Cost-Aware Bayesian Optimization with Adaptive Stopping via Gittins Indices

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INFORMS Annual Meeting 2025 Job Market Showcase

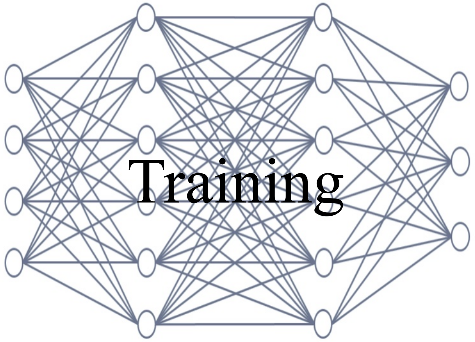
Black-Box Optimization

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

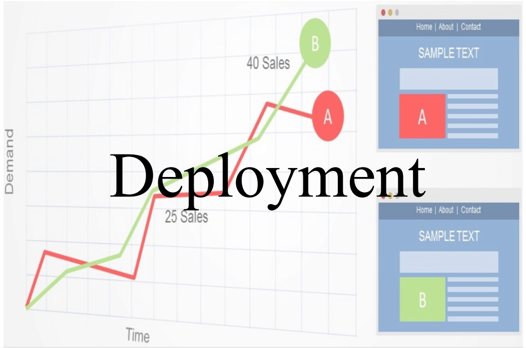
Black-Box Optimization

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

ML model training:

Training hyperparameters ⟶  Training ⟶ Accuracy

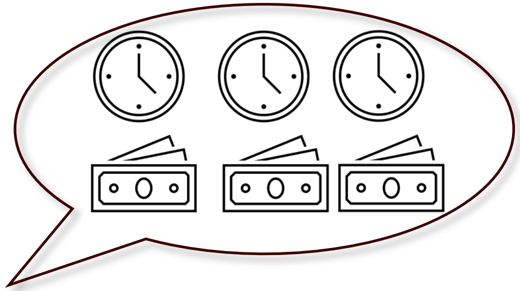
Adaptive experimentation:

Decision/design variables ⟶ 

Deployment ⟶ Revenue

Black-Box Optimization

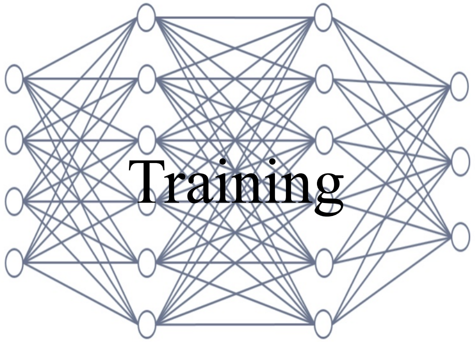
Input x →  → Performance metric $f(x)$

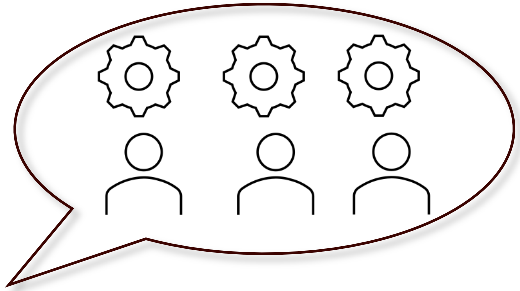


Training time

Compute credits

ML model training:

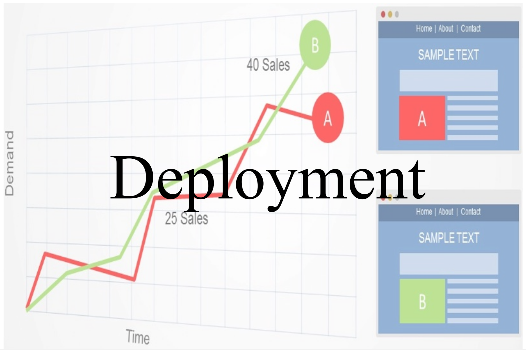
Training hyperparameters →  → Accuracy



Operational cost

User experience

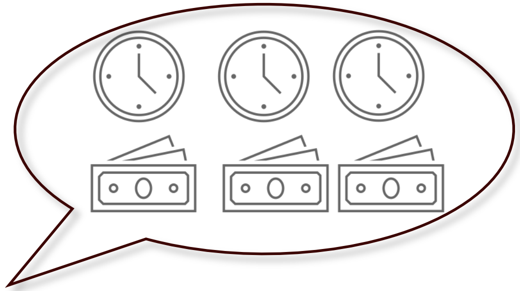
Adaptive experimentation:

Decision/design variables →  → Revenue

Black-Box Optimization

expensive-to-evaluate

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



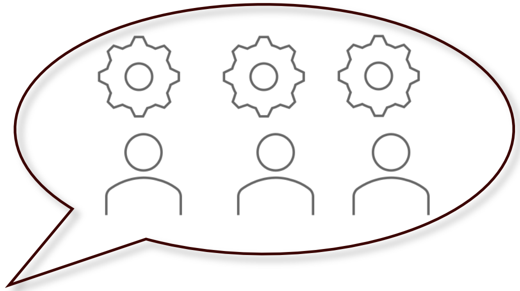
Training time

Compute credits

ML model training:

Training hyperparameters $\longrightarrow$ 

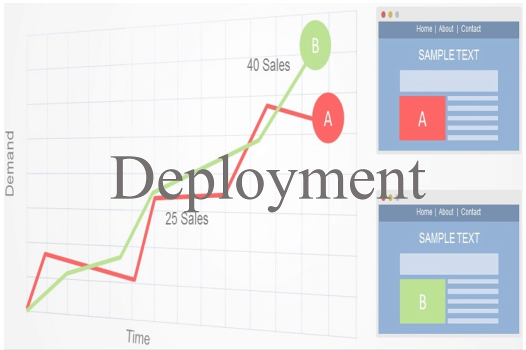
$\longrightarrow$ Accuracy



Operational cost

User experience

Adaptive experimentation:

Decision/design variables $\longrightarrow$ 

$\longrightarrow$ Revenue

Black-Box Optimization

expensive-to-evaluate

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

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

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

Black-Box Optimization

expensive-to-evaluate

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

adaptively

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

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

Fewer #evaluations

Black-Box Optimization

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

expensive-to-evaluate

adaptively

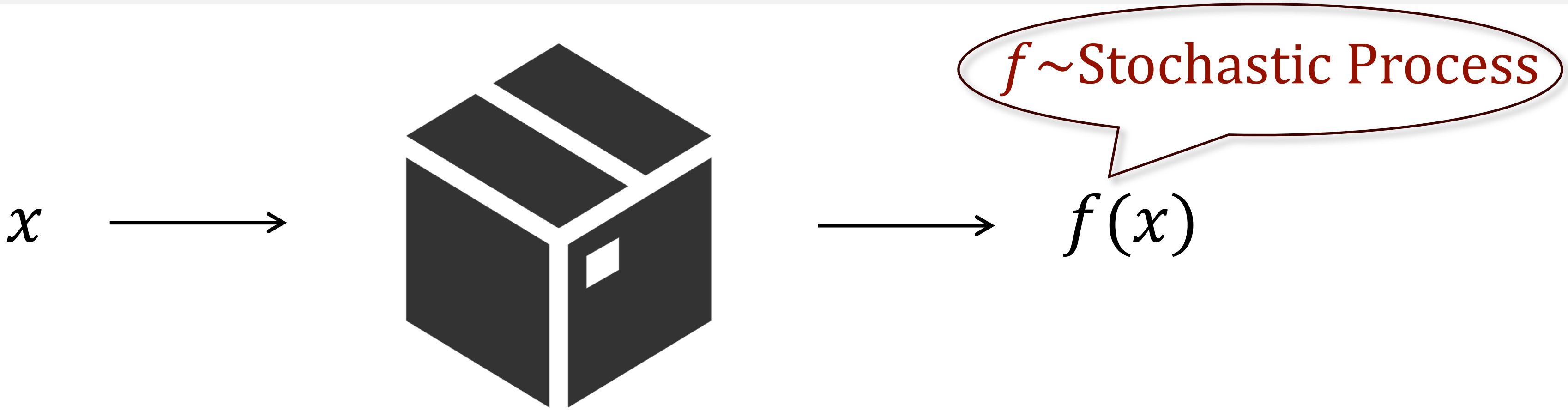
High-level goal: Choose $x_1, \dots, x_T$ to maximize the expected best observed value

