Cost-Aware Bayesian Optimization with Adaptive Stopping via Gittins Indices

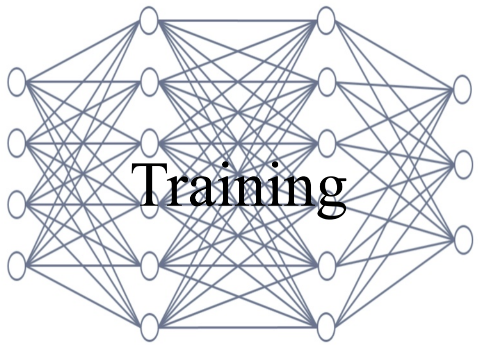
Qian Xie 谢倩 (Cornell ORIE)

INFORMS Annual Meeting 2025 Job Market Showcase

Optimization Under Uncertainty

ML model training:

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



⟶ Accuracy

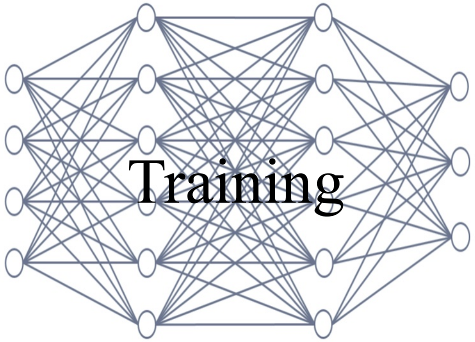
Optimization Under Uncertainty

Black-box optimization:

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

non-analytical & no gradient info

ML model training:

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

$\longrightarrow$ Accuracy

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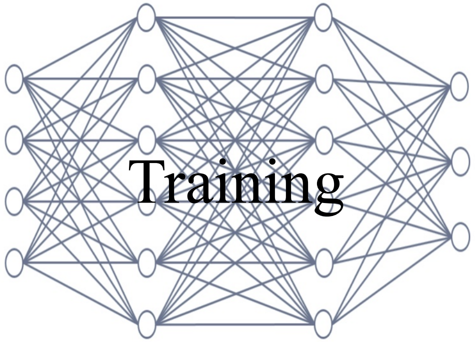
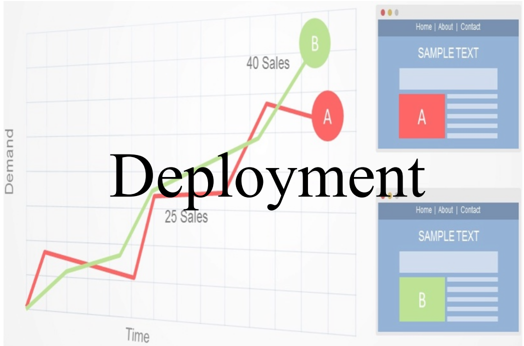
Training hyperparameters (e.g., learning rate, # layers) → 

Training

→ Accuracy

Adaptive experimentation:

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

Deployment

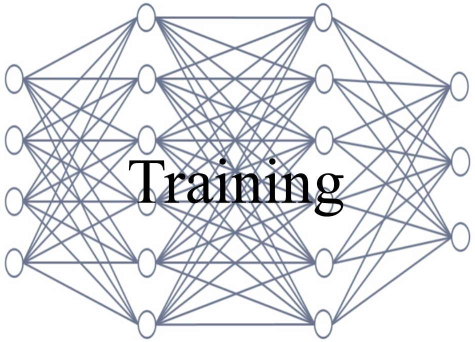
→ Revenue

Black-Box Optimization

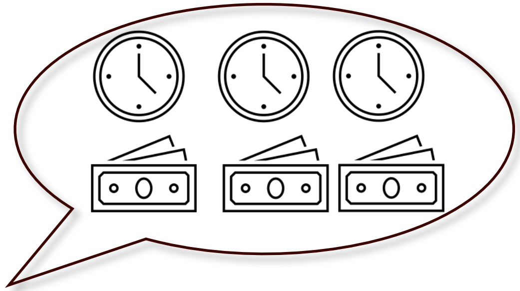
Input x →  → Performance metric $f(x)$

expensive-to-evaluate

ML model training:

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

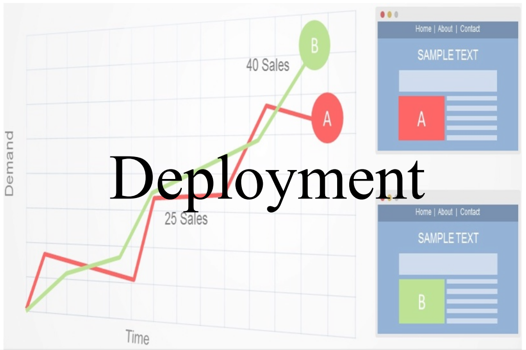
→ Accuracy



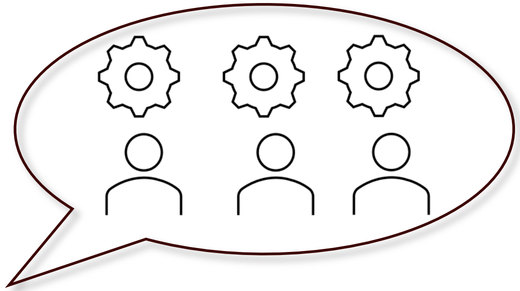
Training time

Compute credits

Adaptive experimentation:

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

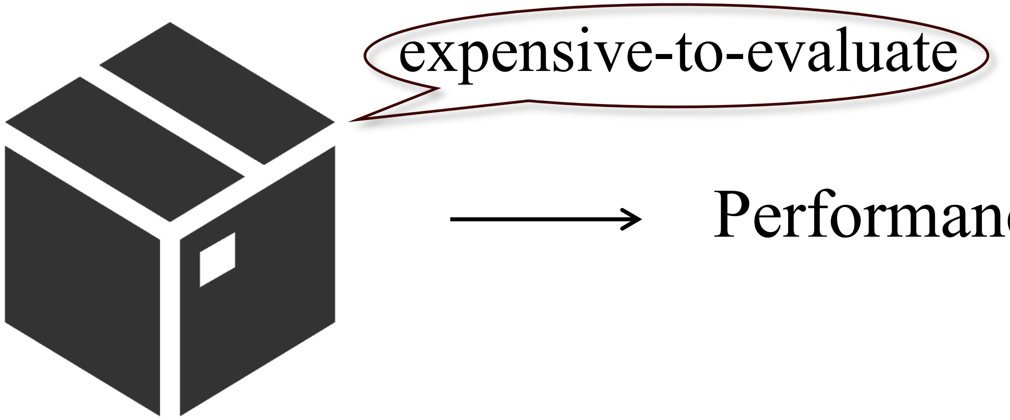
→ Revenue



Operational cost

User experience

Black-Box Optimization



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

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

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

Data-Driven Black-Box Optimization

Input x $\longrightarrow$

expensive-to-evaluate

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

adaptively

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

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

Fewer #evaluations

Data-Driven Black-Box Optimization

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

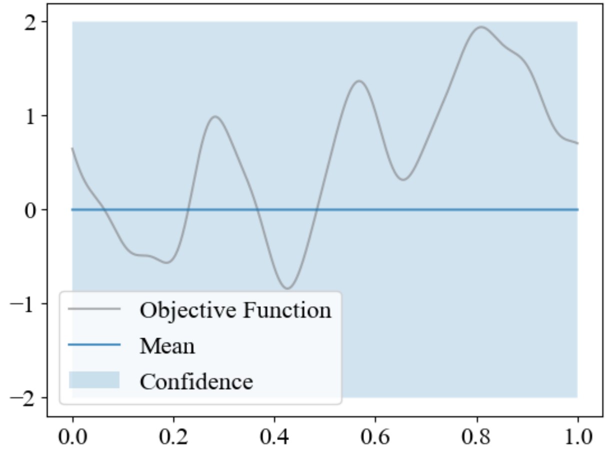
Time 0

$f \sim$Stochastic Process

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

Black-box function

Model belief



Probabilistic model

(e.g., Gaussian process)

Bayesian Optimization

Time t

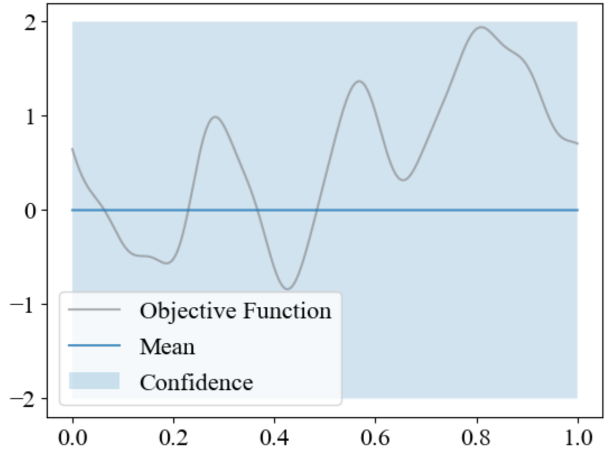
$x_1, \dots, x_t$ $\longrightarrow$

Black-box function

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

$f \sim$Stochastic Process

Model belief



Probabilistic model
(e.g., Gaussian process)

Bayesian Optimization

Time t

$x_1, \ldots, x_t \longrightarrow$

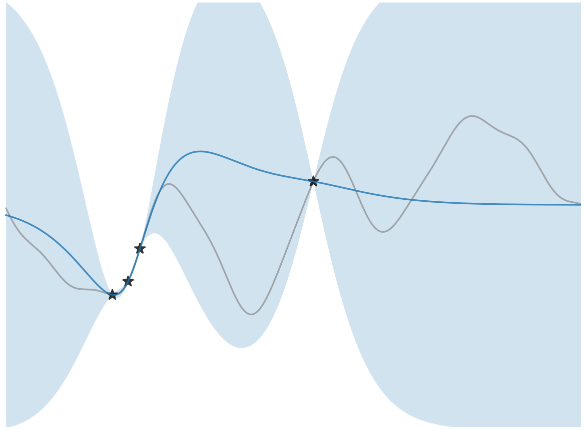
Black-box function

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

$f \sim$Stochastic Process

Update belief

(Bayes' rule)



