Cost-Aware Bayesian Optimization with Adaptive Stopping via Gittins Indices

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INFORMS Annual Meeting 2025 Job Market Showcase

Optimization Under Uncertainty

Black-box optimization:

Input x $\longrightarrow$

non-analytical
& no gradient

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

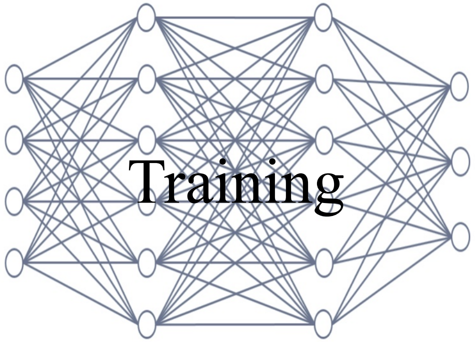
Optimization Under Uncertainty

Black-box optimization:

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

non-analytical & no gradient

ML model training:

Training hyperparameters ⟶  ⟶ Accuracy

Optimization Under Uncertainty

Black-box optimization:

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

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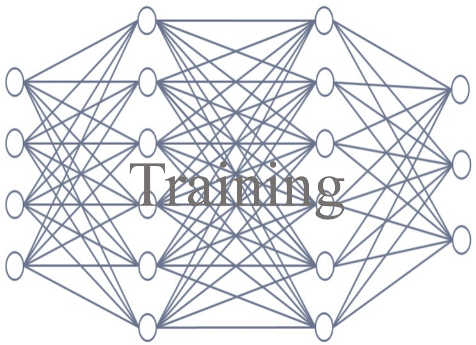
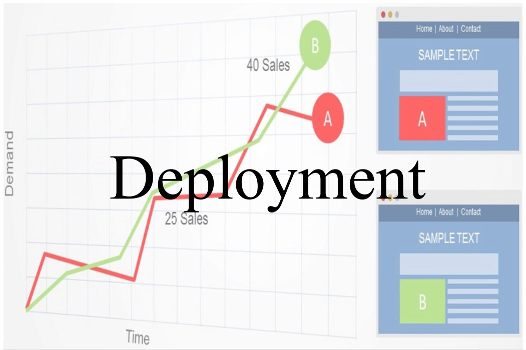
Training hyperparameters ⟶  Training ⟶ Accuracy

Adaptive experimentation:

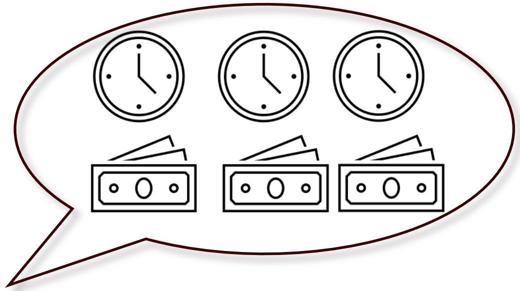
Decision/design variables ⟶ 

Deployment ⟶ Revenue

Black-Box Optimization

expensive-to-evaluate

Input x ⟶ ⟶ Performance metric $f(x)$

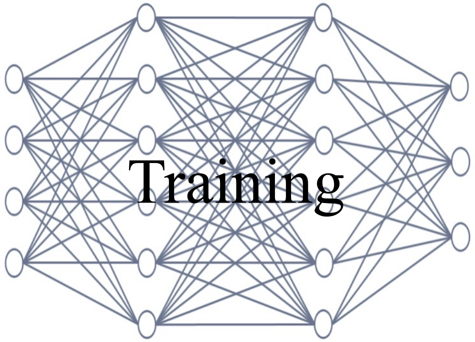


Training time

Compute credits

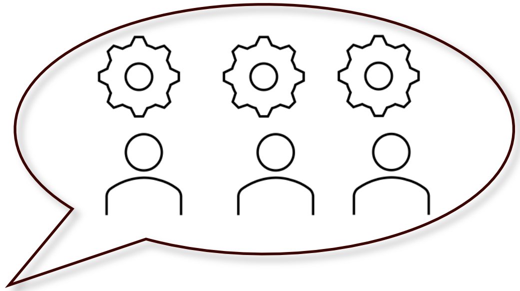
ML model training:

Training hyperparameters ⟶



Training

⟶ Accuracy

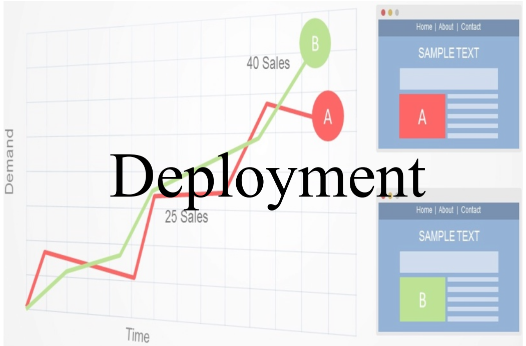


Operational cost

User experience

Adaptive experimentation:

Decision/design variables ⟶



Deployment

⟶ 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

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

Data-Driven Black-Box Optimization

expensive-to-evaluate

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

adaptively

High-level goal: Choose $x_1, \dots, x_T$ 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 $\longrightarrow$ [box] $\longrightarrow$ Performance metric $f(x)$

adaptively

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

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

Fewer #evaluations

Efficient framework: Bayesian optimization

Bayesian Optimization

$f \sim$ Stochastic Process

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

Black-box function

Bayesian Optimization

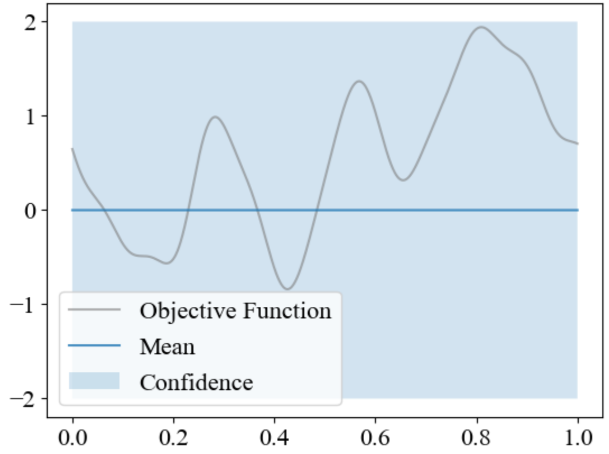
Time 0

$f \sim$Stochastic Process

x →  → $f(x)$

Black-box function

Model belief



Probabilistic model

(e.g., Gaussian process)

Bayesian Optimization

Time t

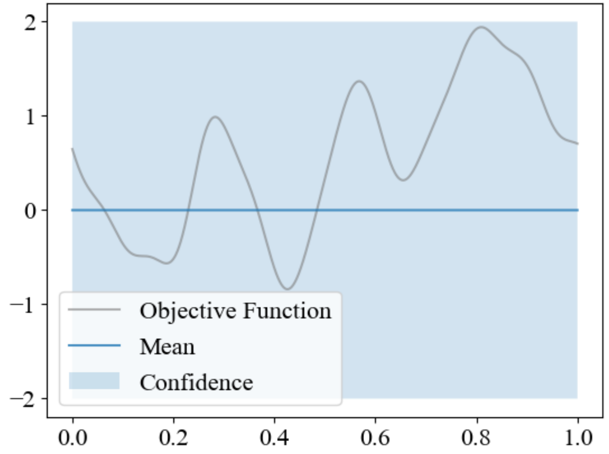
$x_1, \ldots, x_t$ $\longrightarrow$

Black-box function

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

$f \sim$Stochastic Process

Model belief



Probabilistic model
(e.g., Gaussian process)