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

Fewer #evaluations

Efficient framework: Bayesian optimization

Bayesian Optimization



Black-box function

Bayesian Optimization

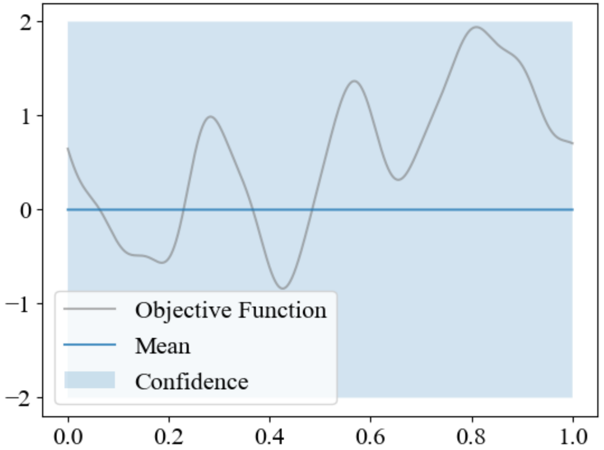
Time 0

$f \sim$ Stochastic Process

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

Black-box function

Model belief



Probabilistic model

(e.g., Gaussian process)

Bayesian Optimization

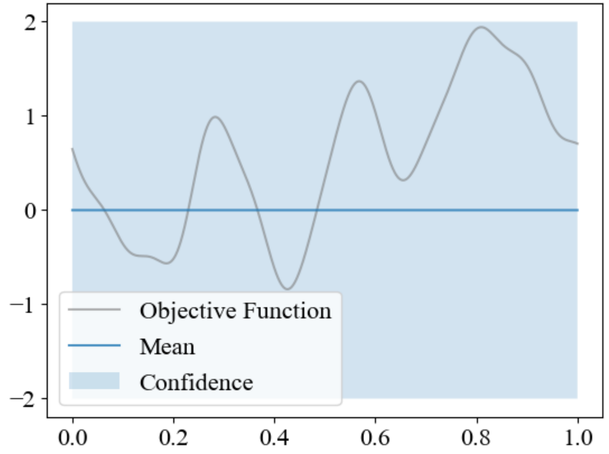
Time t

$f \sim$ Stochastic Process

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

Black-box function

Model belief



Probabilistic model

(e.g., Gaussian process)

Bayesian Optimization

Time t

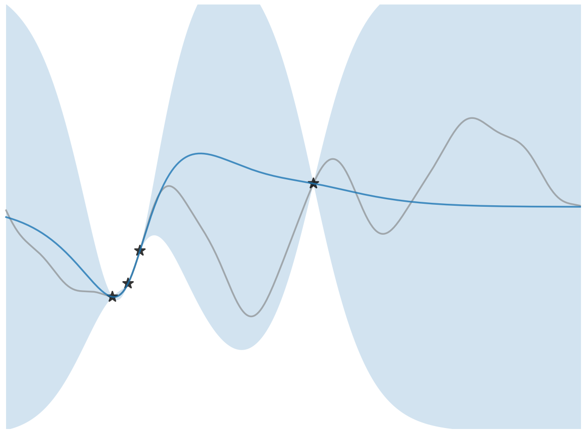
$x_1, \ldots, x_t \longrightarrow$

Black-box function

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

$f \sim$Stochastic Process

Update belief
(Bayes' rule)



Probabilistic model
(e.g., Gaussian process)

Bayesian Optimization

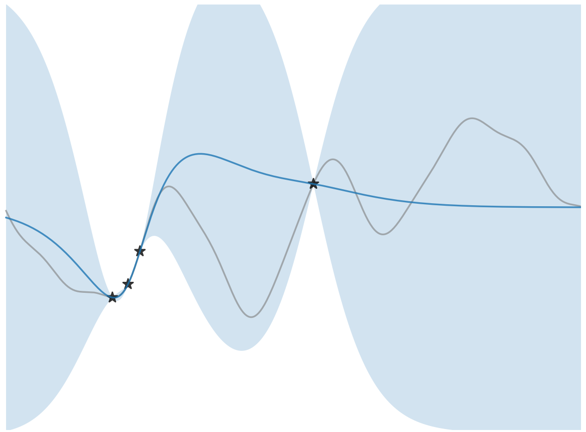
Time t

$x_1, \dots, x_t \longrightarrow$

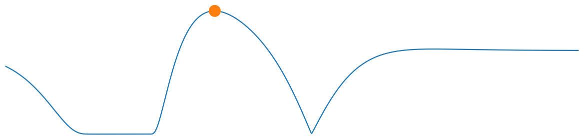
Black-box function

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

Update belief
(Bayes' rule)



Probabilistic model
(e.g., Gaussian process)



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

Bayesian Optimization

Time t

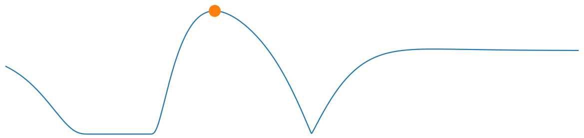
$x_1, \ldots, x_t \longrightarrow$

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

Black-box function

Select next input
(gradient-based optimization)

Update belief
(Bayes' rule)



Decision rule
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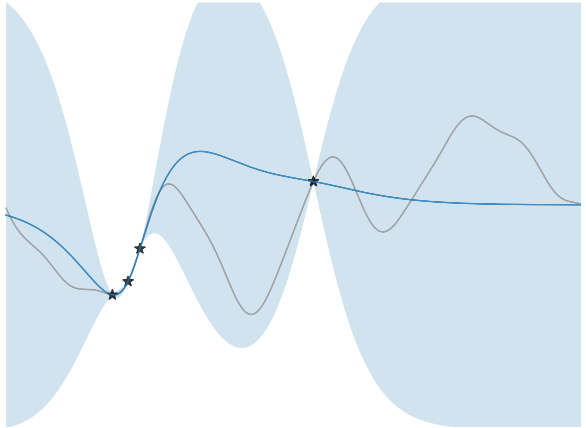


Probabilistic model
(e.g., Gaussian process)

Bayesian Optimization

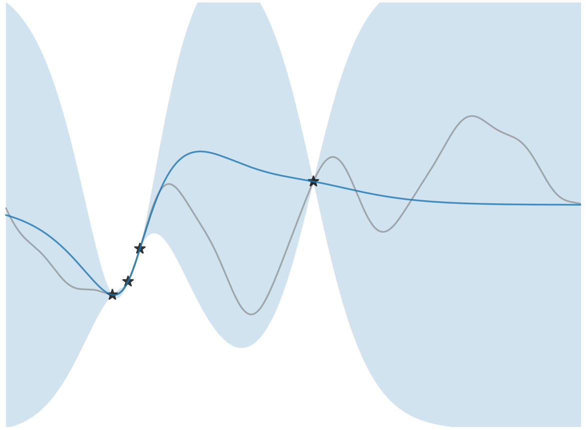
Time $t + 1$

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

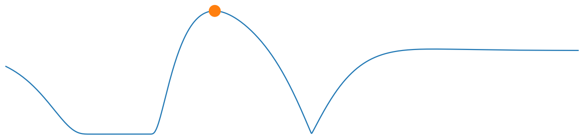
Black-box function

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

Update belief
(Bayes' rule)



Probabilistic model
(e.g., Gaussian process)



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

Select next input
(gradient-based
optimization)