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Black-box function

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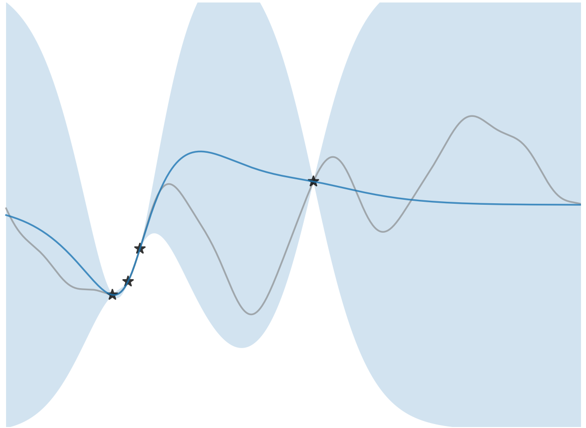

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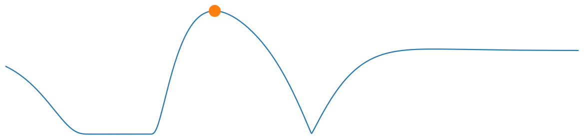
(e.g., Gaussian process)



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

scoring (worth of each point

Bayesian Optimization

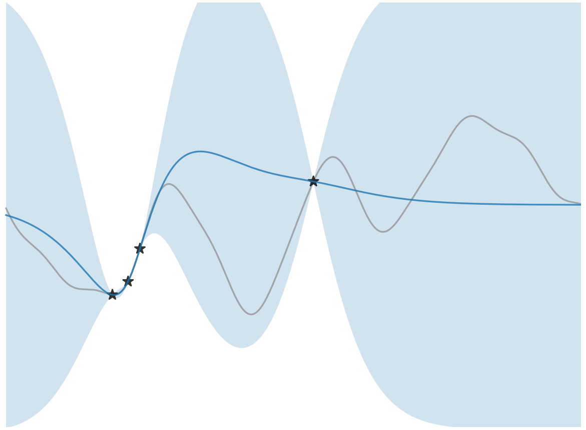
Time t

$x_1, \ldots, x_t$

Black-box function

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

Update belief
(Bayes' rule)



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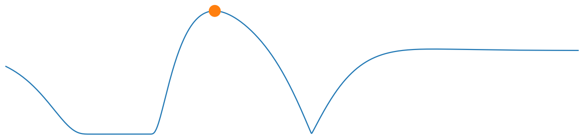


Acquisition function
(e.g., UCB, TS)

scoring (worth of each point

Acquire next data
(gradient-based optimization)

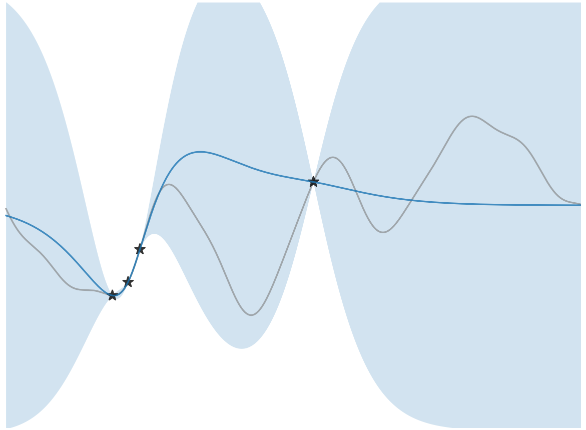
Bayesian Optimization

Time $t+1$

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

Black-box function

Update belief
(Bayes' rule)



Probabilistic model
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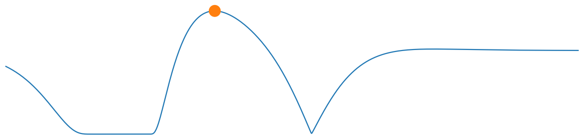

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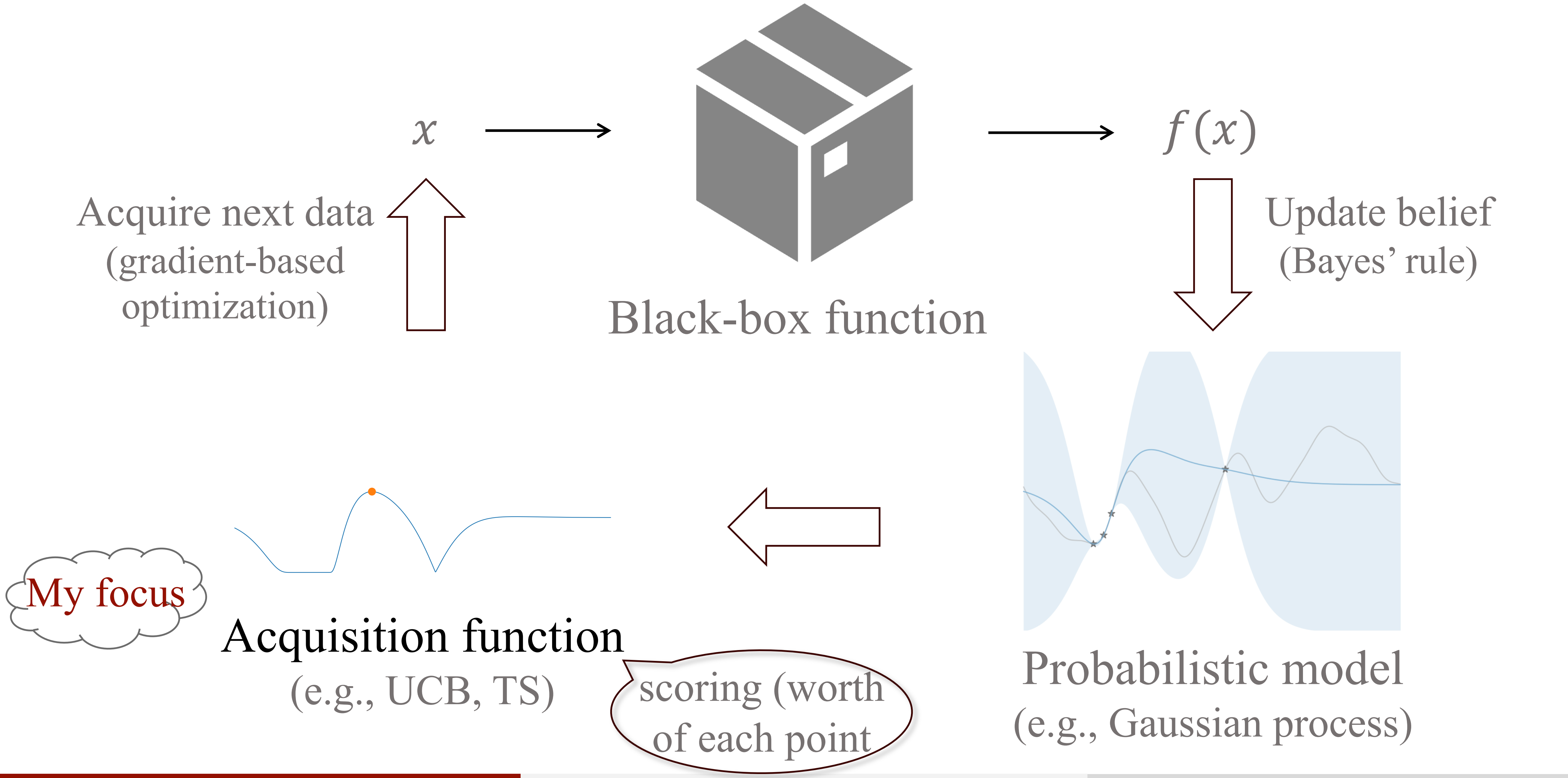
Bayesian Optimization



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

? 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

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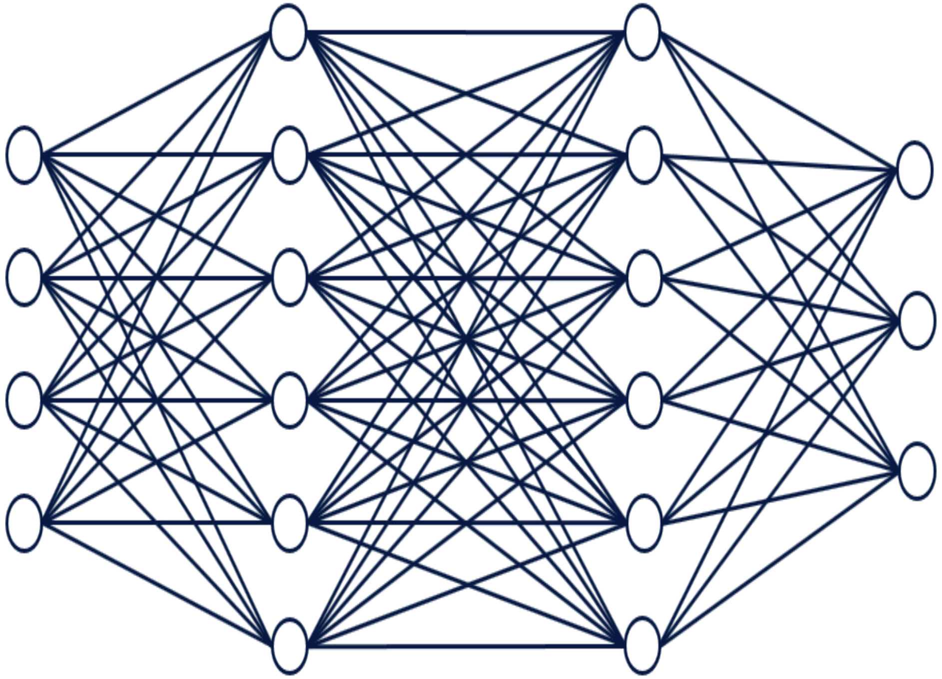
Under-explored Practical Considerations

