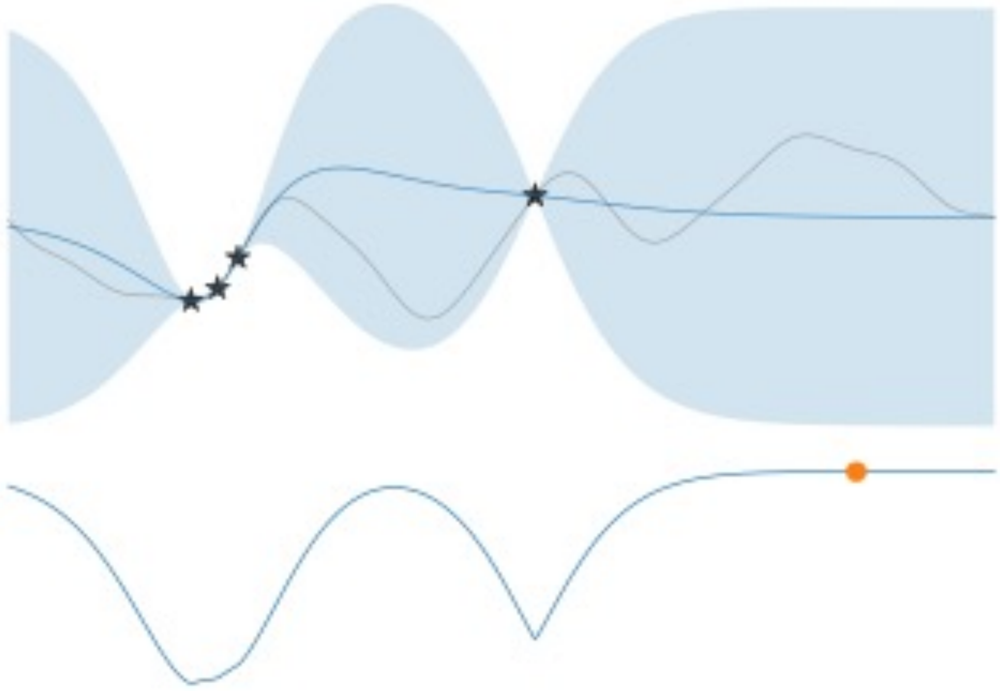
Optimal Policy: Gittins Index

Varying evaluation costs

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

Smart stopping time

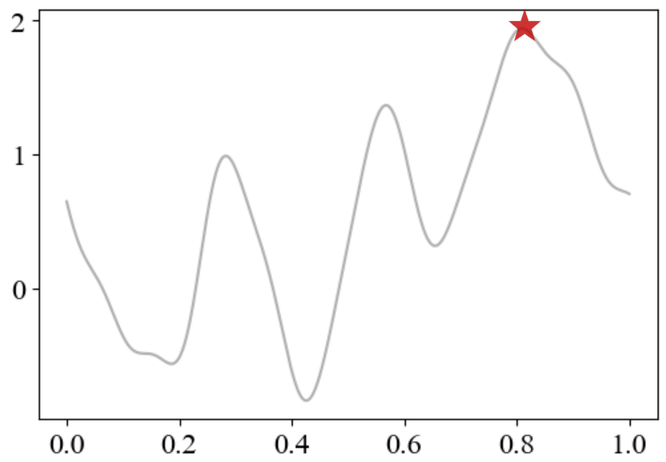
$$\max_x \mathrm{GI}\big(x; c(x)\big) \le \max_x f(x)$$



Gittins index $\mathrm{GI}(x)$

Bayesian Optimization

$f(x)$



Continuous

Correlated

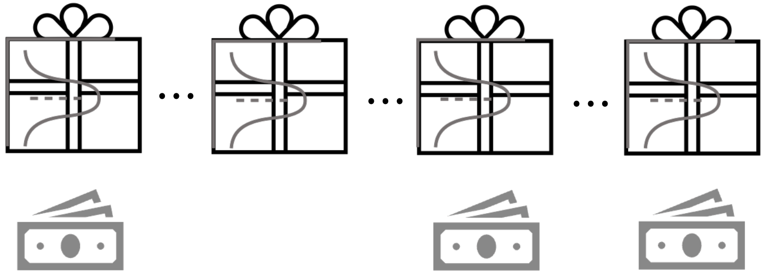
Fixed-budget / Flexible-stopping

Expected (cost-adjusted) regret

Is Gittins index good?