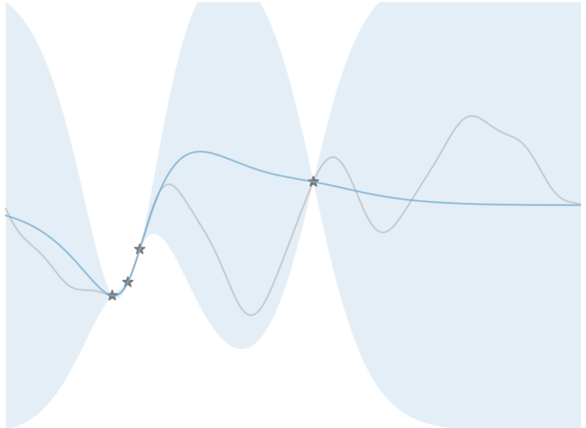
Bayesian Optimization

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

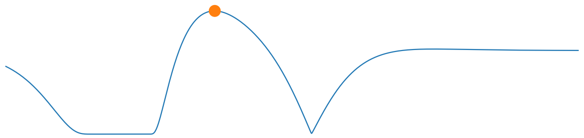
Select next input
(gradient-based
optimization)

Black-box function

Update belief
(Bayes' rule)



Probabilistic model
(e.g., Gaussian process)



My focus

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

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
- **Gittins Index**

New Design Principle: Gittins Index

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

New Design Principle: Gittins Index

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

Why another principle?

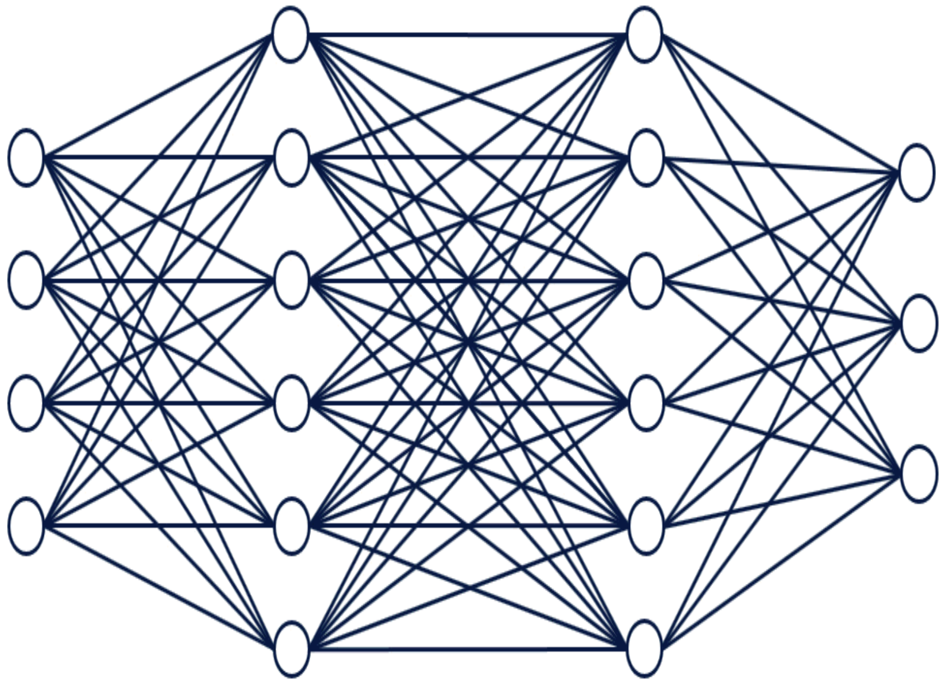
1. Naturally handles practical considerations
2. Performs competitively on benchmarks
3. Comes with theoretical guarantees

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

New design principle:
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New design principle:
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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

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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

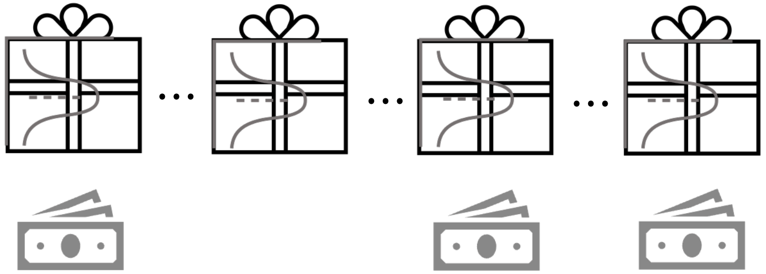
Features in Pandora's box

Observable multi-stage feedback

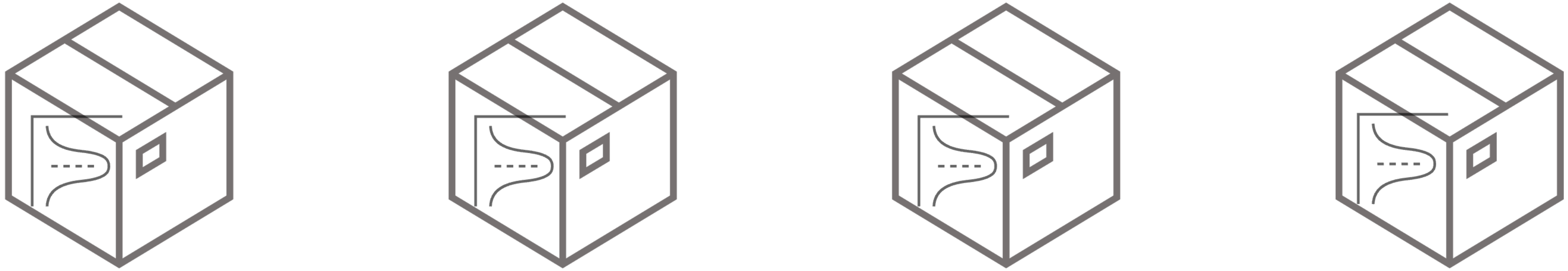
Features in Markovian bandits

New design principle:
Gittins index

Optimal in related sequential decision problems



Pandora's Box



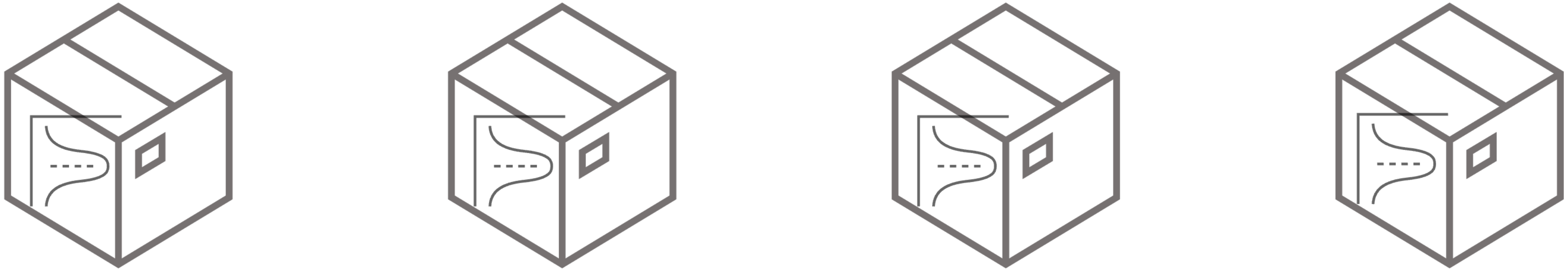
High-level goal: Choose $x_1, \ldots, x_T$ to maximize the expected utility