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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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

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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

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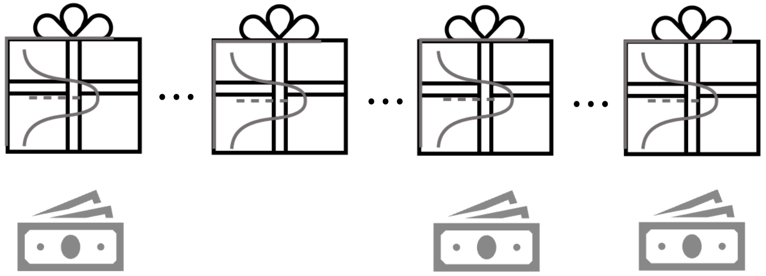
Observable multi-stage feedback

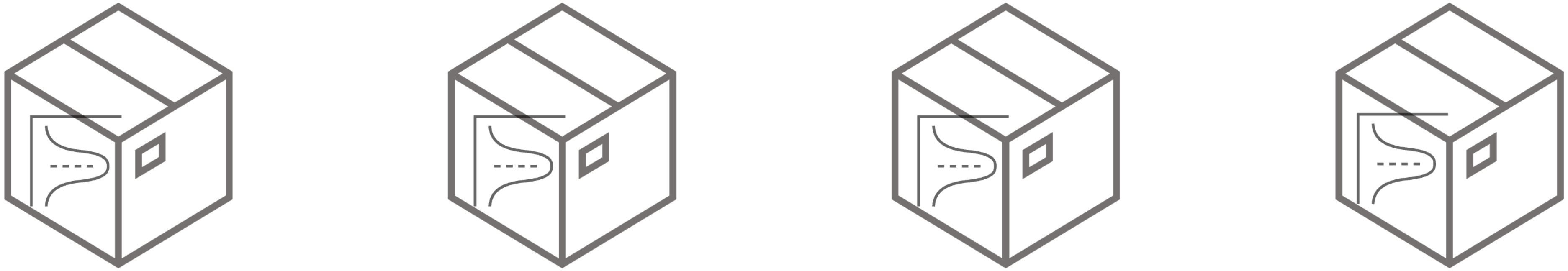
Features in Markovian bandits

New design principle:
Gittins index

Optimal in related sequential decision problems



Pandora's Box



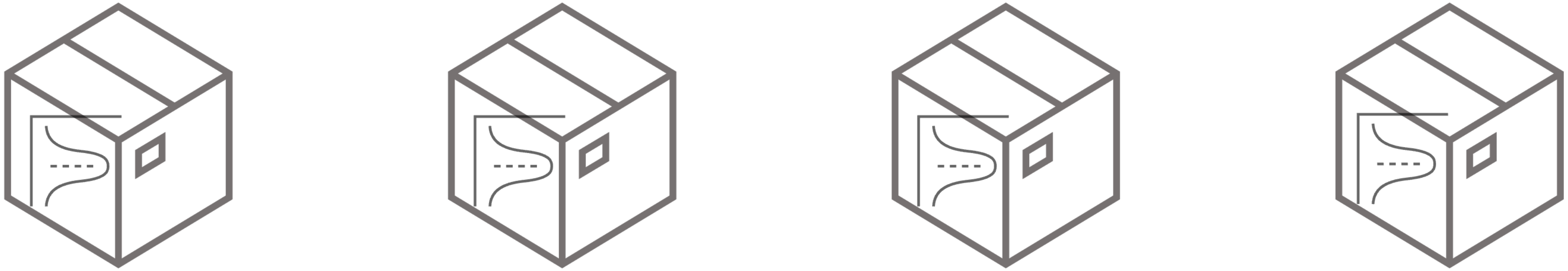
High-level goal: Choose $x_1, \ldots, x_T$ to maximize the expected utility

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

Flexible stopping time

Pandora's Box

$t = 0$



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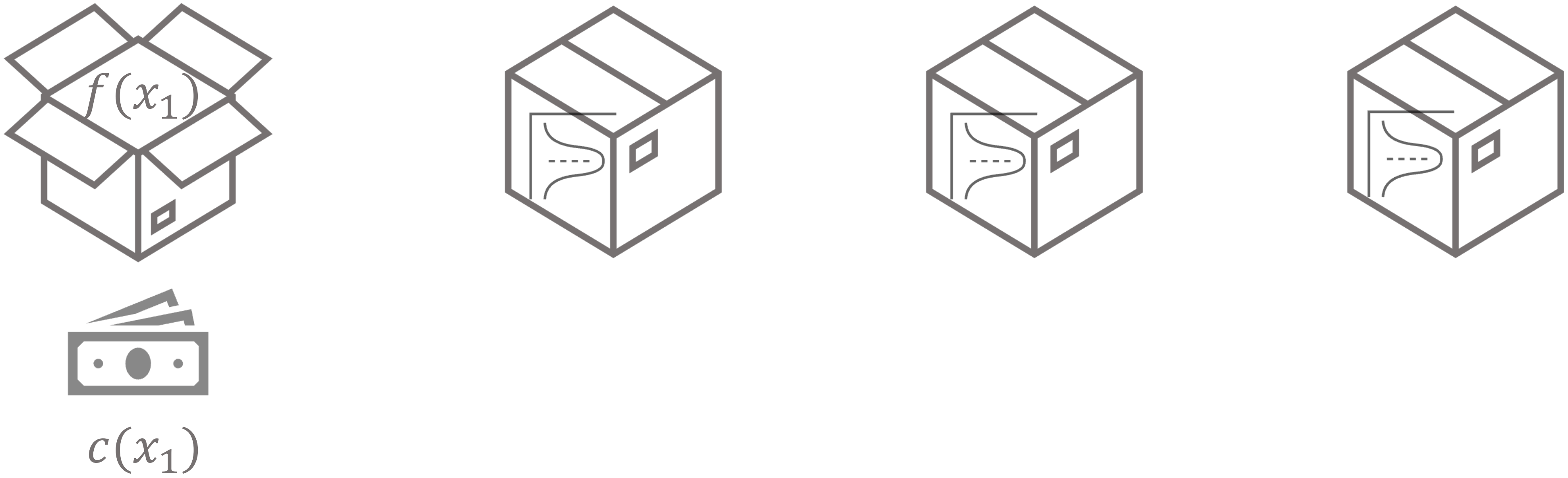
Pandora's Box