Pandora’s Box

[Weitzman’79]



$f(x)$

$c(x)$

Discrete

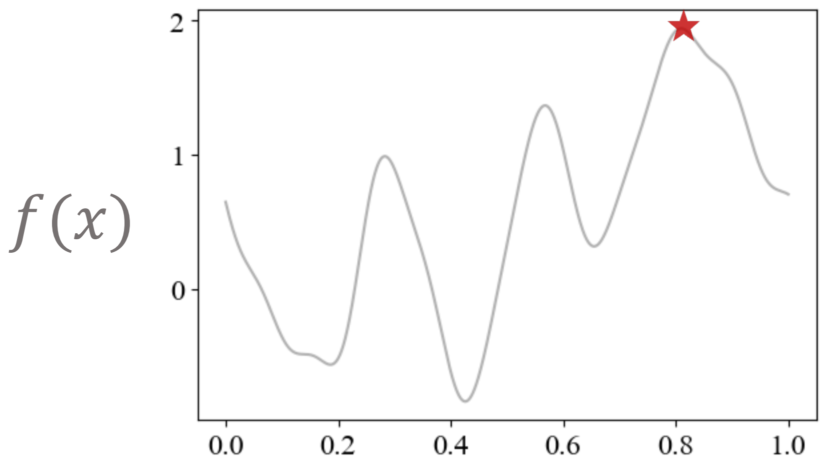
Independent

Flexible-stopping

Expected cost-adjusted regret

Gittins index is optimal

Bayesian Optimization



Continuous

Correlated

Fixed-budget / Flexible-stopping

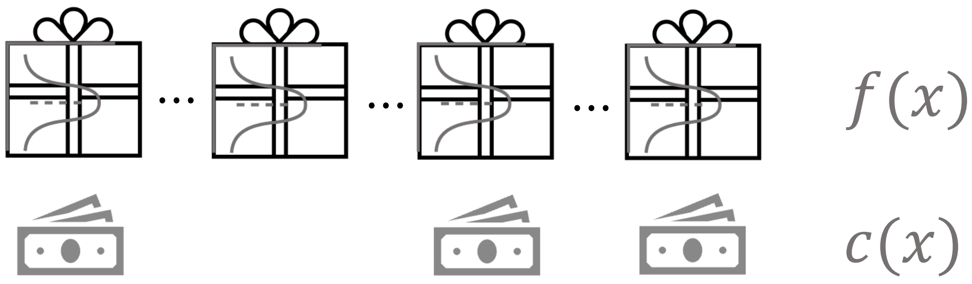
Expected (cost-adjusted) regret

Is Gittins index good?

empirically

Pandora's Box

[Weitzman'79]