Bayesian Optimization

Time t

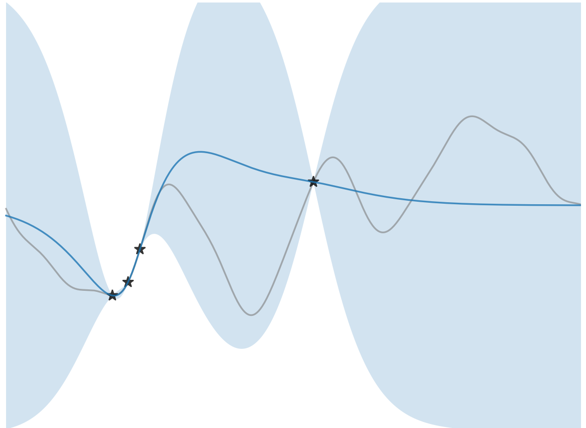
$f \sim$Stochastic Process

$x_1, \dots, x_t$

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

Black-box function

Update belief
(Bayes' rule)



Probabilistic model
(e.g., Gaussian process)

Bayesian Optimization

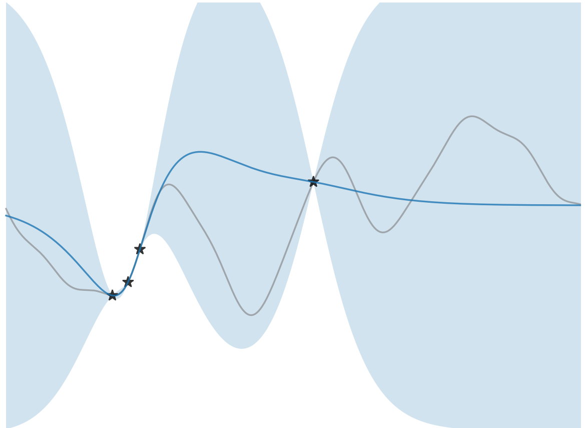
Time t

$x_1, \ldots, x_t \longrightarrow$

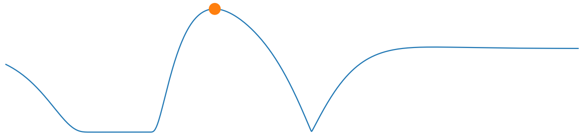
Black-box function

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

Update belief
(Bayes' rule)



Probabilistic model
(e.g., Gaussian process)



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

rating across search space

Bayesian Optimization

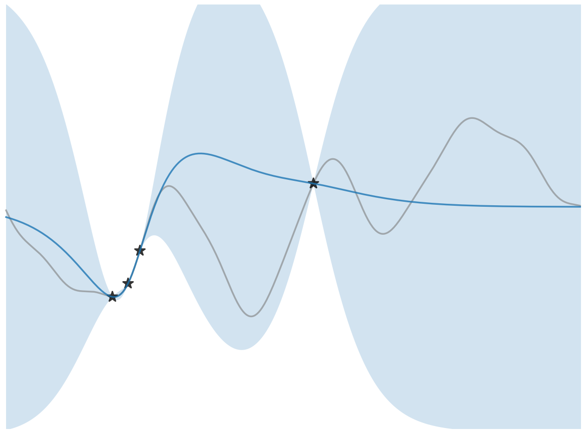
Time t

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

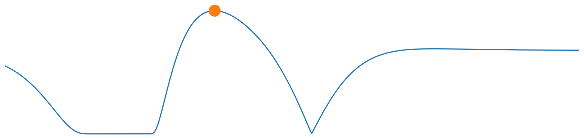
Black-box function

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

Update belief
(Bayes' rule)



Probabilistic model
(e.g., Gaussian process)



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

rating across search space

Acquire next data
(gradient-based optimization)

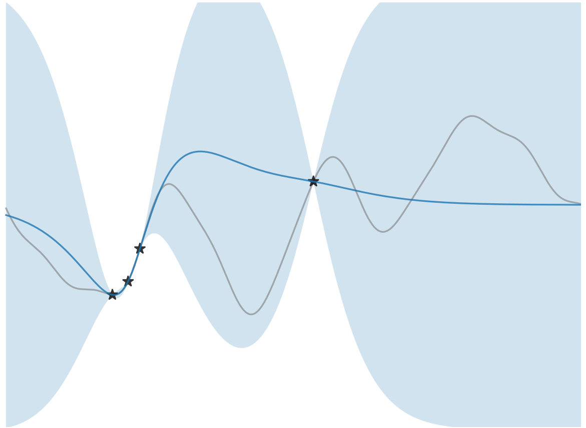
Bayesian Optimization

Time $t + 1$

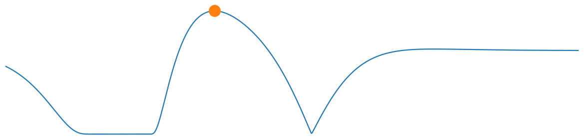
$x_1, \ldots, x_{t+1}$ → Black-box function → $f(x_1), \ldots, f(x_{t+1})$