$t = 1$

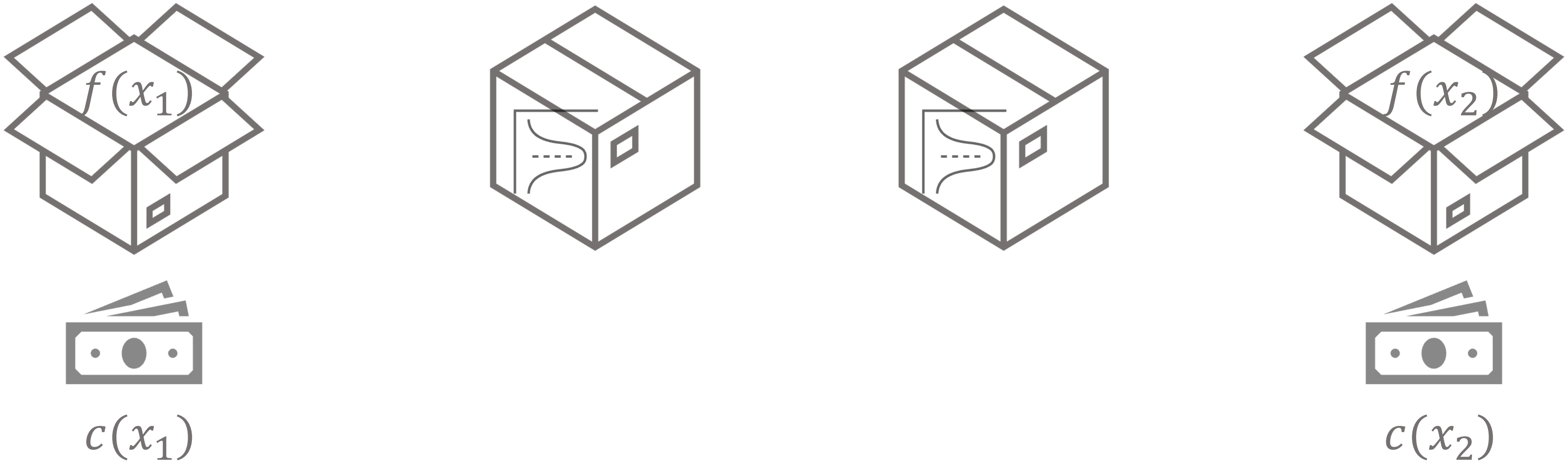


High-level goal: Choose $x_1, \ldots, x_T$ to maximize the expected utility

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

Pandora's Box

$t = 2$

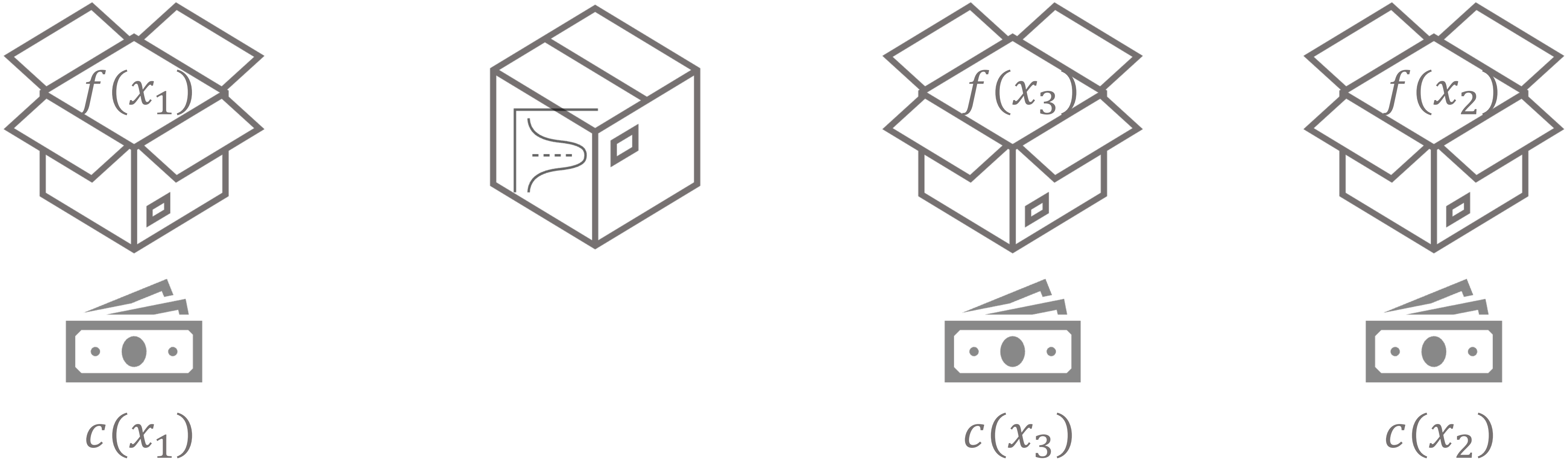


High-level goal: Choose $x_1, \ldots, x_T$ to maximize the expected utility

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

Pandora's Box

$t = 3$

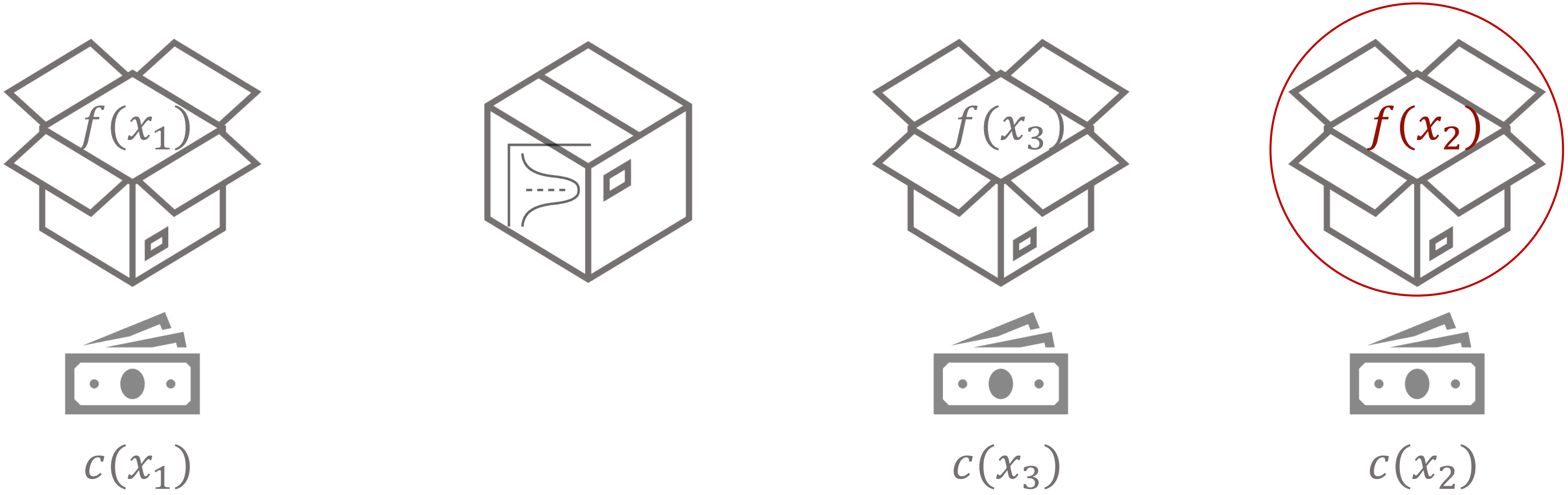


High-level goal: Choose $x_1, \dots, x_T$ to maximize the expected utility

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

Pandora's Box

$t = T$, stop

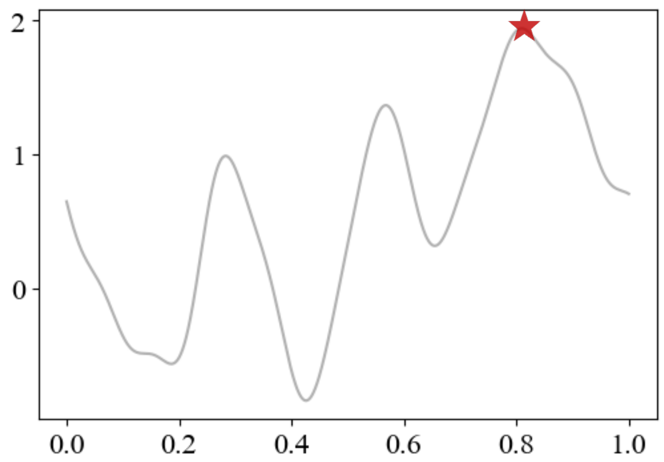


High-level goal: Choose $x_1, \dots, x_T$ to maximize the expected utility

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

Bayesian Optimization

$f(x)$



Continuous

Correlated

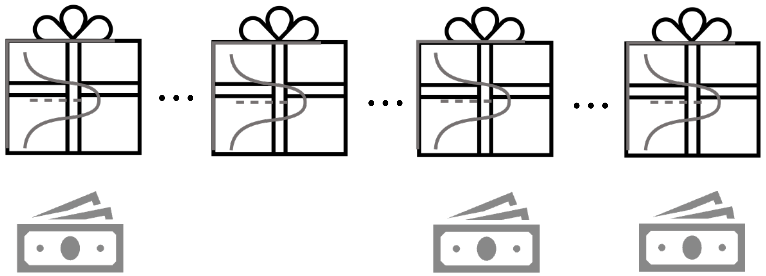
Fixed-iteration

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

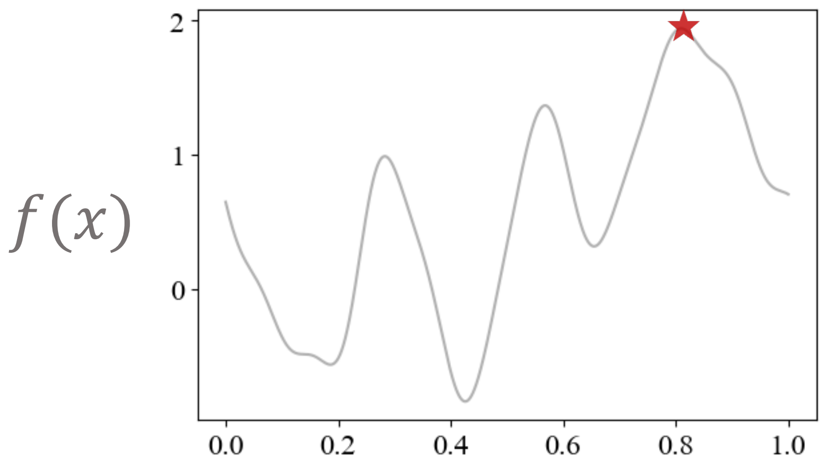
Flexible-stopping

Expected utility

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

cumulative cost

Bayesian Optimization



Continuous

Correlated

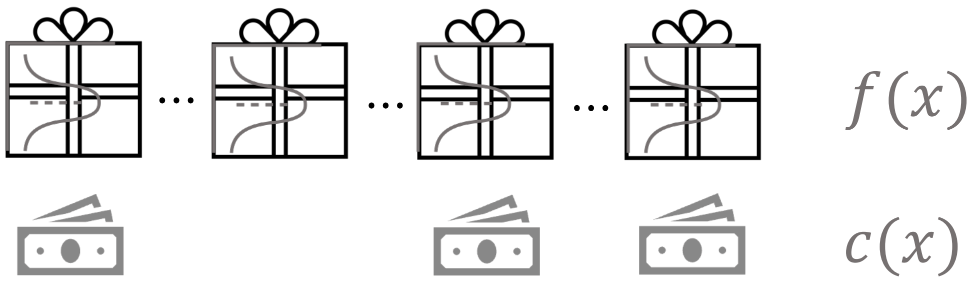
Fixed-iteration

Expected best-observed value

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

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

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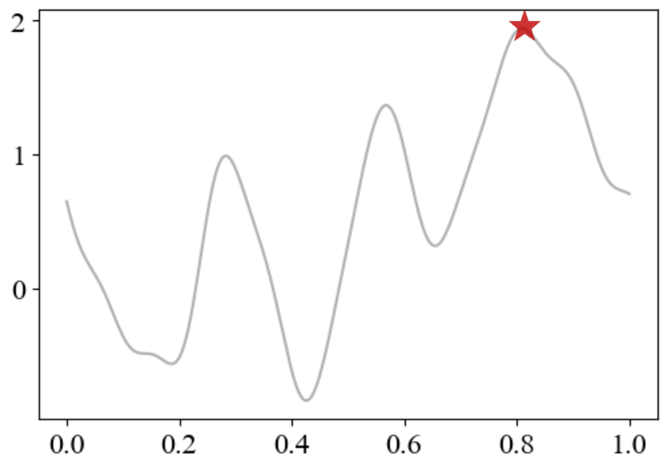