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

Flexible stopping time

Pandora's Box

$t = 0$



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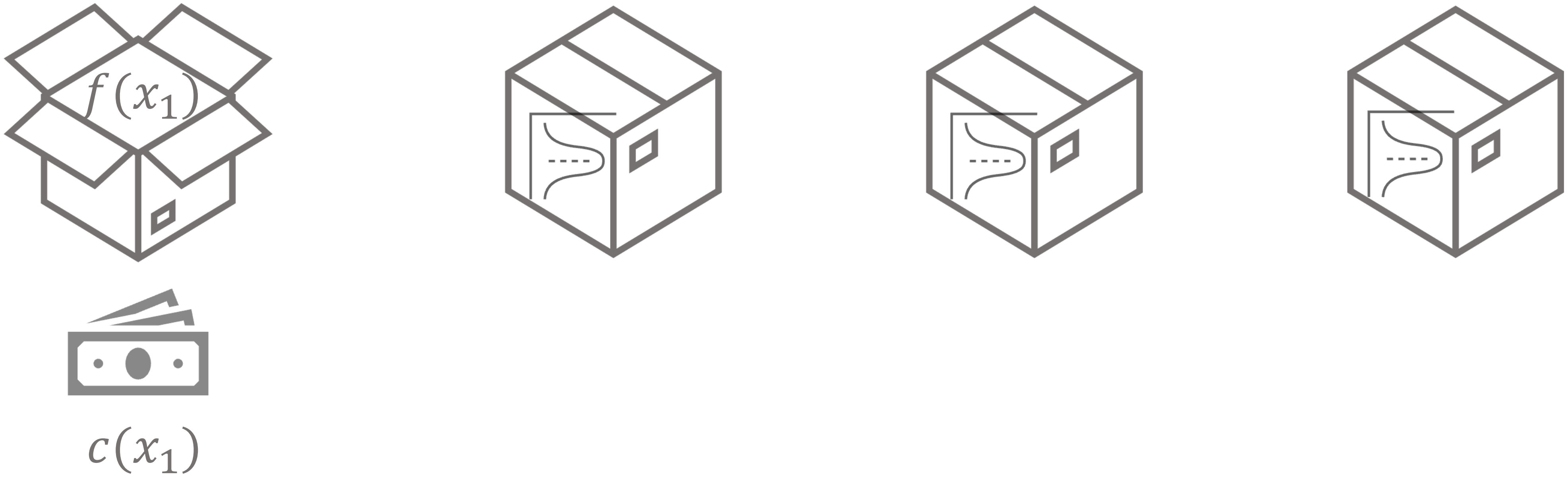
Pandora's Box