Discrete

Independent

Flexible-stopping

Expected cost-adjusted regret

Gittins index is optimal

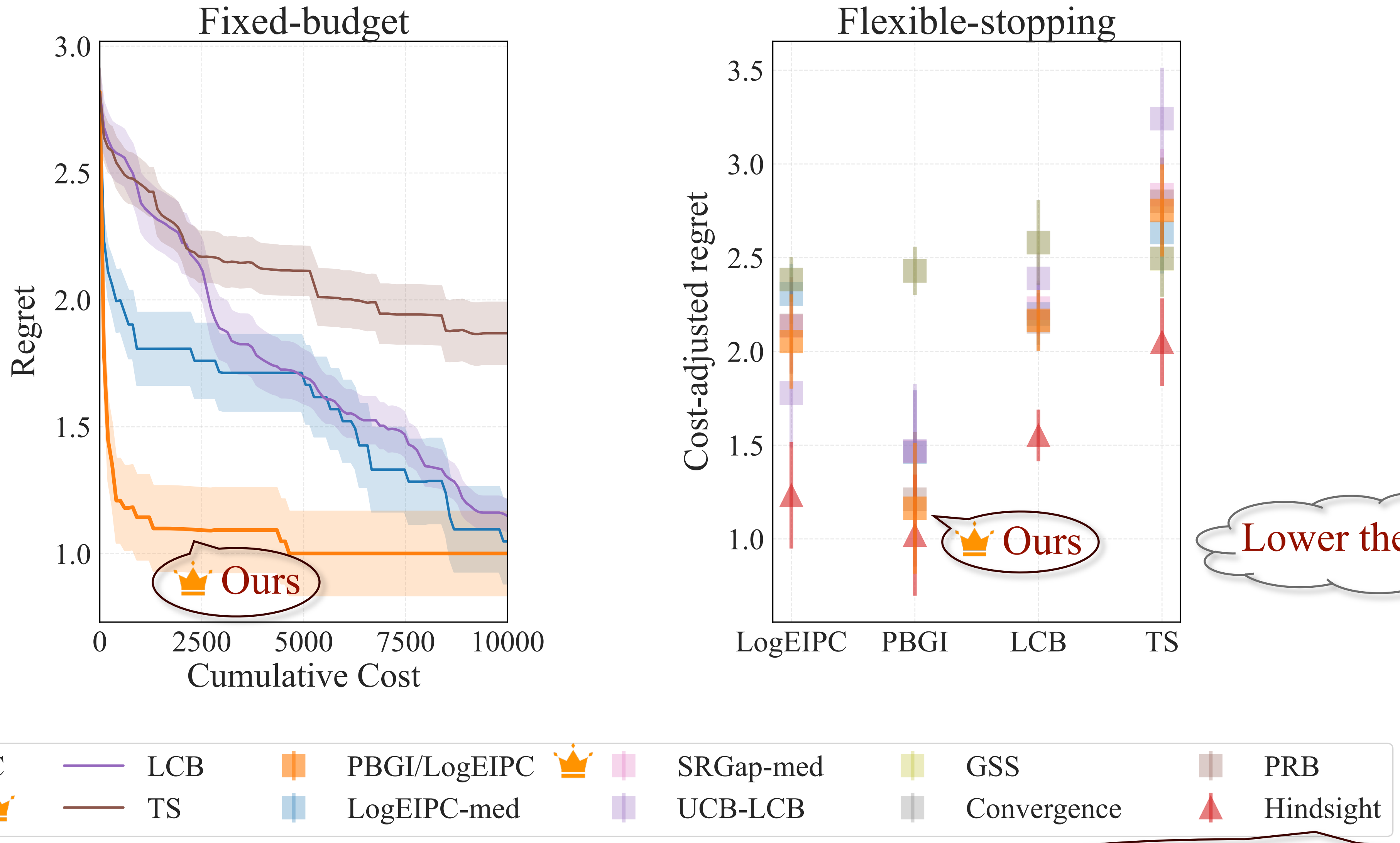
Our Contribution: Gittins Index Principle

- 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

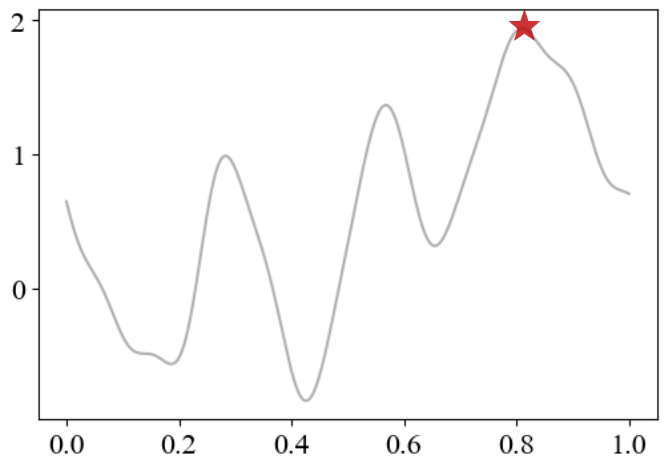
Gittins Index vs Baselines on AutoML Benchmark