Continuous

Correlated

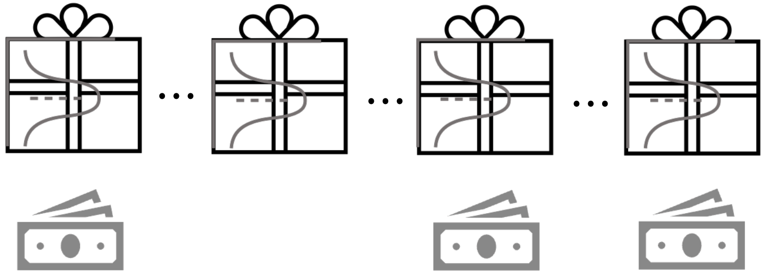
Fixed-iteration

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

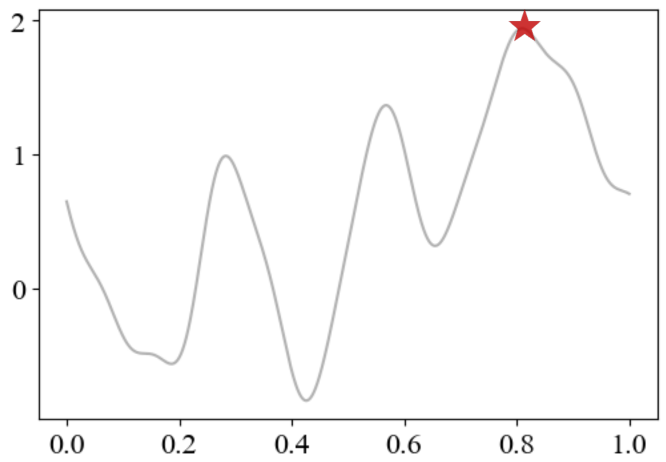
Expected utility

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

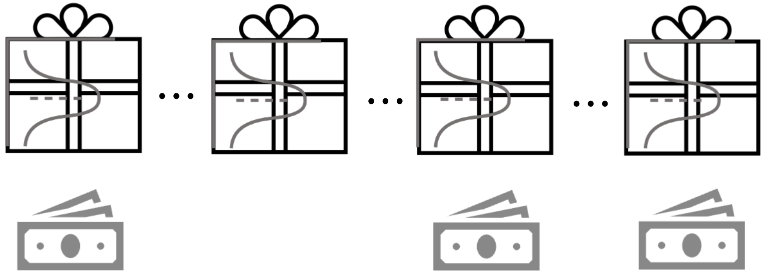
Fixed-iteration

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

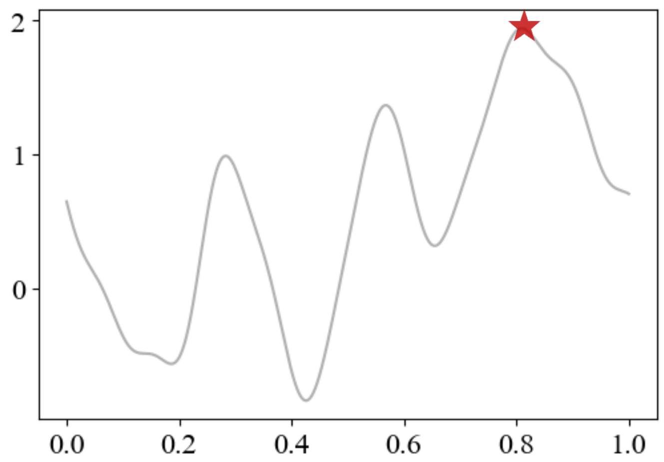
Expected cost-adjusted regret

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

cumulative cost

Bayesian Optimization

$f(x)$



Continuous

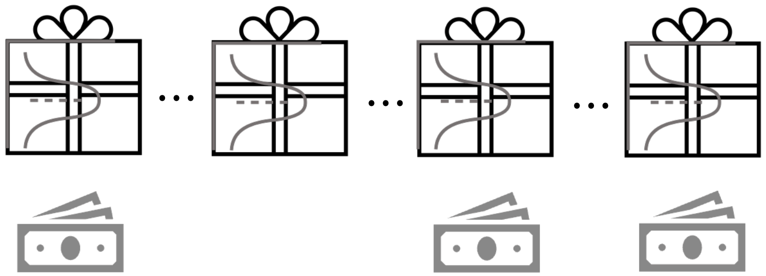
Correlated

Fixed-budget / Flexible-stopping

Expected (cost-adjusted) regret

Pandora's Box

[Weitzman'79]



$f(x)$

$c(x)$

Discrete

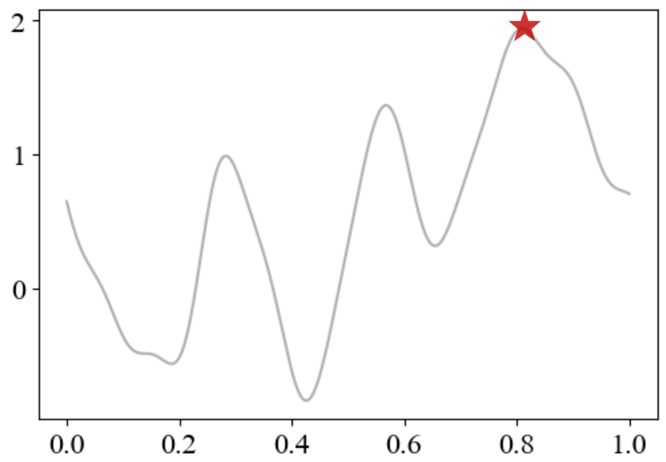
Independent

Flexible-stopping

Expected cost-adjusted regret

Bayesian Optimization

$f(x)$



Continuous

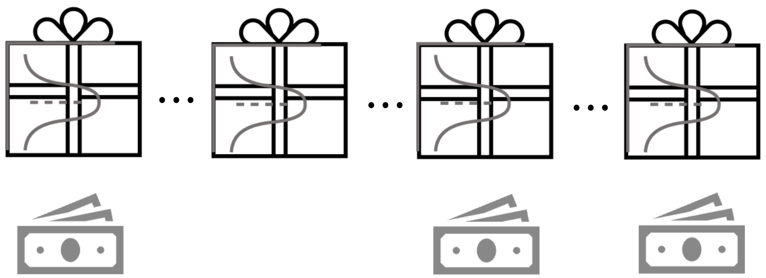
Correlated

Fixed-budget / Flexible-stopping

Expected (cost-adjusted) regret

Pandora's Box

[Weitzman'79]



$f(x)$

$c(x)$

Discrete

Independent

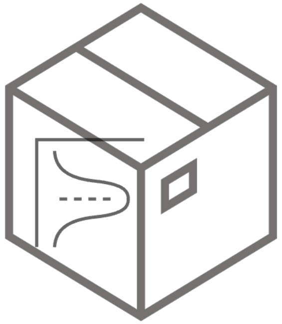
Flexible-stopping

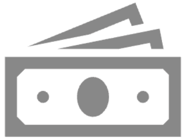
Expected cost-adjusted regret

Optimal policy: Gittins index

Optimal Policy: Gittins Index

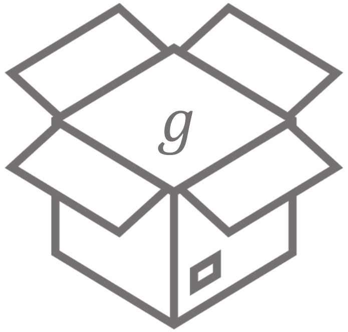
Step 1: Assign each box a Gittins index (higher is better)