Black-box function

Update belief
(Bayes' rule)



Probabilistic model
(e.g., Gaussian process)



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

Acquire next data
(gradient-based optimization)

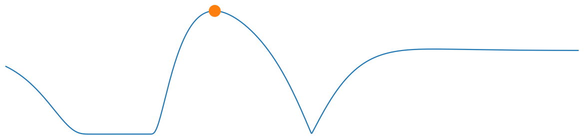
Bayesian Optimization

x →  → $f(x)$

Black-box function

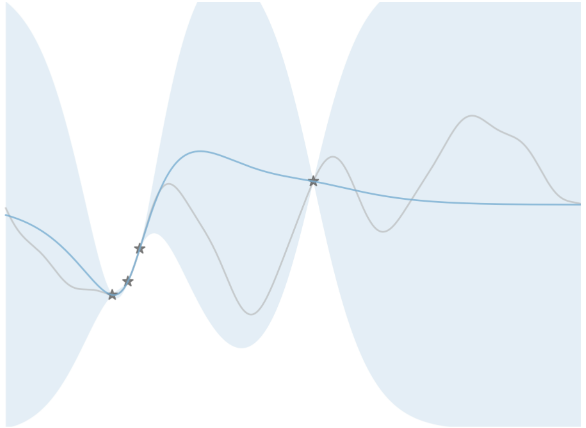
Acquire next data
(gradient-based
optimization)

Update belief
(Bayes' rule)



My focus

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



Probabilistic model
(e.g., Gaussian process)

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

? Why another principle?

New Design Principle: Gittins Index

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

Why another principle?

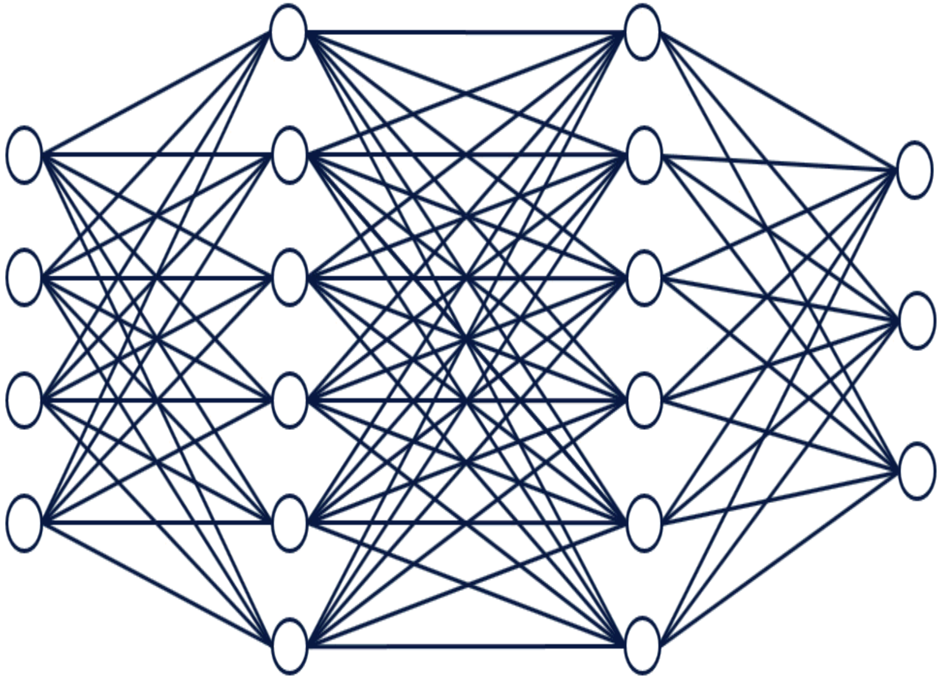
1. Naturally handles practical considerations
2. Performs competitively on benchmarks
3. Comes with theoretical guarantees

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:
Gittins index

Why Gittins index?