$t = 1$

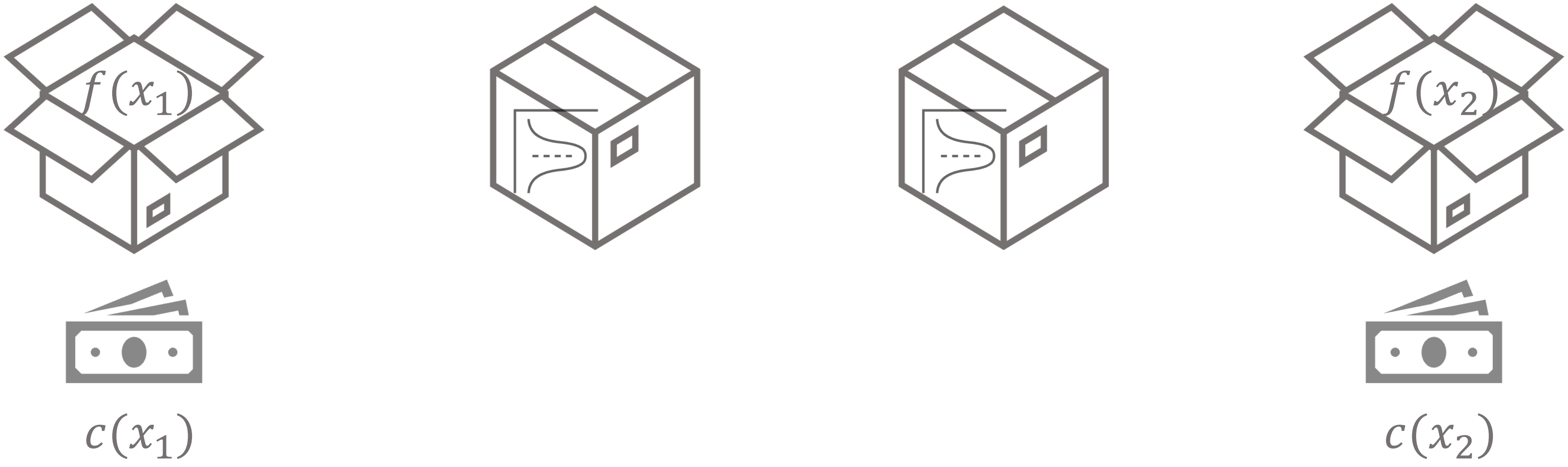


High-level goal: Choose $x_1, \dots, x_T$ to maximize the expected utility

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

Pandora's Box

$t = 2$

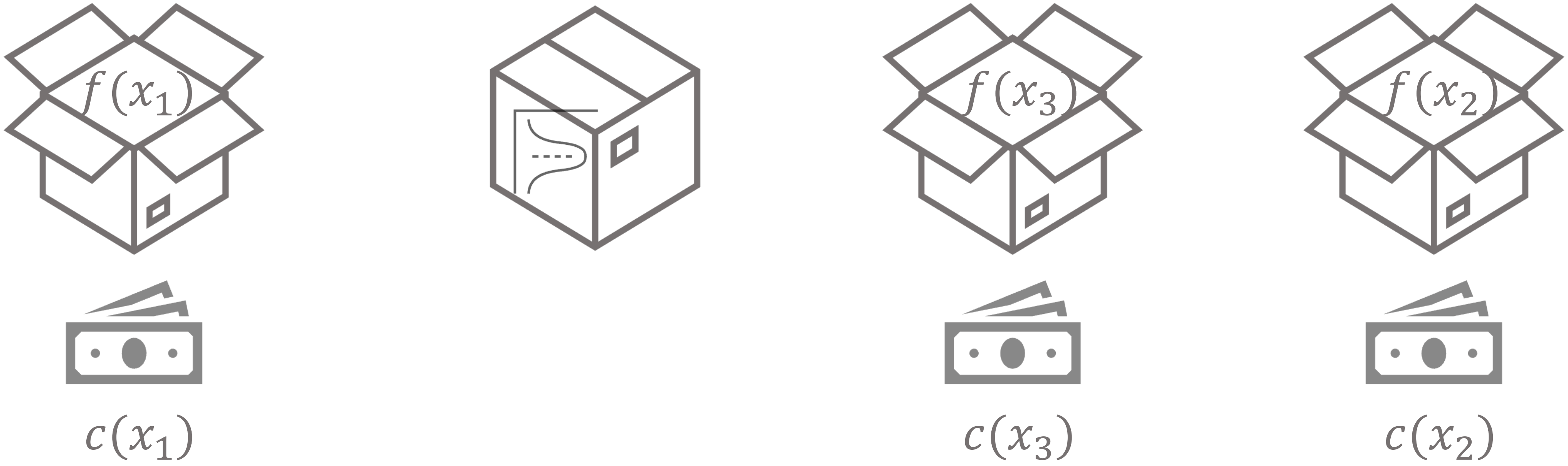


High-level goal: Choose $x_1, \ldots, x_T$ to maximize the expected utility

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

Pandora’s Box

$t = 3$

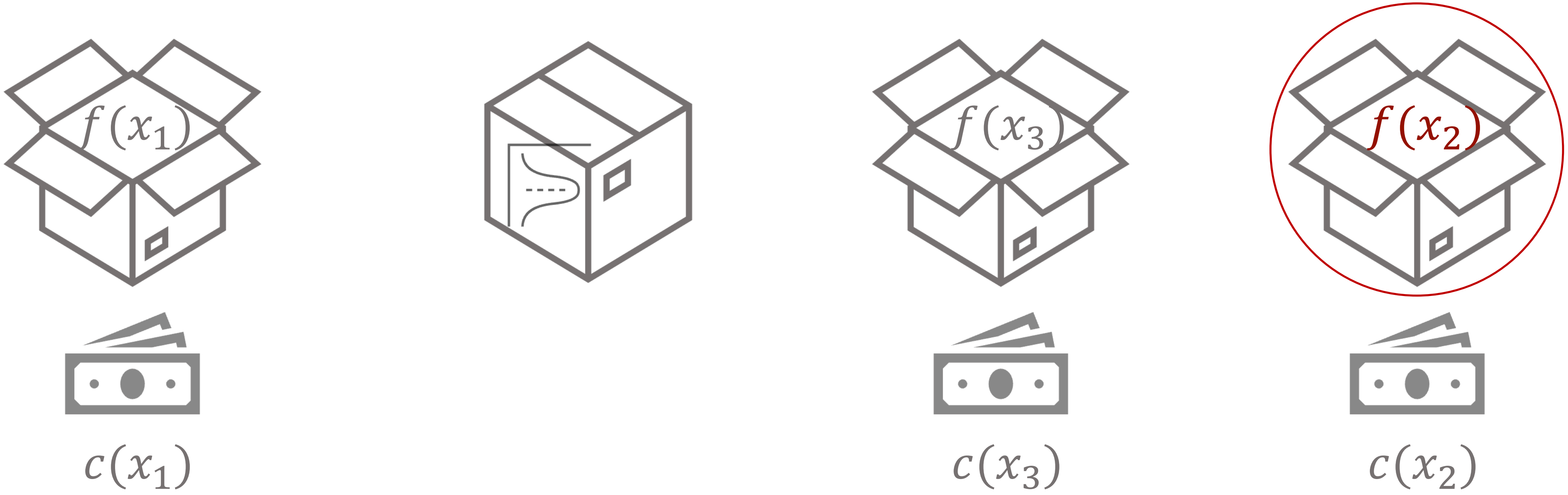


High-level goal: Choose $x_1, \ldots, x_T$ to maximize the expected utility

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

Pandora's Box

$t = T$, stop

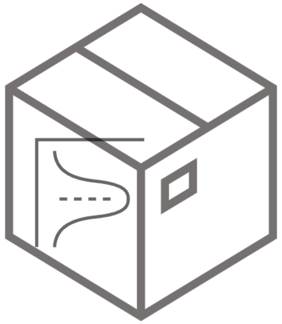


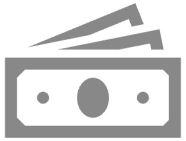
High-level goal: Choose $x_1, \ldots, x_T$ to maximize the expected utility

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

Optimal Policy: Gittins Index

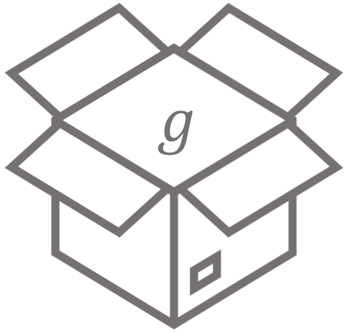
Step 1: Assign each box a Gittins index (higher is better)

$f(x)$ 

$c(x)$ 

$\downarrow$

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

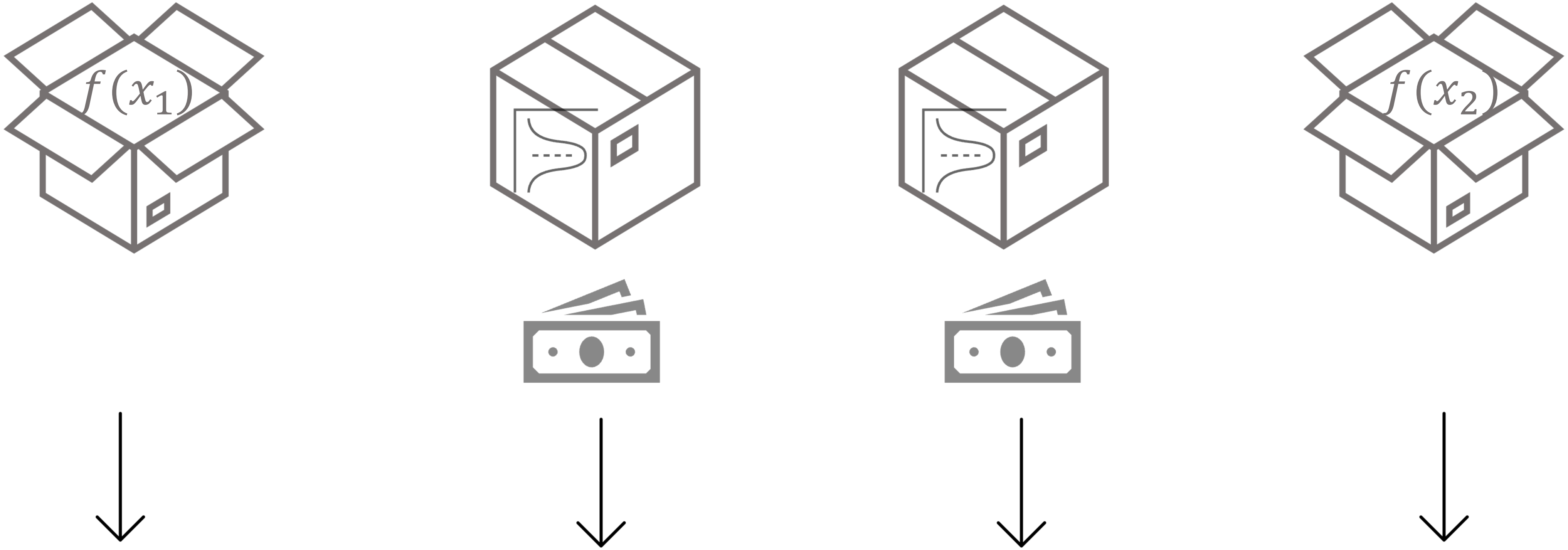


$\downarrow$

g

Optimal Policy: Gittins Index

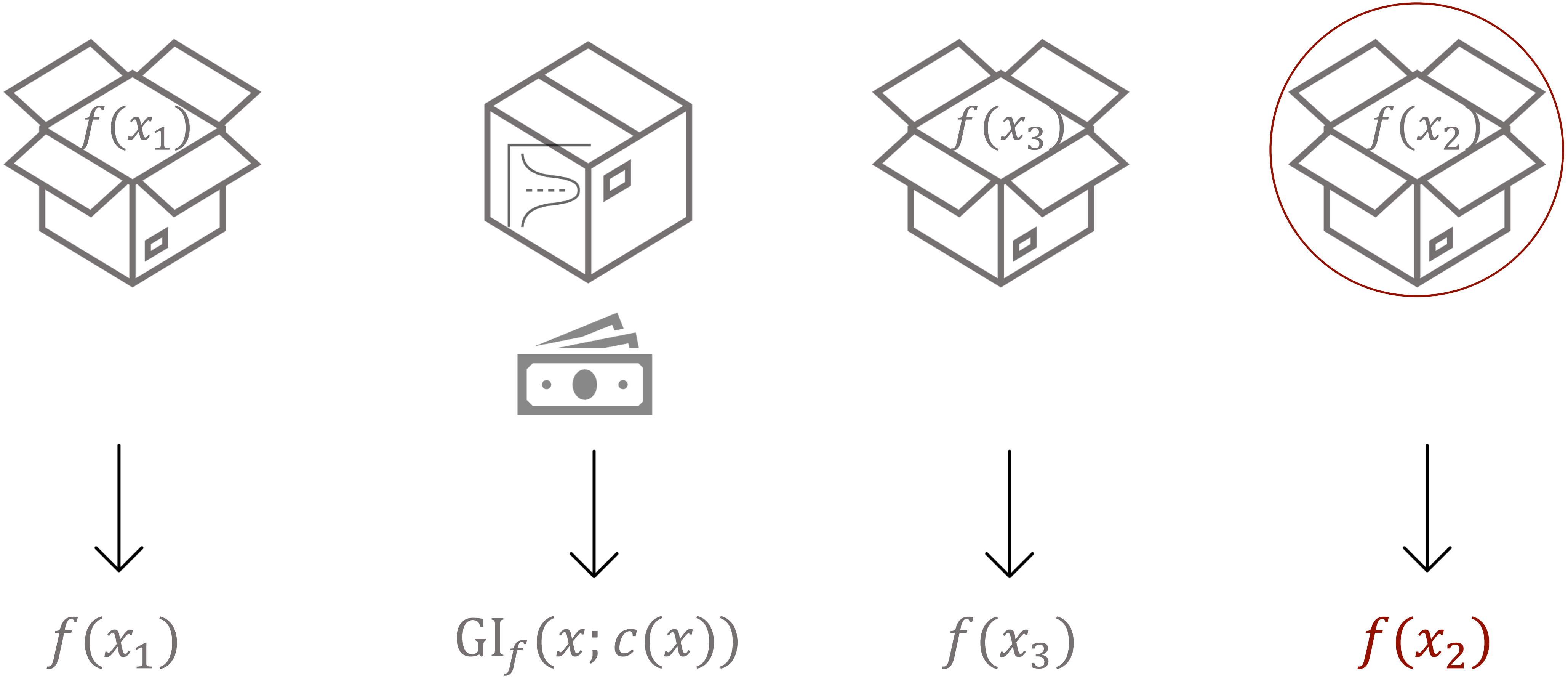
Step 2: Open the box with highest index if it is closed