$f(x)$ 

$c(x)$ 

$\downarrow$

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

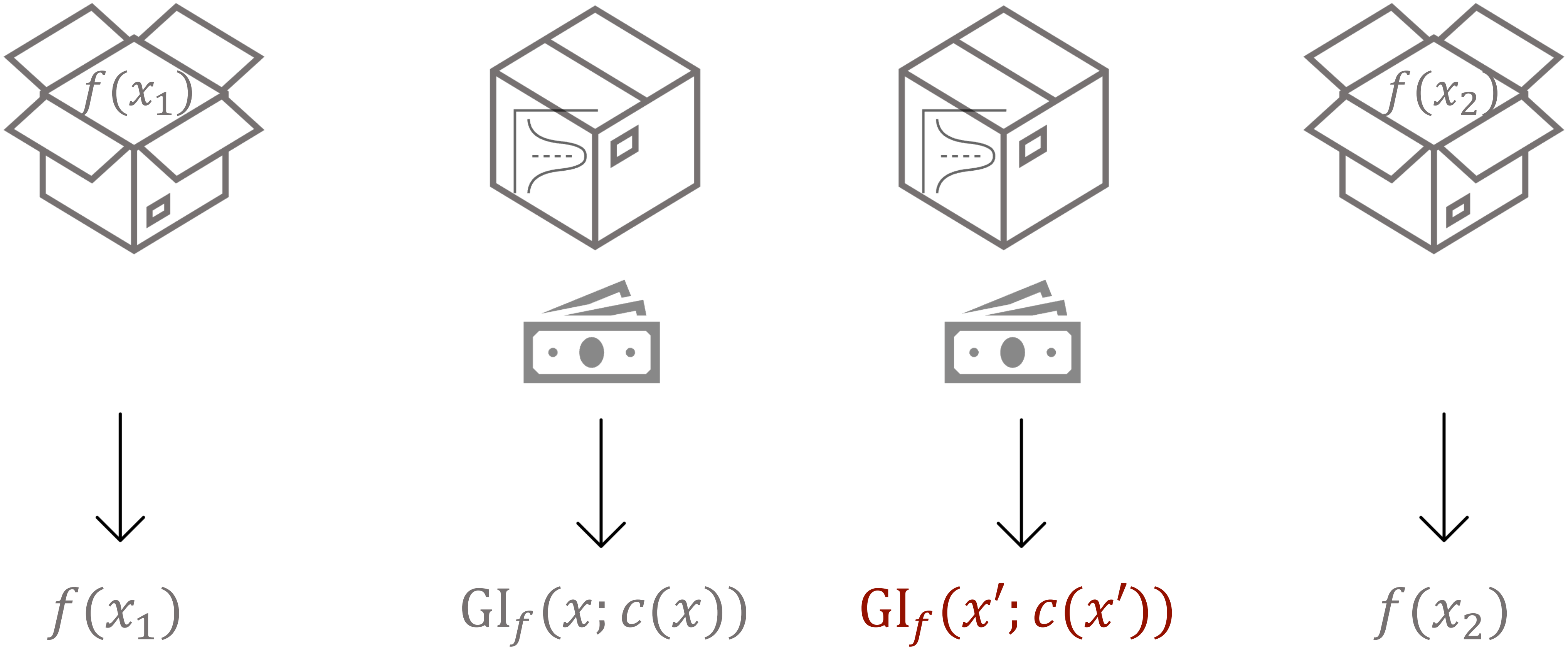


$\downarrow$

g

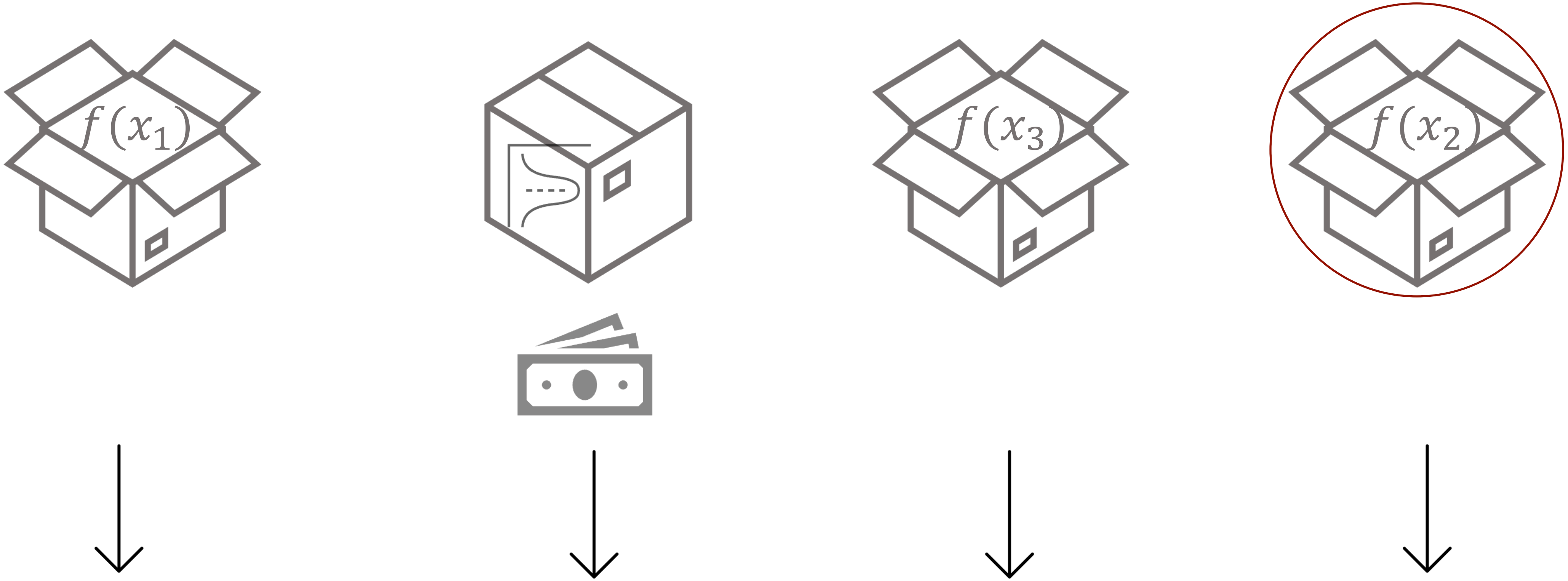
Optimal Policy: Gittins Index

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



Optimal Policy: Gittins Index

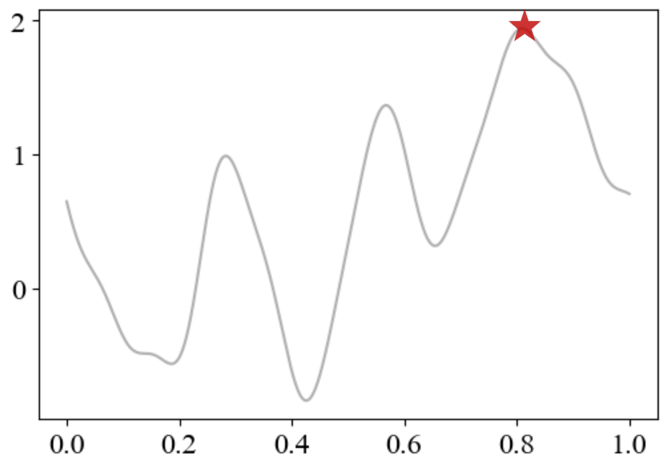
Step 2’: Select the box with highest index if it is opened and stop



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

Bayesian Optimization

$f(x)$



Continuous

Correlated

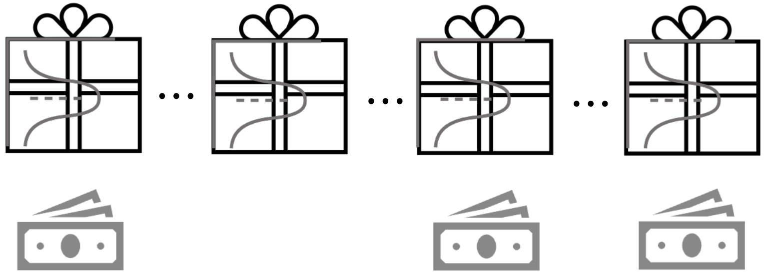
Fixed-budget / Flexible-stopping

Expected (cost-adjusted) regret

Is Gittins index good?

Pandora's Box

[Weitzman'79]



$f(x)$

$c(x)$

Discrete

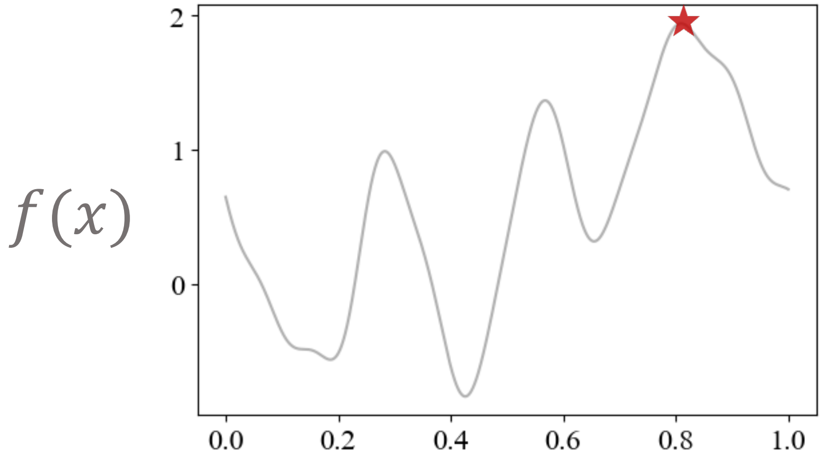
Independent

Flexible-stopping

Expected cost-adjusted regret

Gittins index is optimal

Bayesian Optimization



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empirically

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Discrete

Independent

Flexible-stopping

Expected cost-adjusted regret

Gittins index is optimal

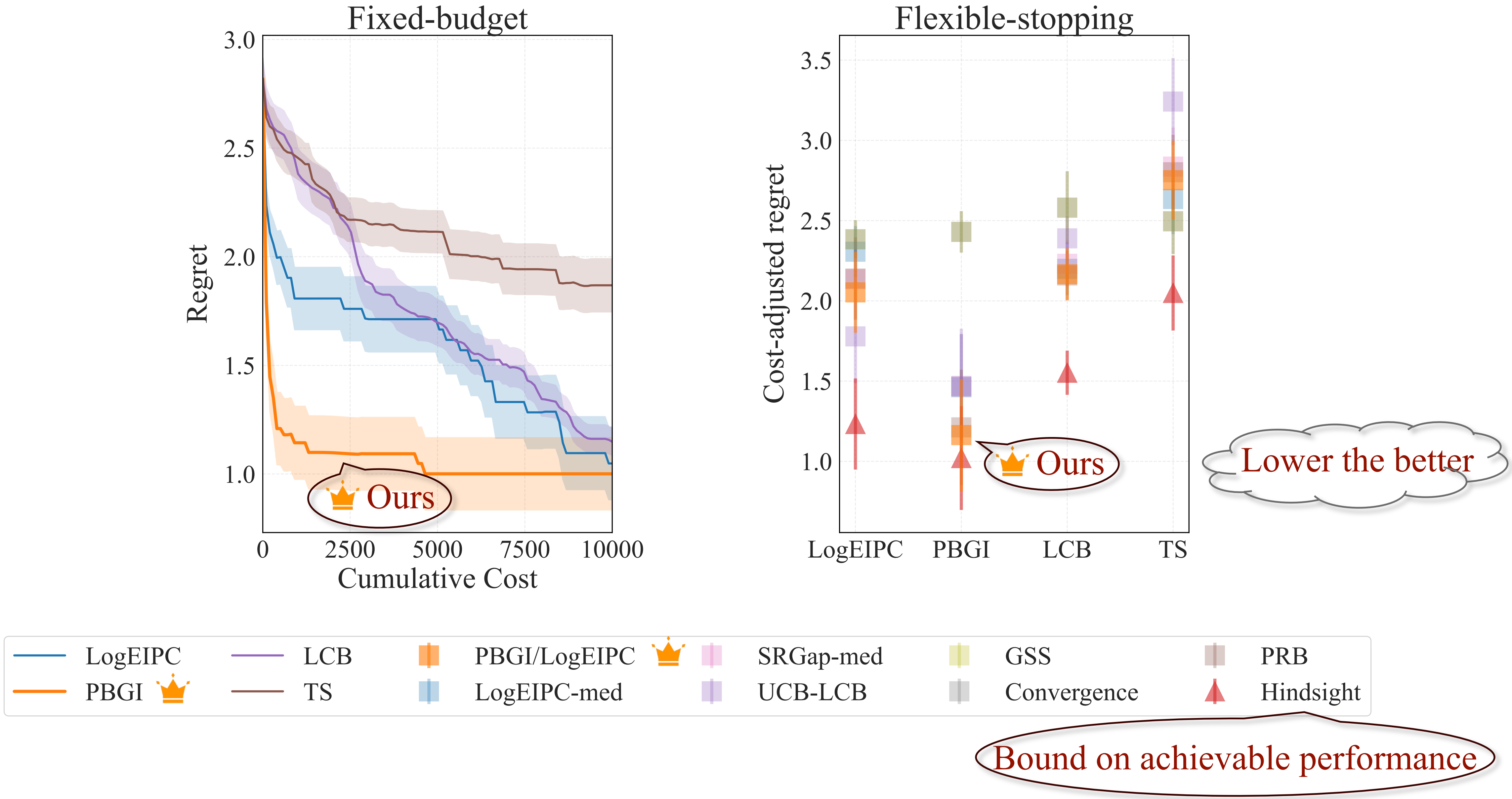
Our Contribution: Gittins Index Principle