Varying evaluation costs

Smart stopping time

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

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

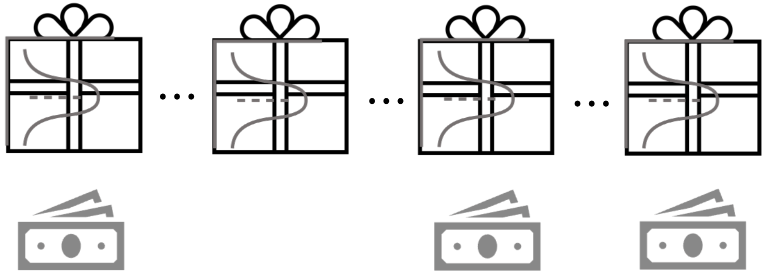
Features in Pandora's box

Observable multi-stage feedback

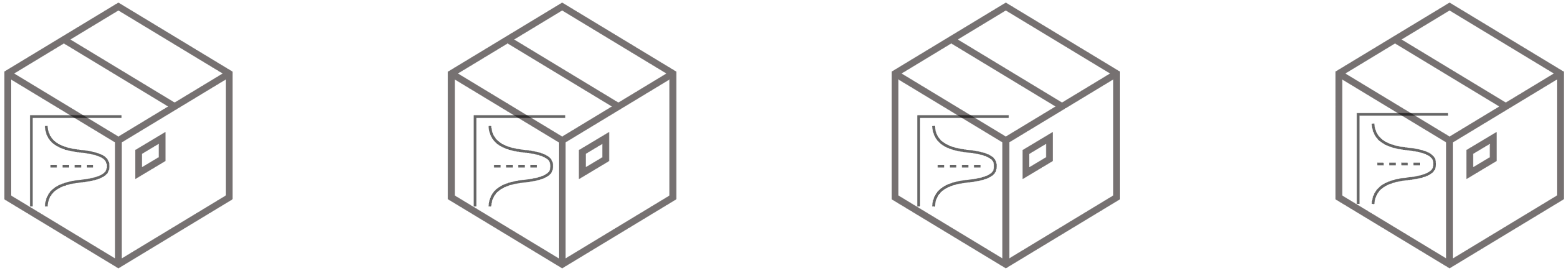
Features in Markovian bandits

New design principle:
Gittins index

Optimal in related sequential decision problems



Pandora's Box



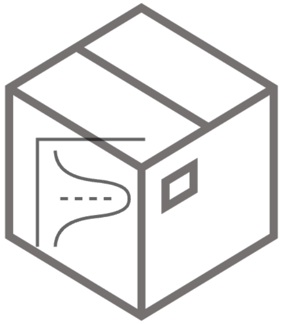
High-level goal: Choose $x_1, \dots, x_T$ to maximize the expected utility

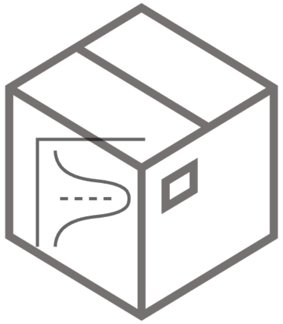
$$\mathbb{E}\max_{t=1,2,\dots,T} f(x_t) - \mathbb{E}\sum_{t=1}^{T} c(x_t)$$