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

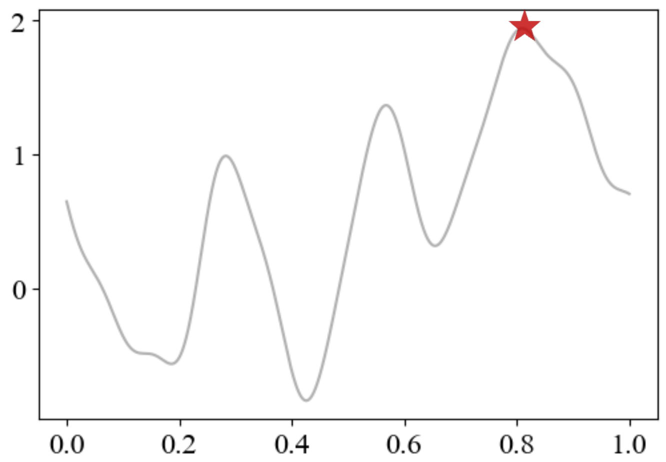
Optimal Policy: Gittins Index

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



Bayesian Optimization

$f(x)$



Continuous

Correlated

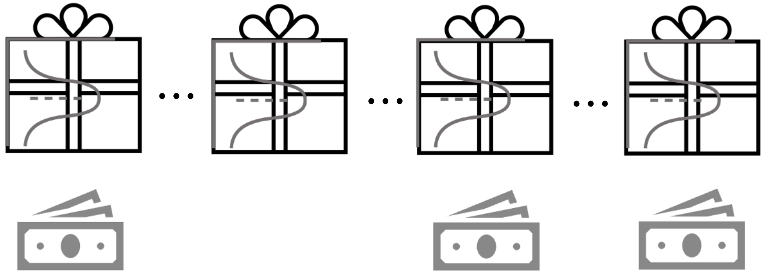
Fixed-iteration

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

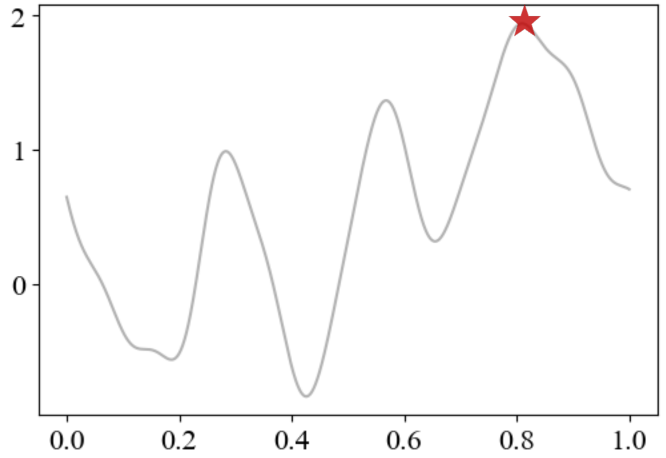
Expected utility

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

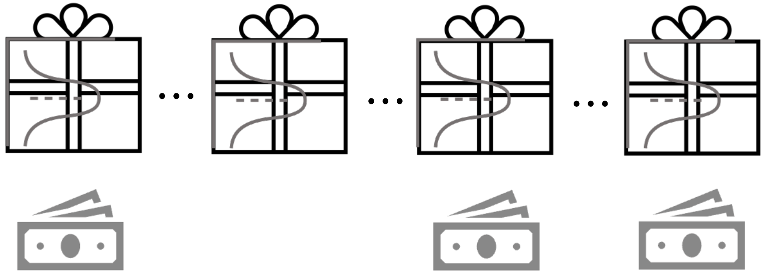
Fixed-iteration

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 cost-adjusted regret

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

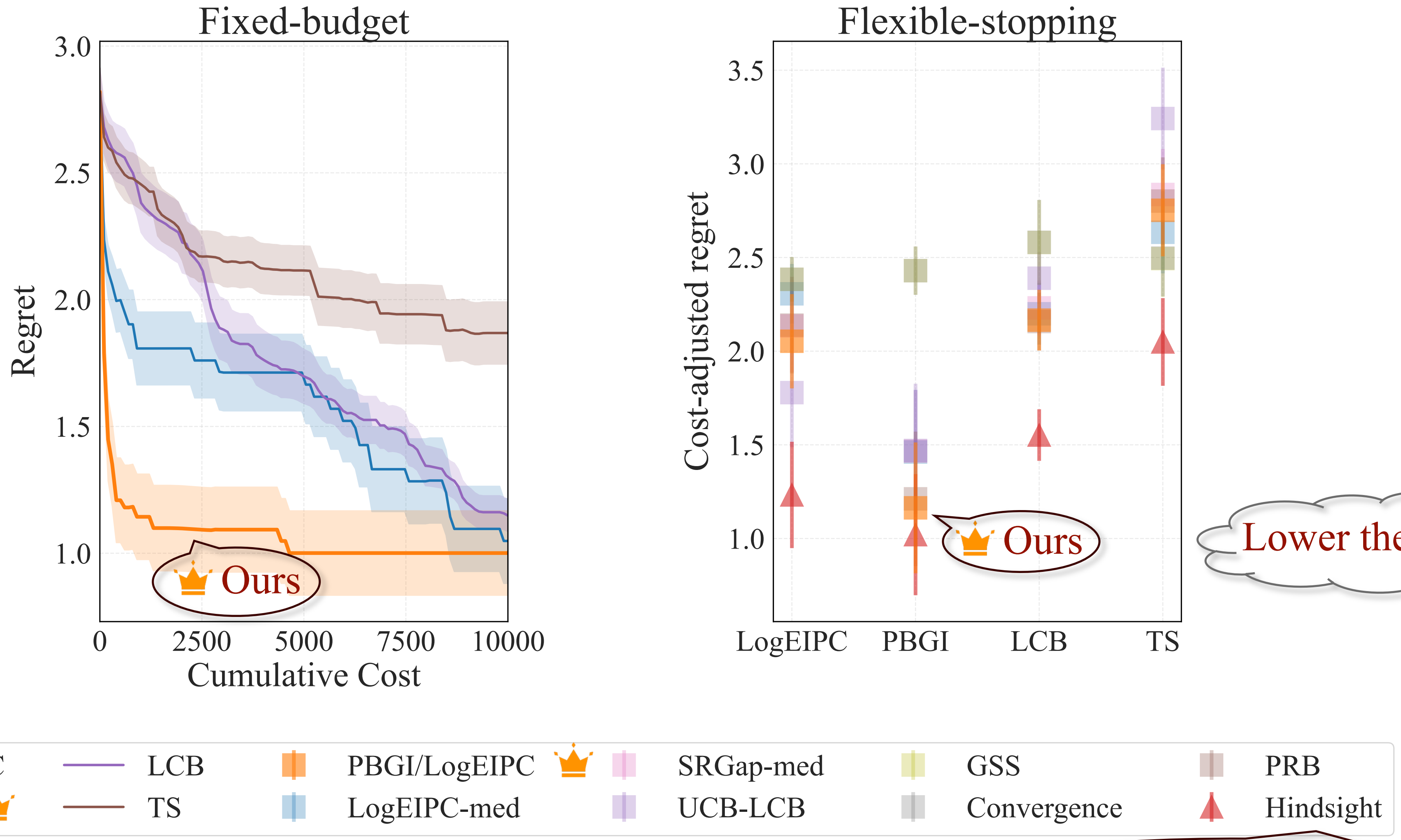
New Design Principle: Gittins Index

- 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



Lower the better

Bound on achievable performance

New Design Principle: Gittins Index

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

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Theoretical Guarantee and Empirical Validation