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

? Why another principle?

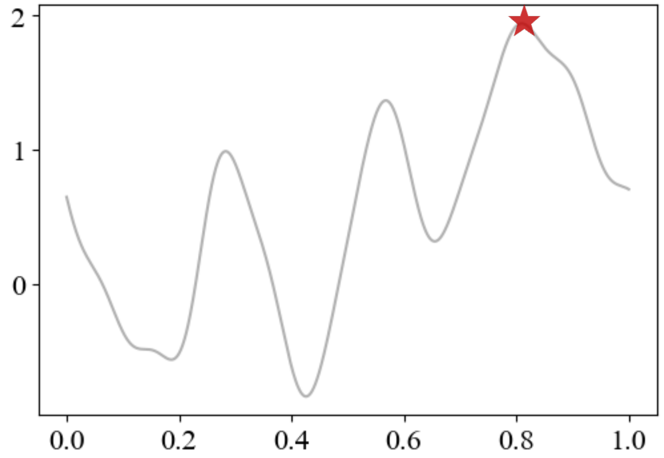
1. Naturally handles practical considerations
2. Performs competitively on benchmarks
3. Comes with theoretical guarantees

Gittins Index vs Baselines on AutoML Benchmark



Bayesian Optimization

$f(x)$



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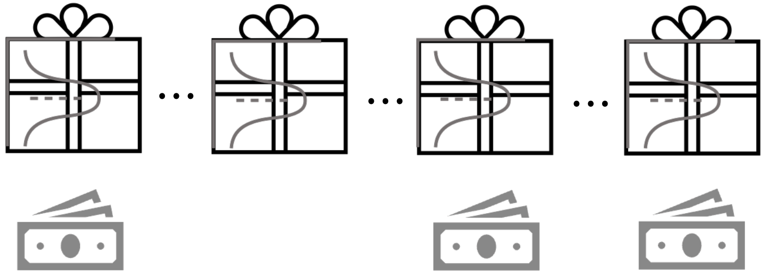

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Theoretical Guarantee and Empirical Validation

Theorem (No worse than stopping-immediately)

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

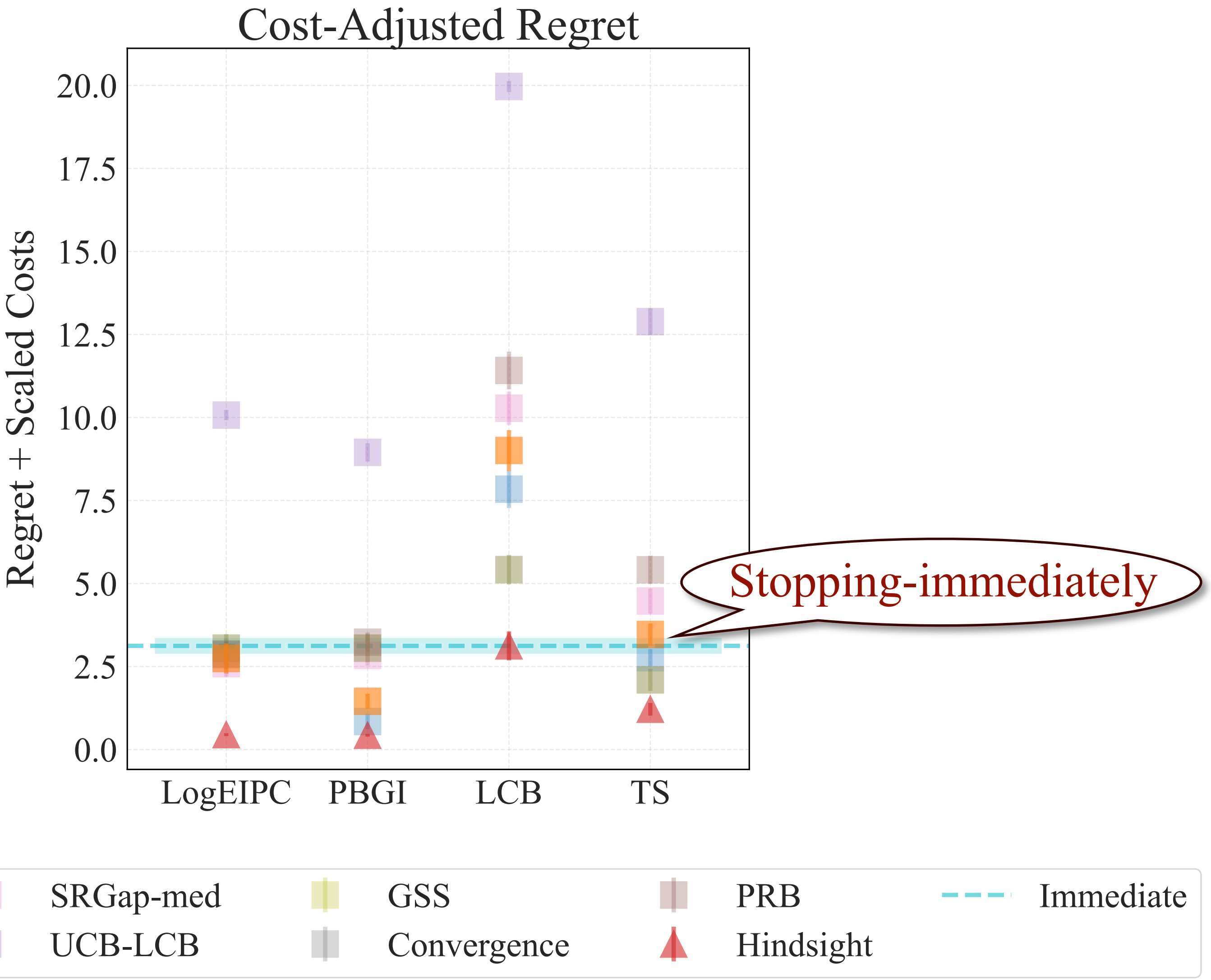
or LogEIPC

cost-adjusted regret

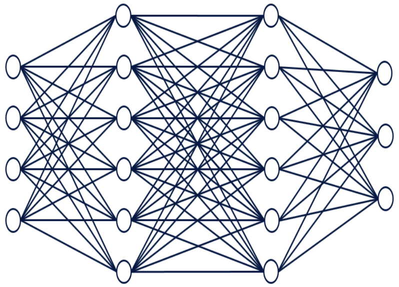
Implication:

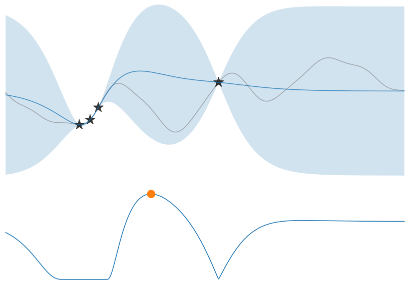
- Matches the best achievable performance in the worst case (evaluations are all very costly).

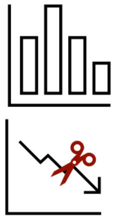
- Avoids over-spending — a property many cost-unaware stopping rules lack.