Lower the better

Bound on achievable performance

Bayesian Optimization



$f(x)$

Continuous

Correlated

Fixed-budget / Flexible-stopping

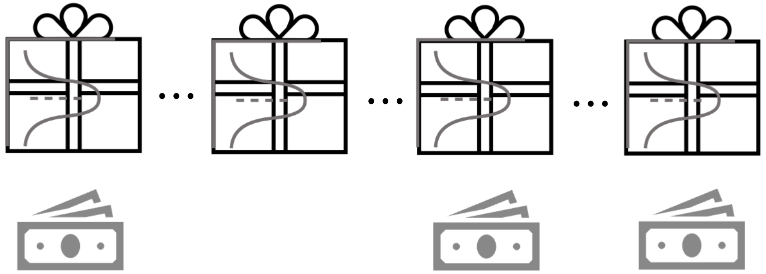
Expected (cost-adjusted) regret

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?

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3. Comes with theoretical guarantees

Theoretical Guarantee and Empirical Validation

Theorem (No worse than stopping-immediately)

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

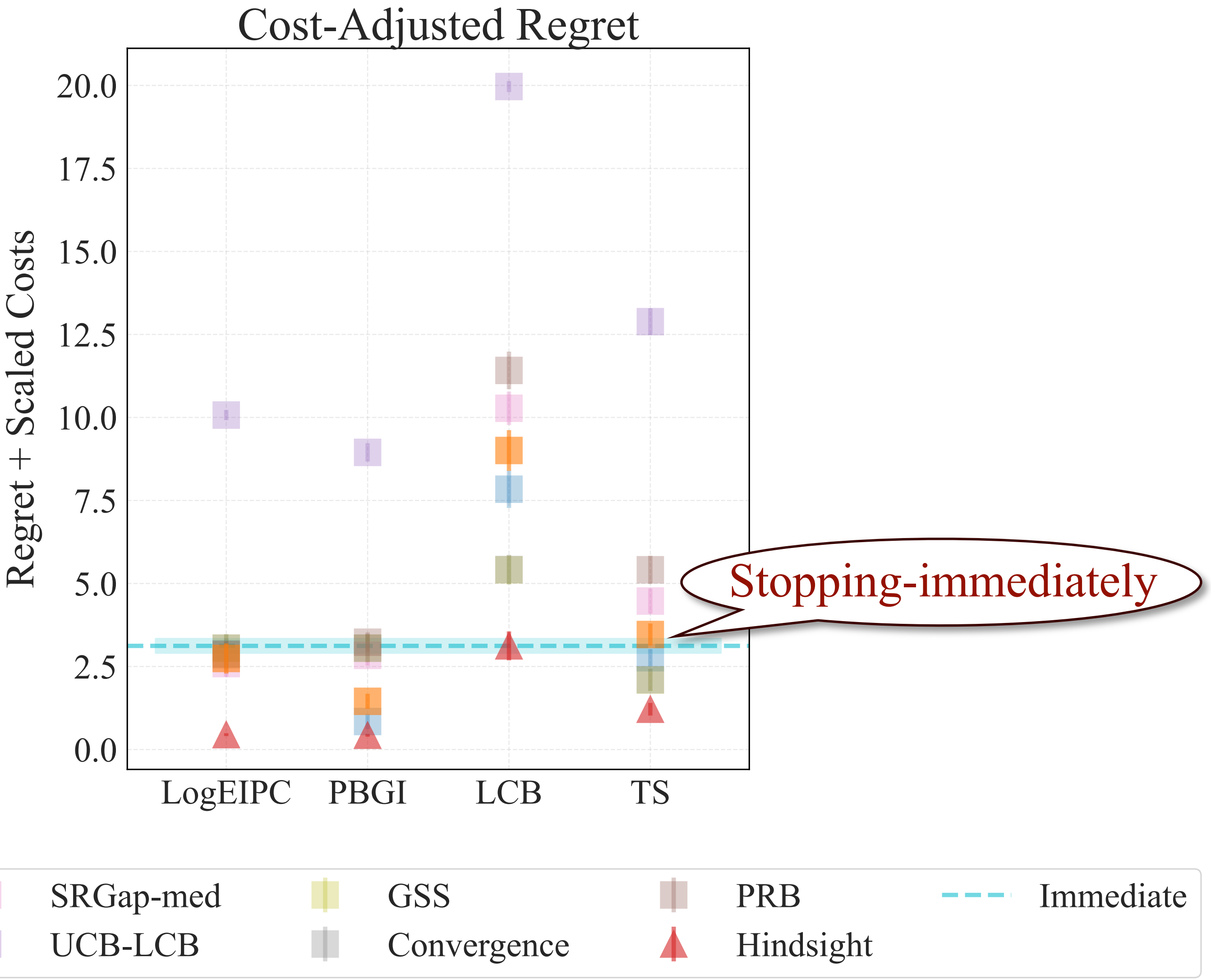
or LogEIPC

cost-adjusted regret

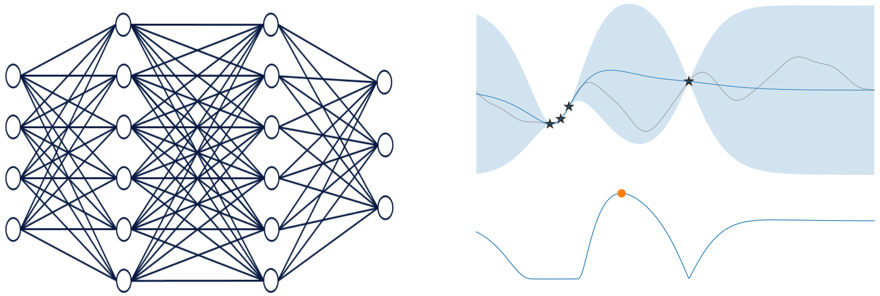
Implication:

- 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.