Theorem (No worse than stopping-immediately)

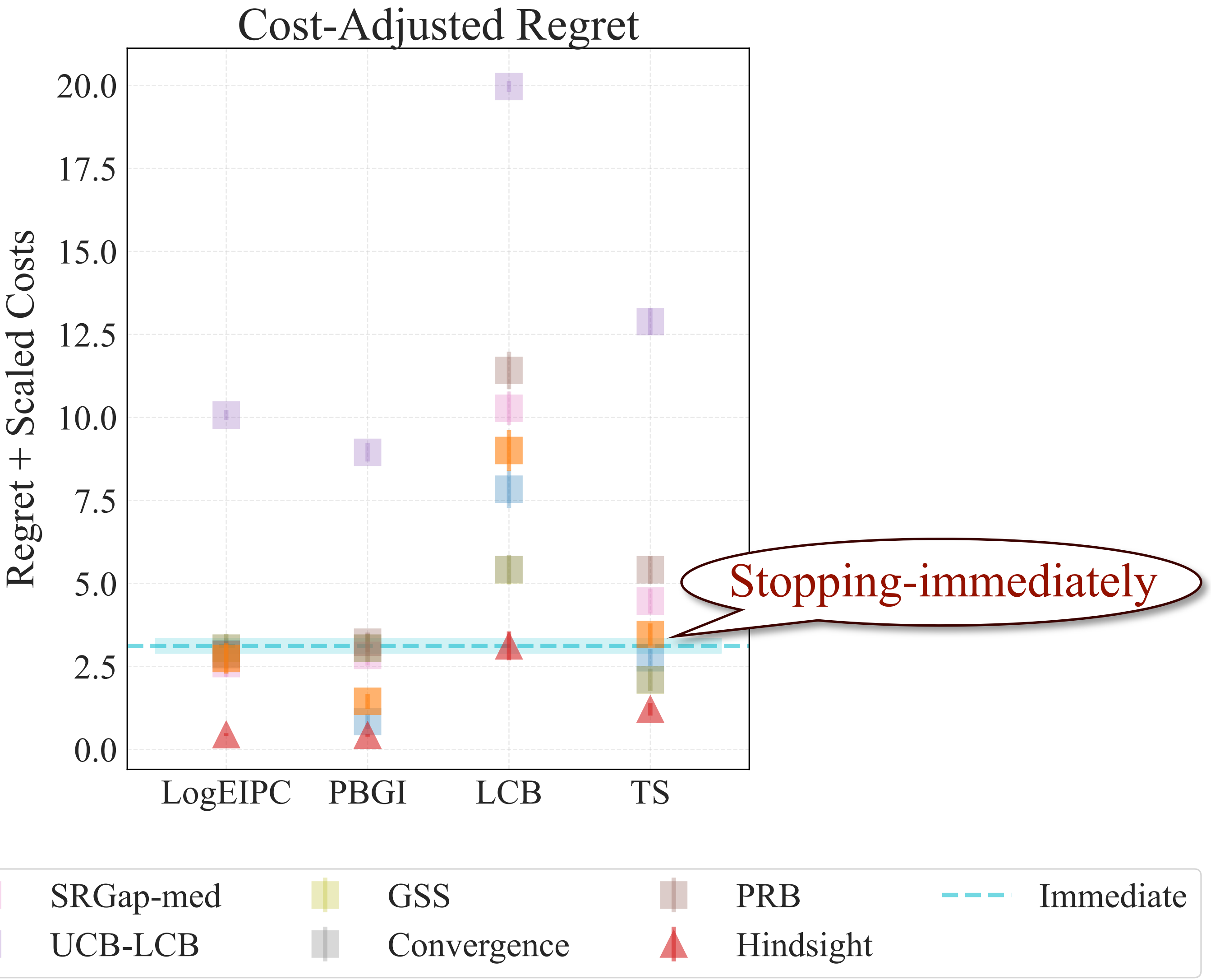
$$\mathbb{E}[R(\text{ours}; \text{PBGI})] \leq R[\text{stopping immediately}]$$

or LogEIPC

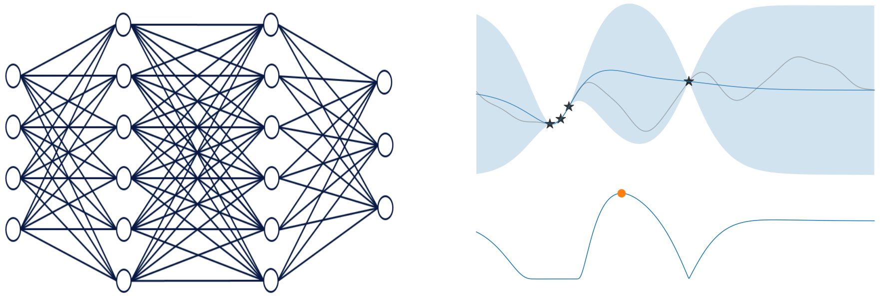
cost-adjusted regret

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.



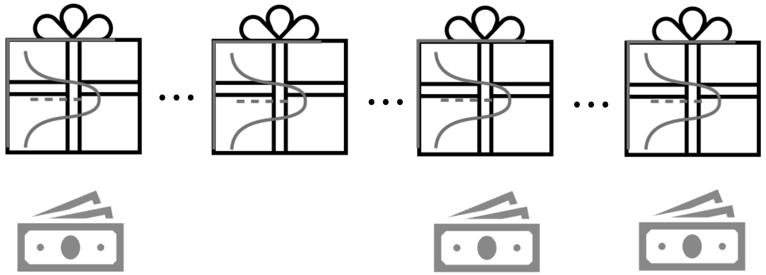
Studied problem



Varying evaluation costs

Adaptive stopping time

Key idea



Link to Pandora's Box problem
& Gittins index theory

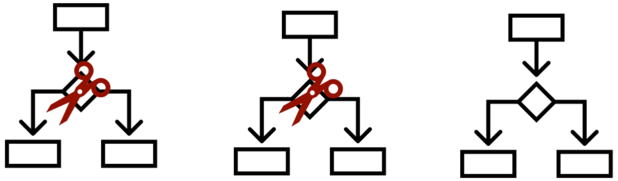
Impact

Meta

BoTorch Ax

Competitive empirical performance &
interests from practitioners

Ongoing work

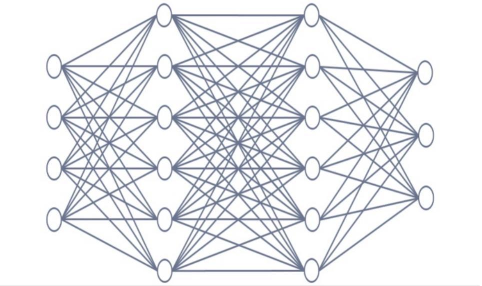


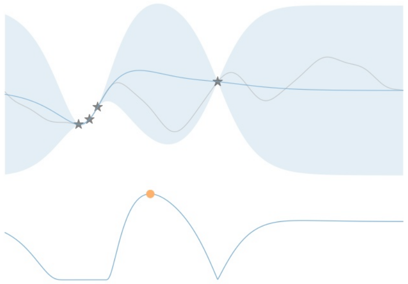
Sharper theoretical guarantees & black-box optimization w/ multi-stage feedback