Studied problem



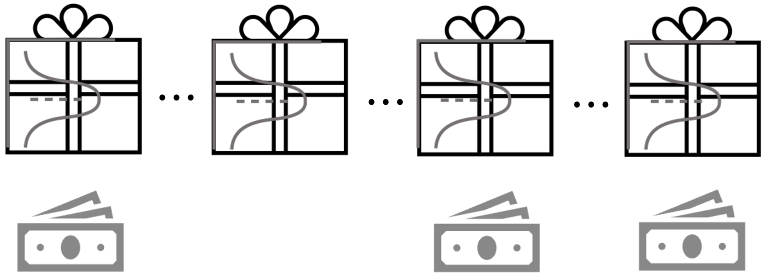




Varying evaluation costs

Adaptive stopping time

Key idea



Link to Pandora's Box problem
& Gittins index theory

Impact

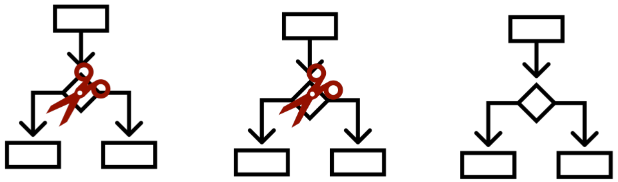
Meta

BoTorch Ax

Competitive empirical performance &
interests from practitioners

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

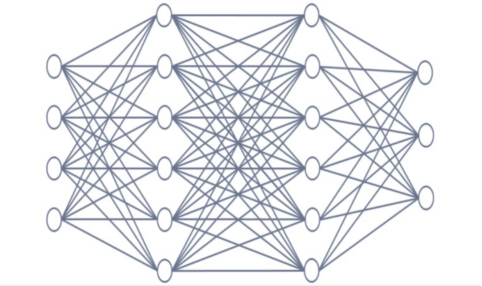
Ongoing work

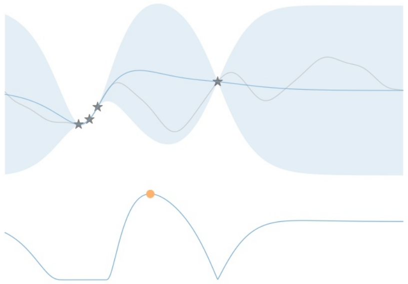


Sharper theoretical guarantees & black-box optimization w/ multi-stage feedback

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

Studied problem





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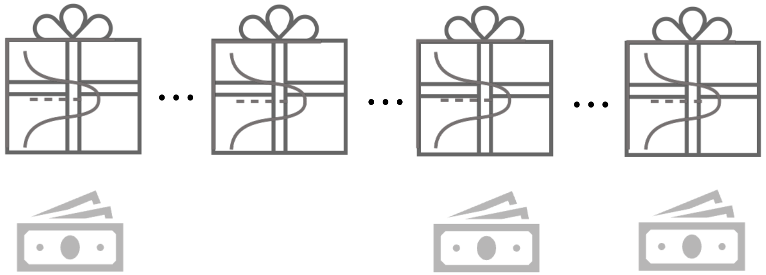

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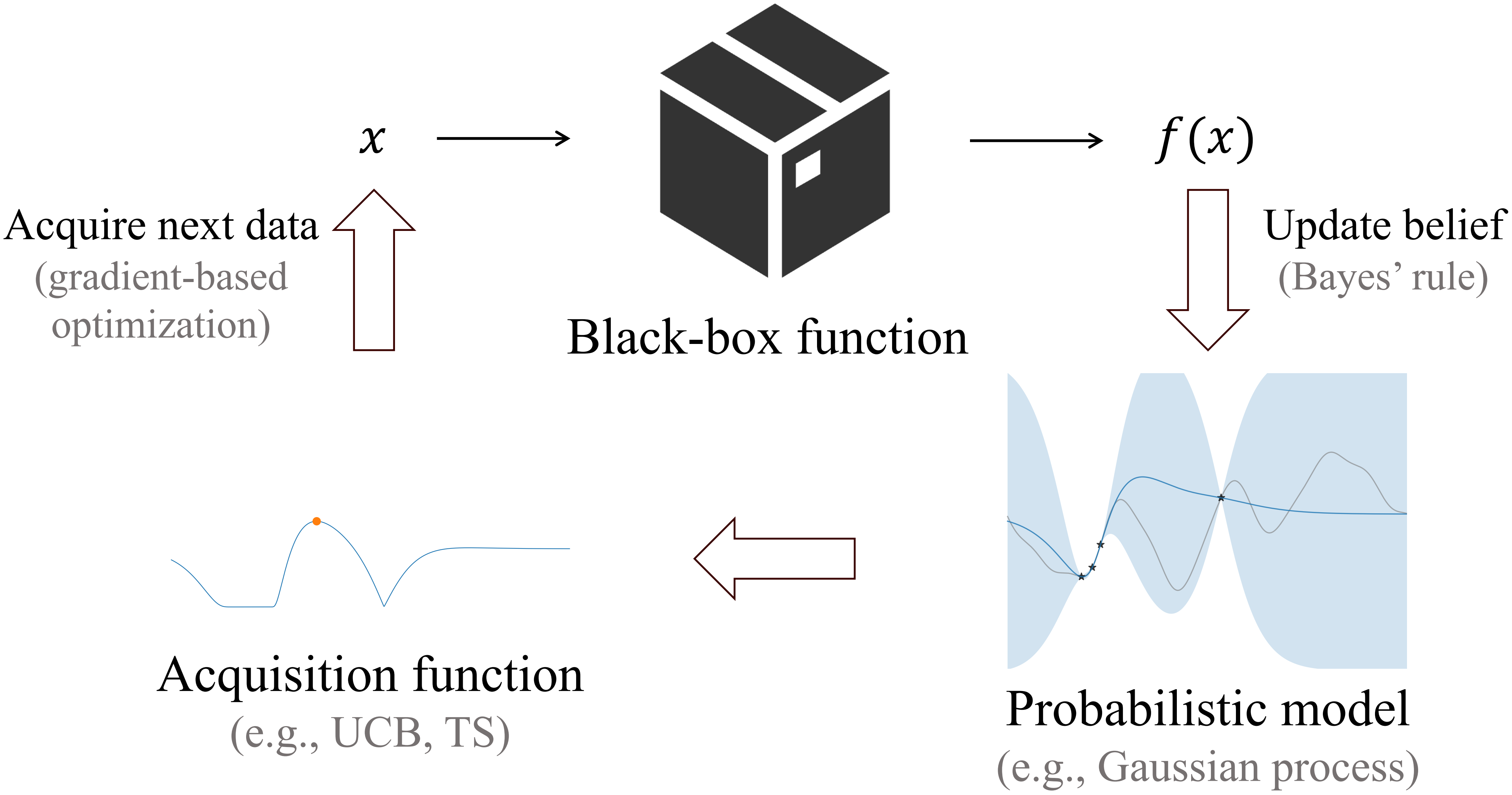
ChatGPT Gemini

deepseek Claude

LLM-driven black-box optimization

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

Recap: Bayesian Optimization



Ongoing: LLM-Driven Black-Box Optimization

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

Acquire next data
(LLM proposal)

Black-box function

Update belief
(feedback-augmented context)

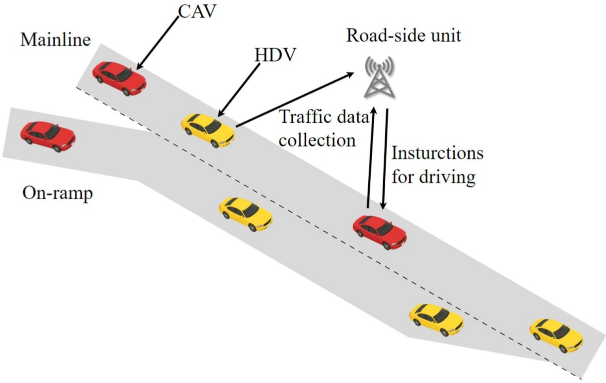
Acquisition function
(e.g., Softmax sampling)

Probabilistic model
(e.g., autoregressive model)

Ongoing: LLM-Driven RL Training Optimization

Mixed-autonomy traffic control:

(e.g., Transformer config)
x ⟶

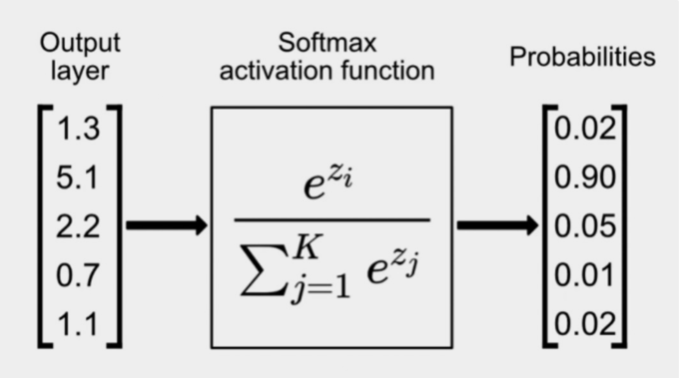


⟶ (e.g., average speed)
$f(x)$

Acquire next data
(LLM proposal)

Update belief
(feedback-augmented context)

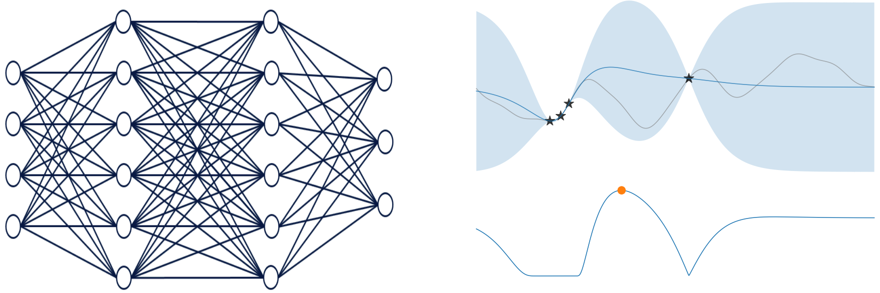
Black-box function
(RL training & evaluation)



Acquisition function
(e.g., Softmax sampling)

Probabilistic model
(large language model)

Studied problem



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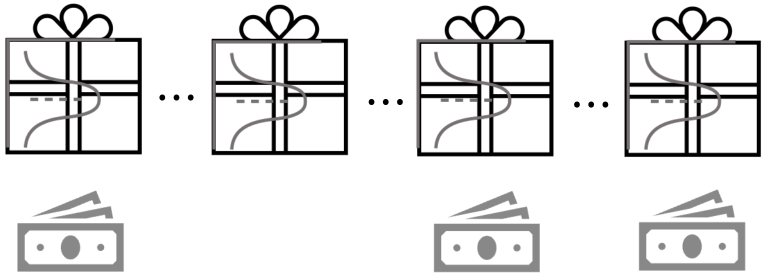

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