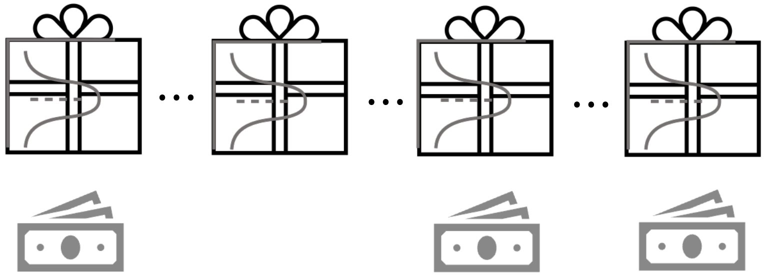
Studied problem



Varying evaluation costs

Adaptive stopping time

Key idea



Link to Pandora's Box problem
& Gittins index theory

Impact

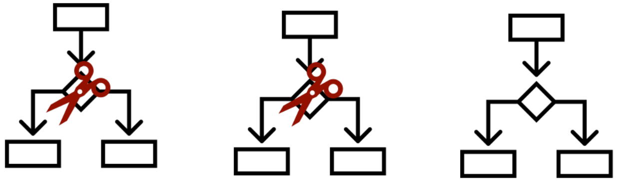
Meta

BoTorch Ax

Competitive empirical performance &
interests from practitioners

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

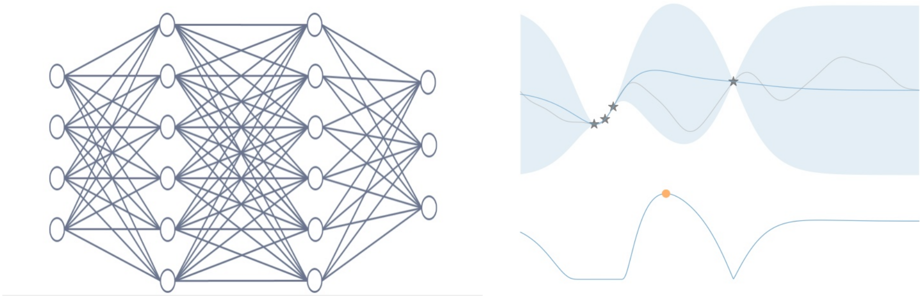
Ongoing work



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

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

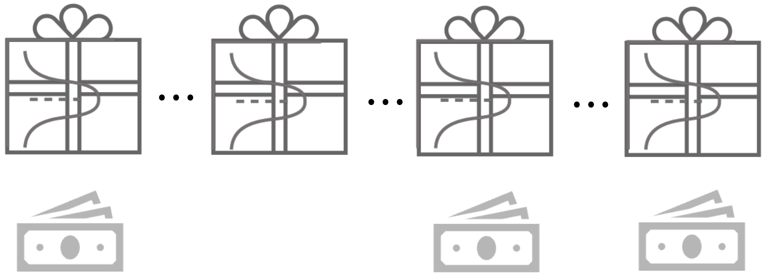