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

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

Studied problem

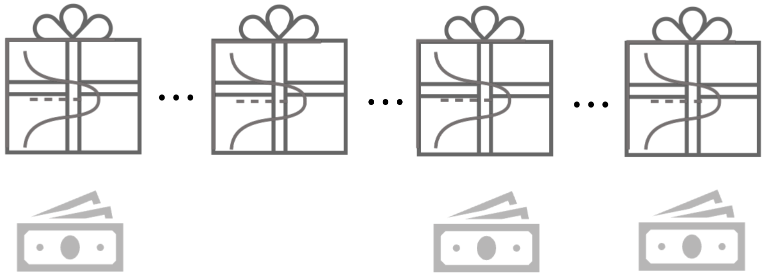




Varying evaluation costs

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

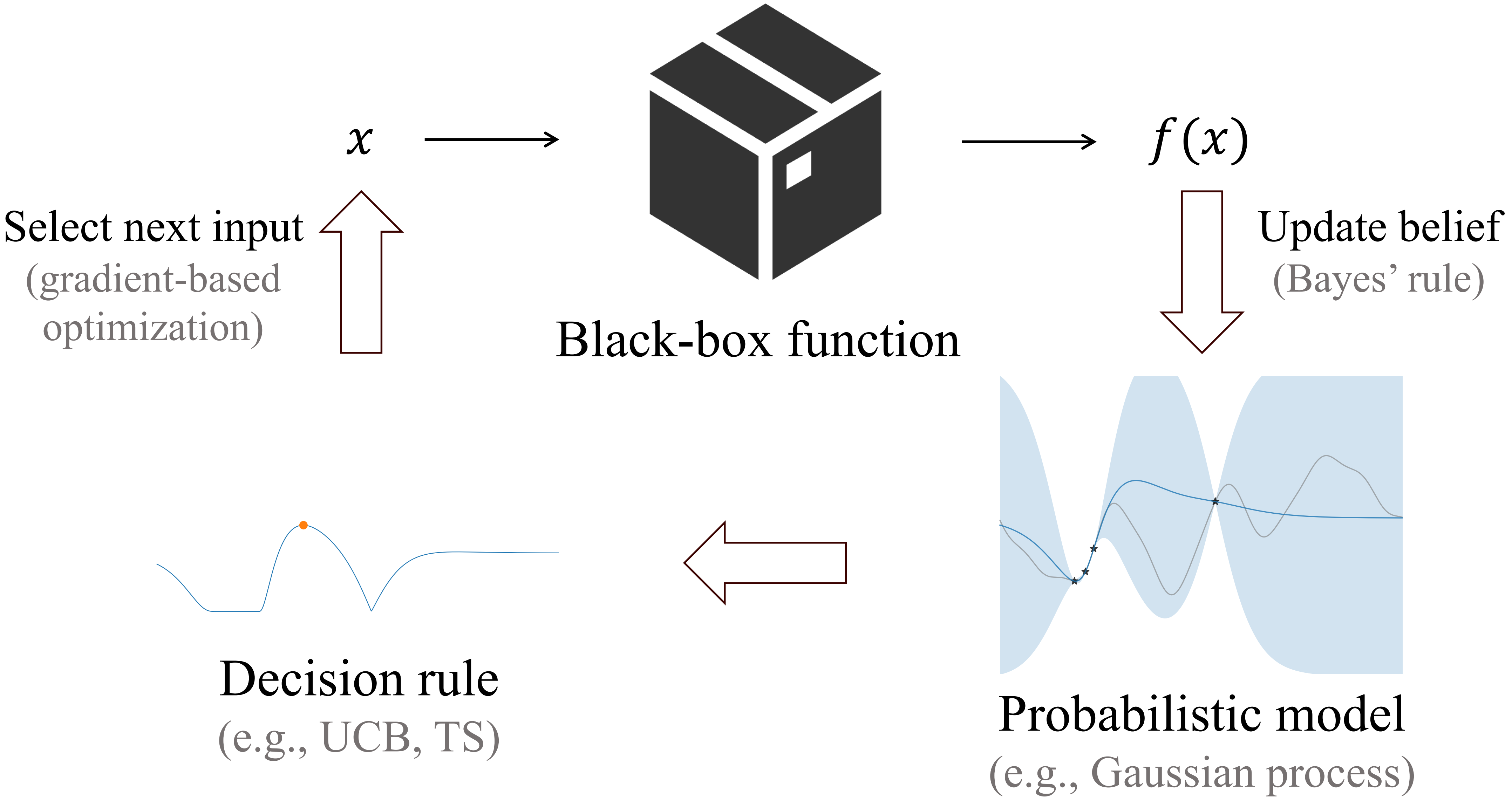
ChatGPT Gemini

deepseek Claude

LLM-driven black-box optimization

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

Recap: Bayesian Optimization



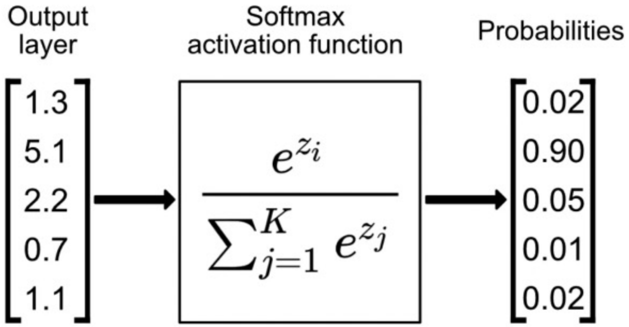
Ongoing: LLM-Driven Black-Box Optimization

x →  → $f(x)$

Black-box function

Select next input
(LLM proposal)

Update belief
(feedback-augmented context)



Decision rule
(e.g., Softmax sampling)

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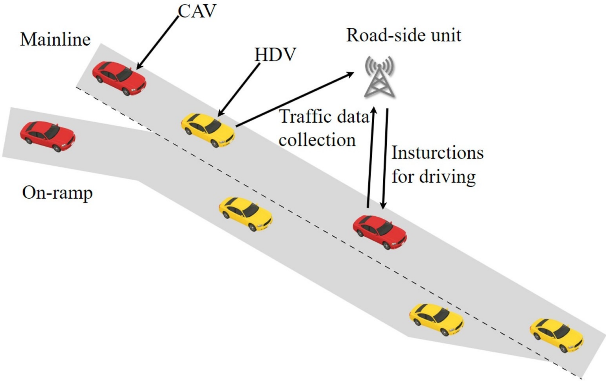
Probabilistic model
(large language model)

Ongoing: LLM-Driven RL Training Optimization

Mixed-autonomy traffic control:

(e.g., Transformer config)

x



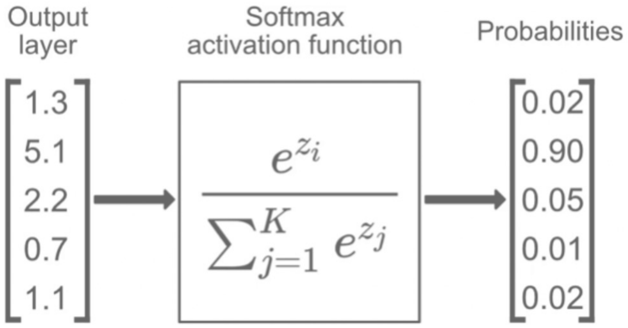
(e.g., average speed)

$f(x)$

Select next input
(LLM proposal)

Update belief
(feedback-augmented context)

Black-box function
(RL training & evaluation)



Decision rule
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Probabilistic model
(large language model)