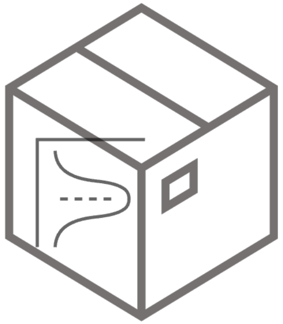
Flexible stopping time

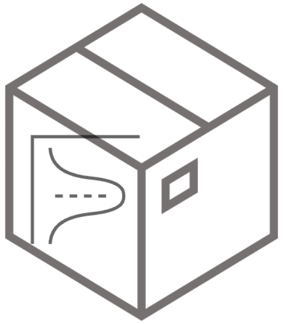
Pandora's Box

$t = 0$







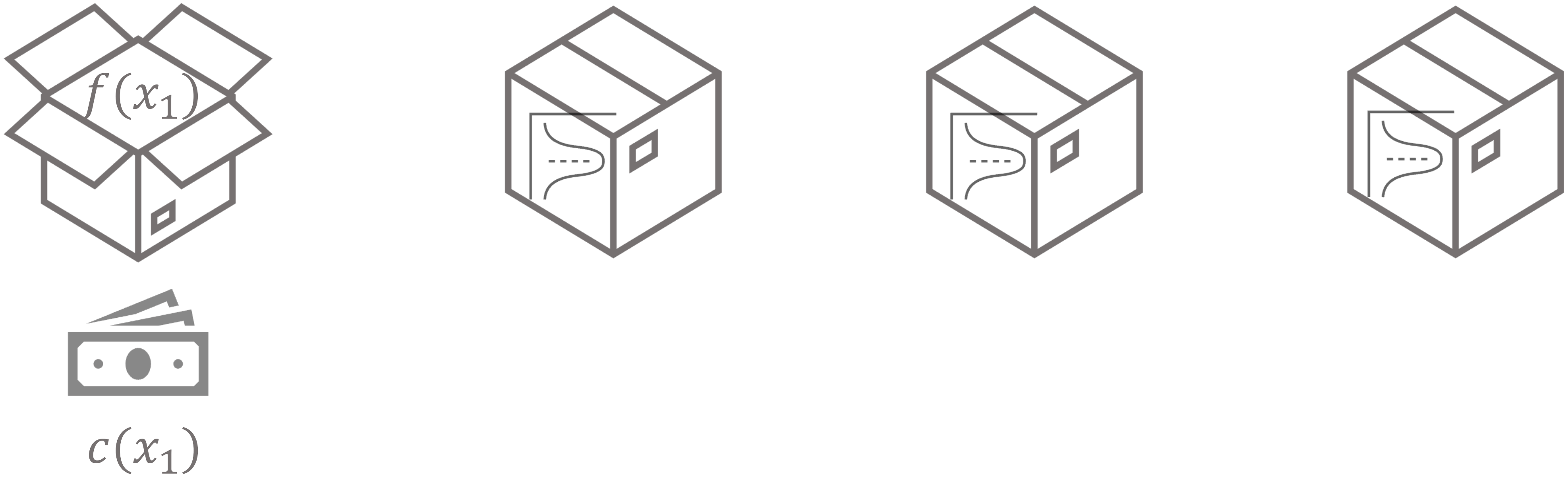


High-level goal: Choose $x_1, \ldots, x_T$ to maximize the expected utility

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

Pandora's Box

$t = 1$

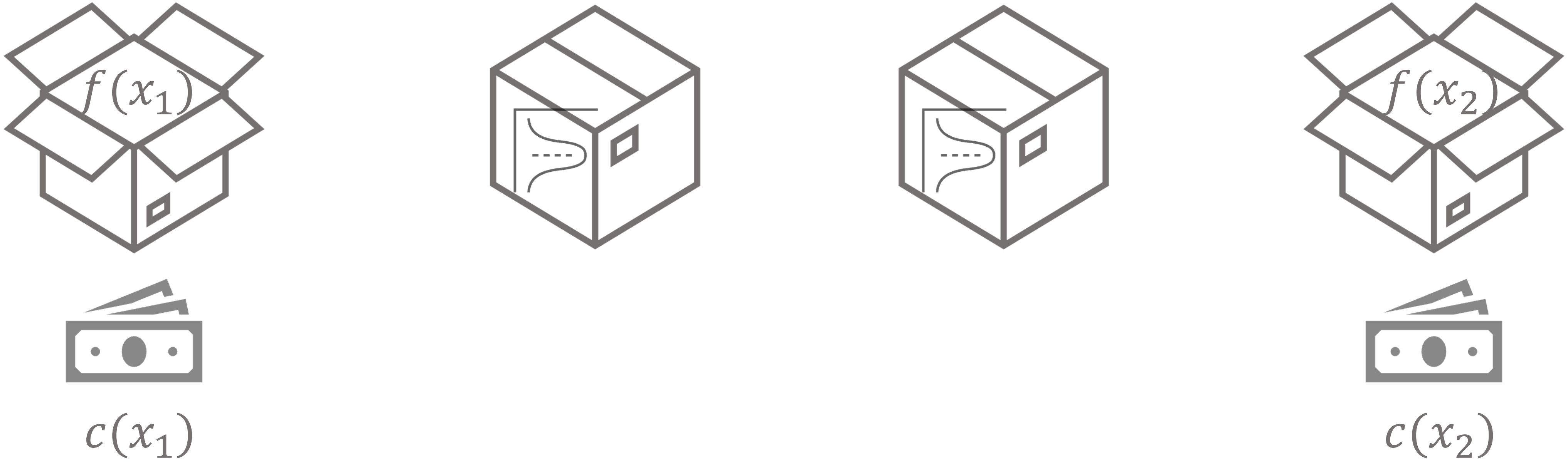