Studied problem



Varying evaluation costs

Adaptive stopping time

Key idea



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Ongoing work

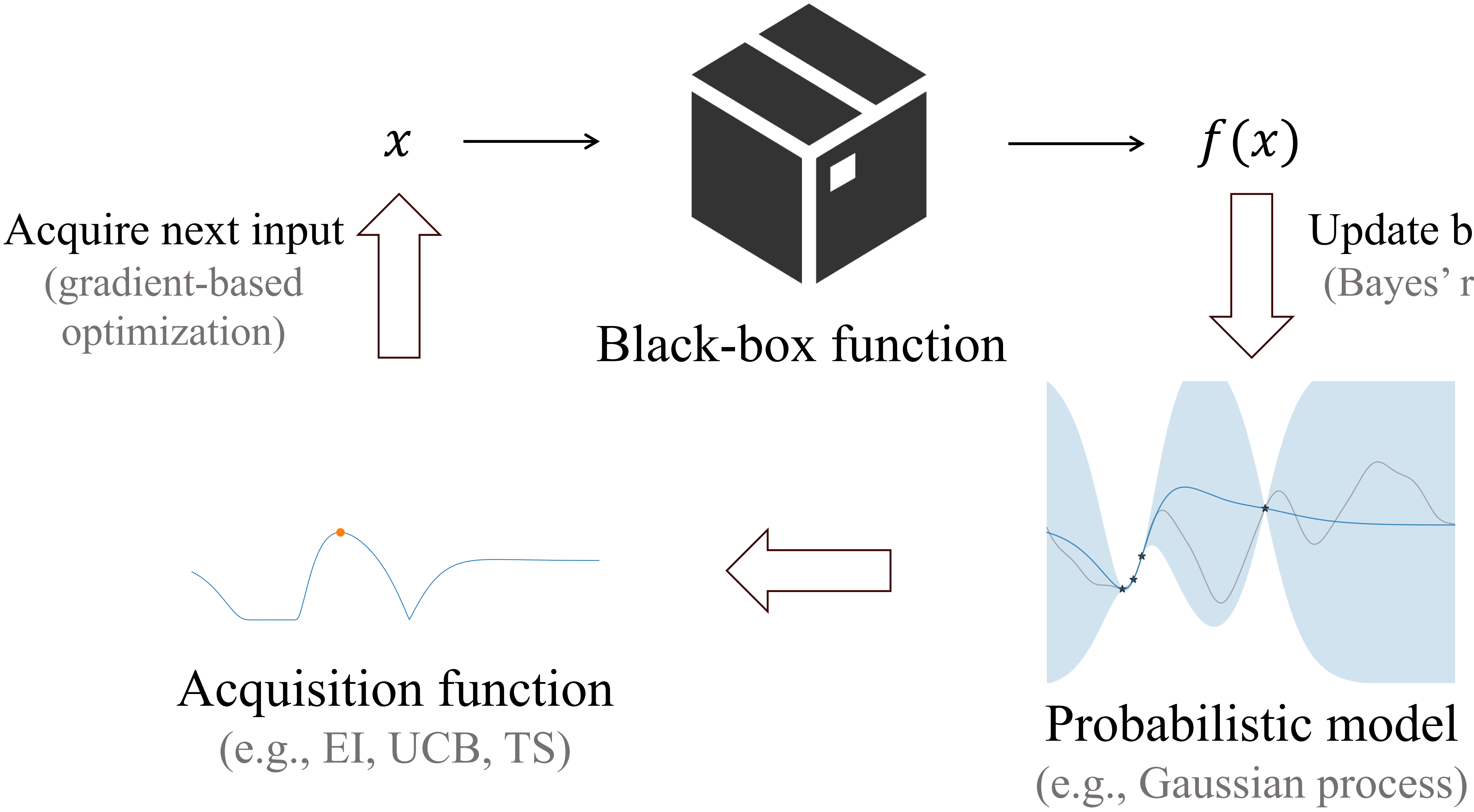
ChatGPT Gemini

deepseek Claude

LLM-driven black-box optimization

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

Recap: Bayesian Optimization



Ongoing: LLM-Driven Black-Box Optimization

Joint work with Yu Yu and Li Jin (SJTU)

x →  → $f(x)$

Acquire next input
(LLM proposal)

Black-box function

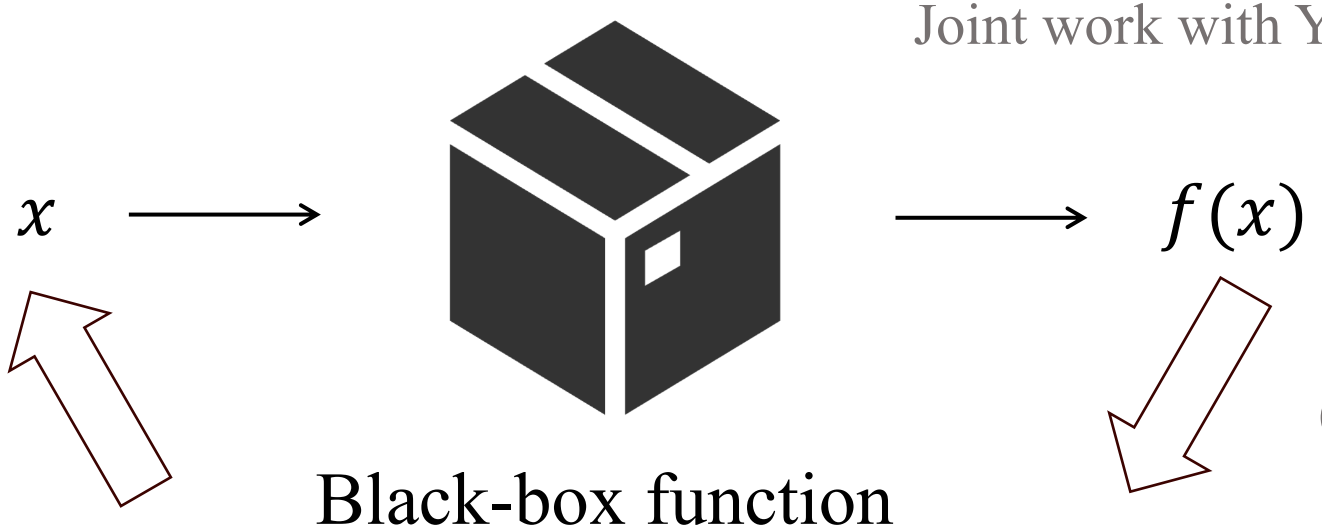
Update belief
(feedback-augmented context)

Acquisition function
(e.g., Softmax sampling)

Probabilistic model
(e.g., autoregressive model)

Ongoing: LLM-Driven Black-Box Optimization

Joint work with Yu Yu and Li Jin (SJTU)



Acquire next input
(LLM proposal)

Black-box function

Update belief
(feedback-augmented context)

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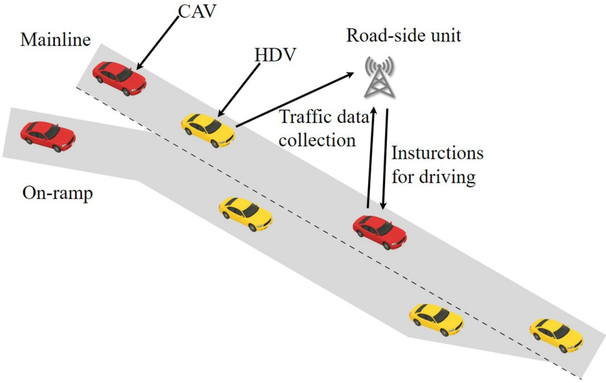
Large language model

Ongoing: LLM-Driven Black-Box Optimization

Mixed-autonomy traffic control:

Joint work with Yu Yu and Li Jin (SJTU)

(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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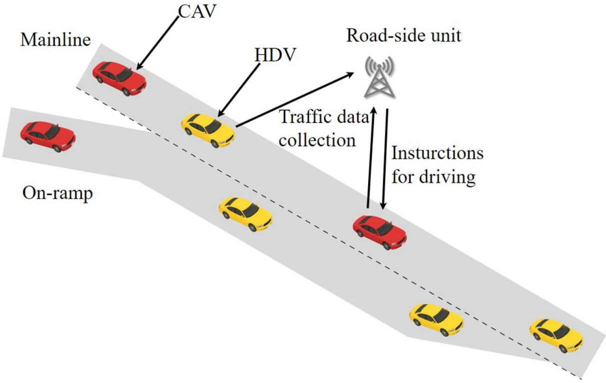
Ongoing: LLM-Driven Black-Box Optimization

Mixed-autonomy traffic control:

Joint work with Yu Yu and Li Jin (SJTU)

(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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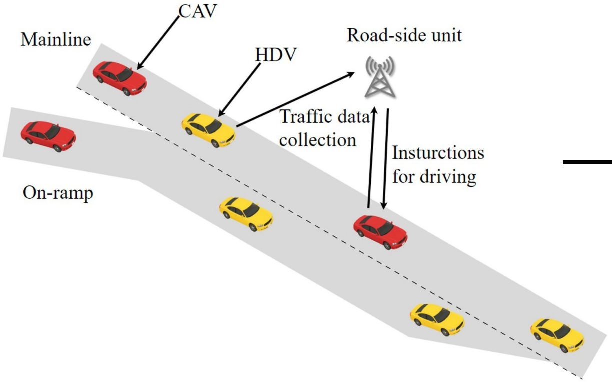
Our LLM-Driven Method: Incorporate Side Info

Mixed-autonomy traffic control:

Joint work with Yu Yu and Li Jin (SJTU)



(e.g., Transformer config)
RL state representation → Average speed

Update belief
(feedback-augmented context)

performance metric +
representation quality

Black-box function
(RL training & evaluation)

Acquire next input
(LLM proposal)

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Large language model

Find our papers on arXiv!

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

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