High-level goal: Choose $x_1, \ldots, x_T$ to maximize the expected utility

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

Pandora's Box

$t = 2$

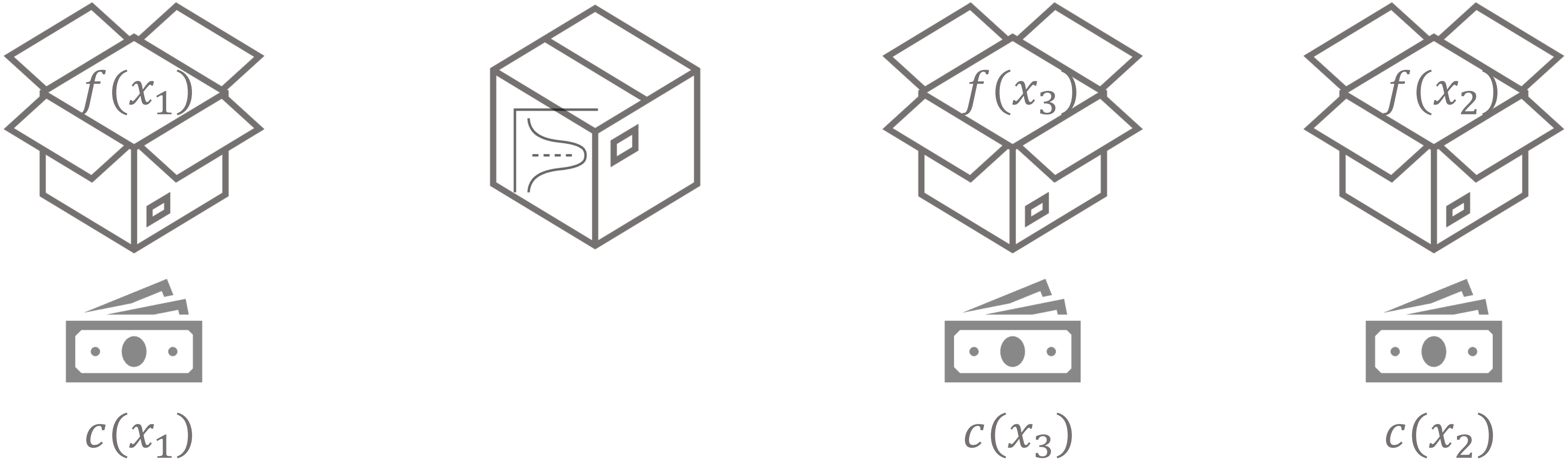


High-level goal: Choose $x_1, \dots, x_T$ to maximize the expected utility

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

Pandora's Box

$t = 3$

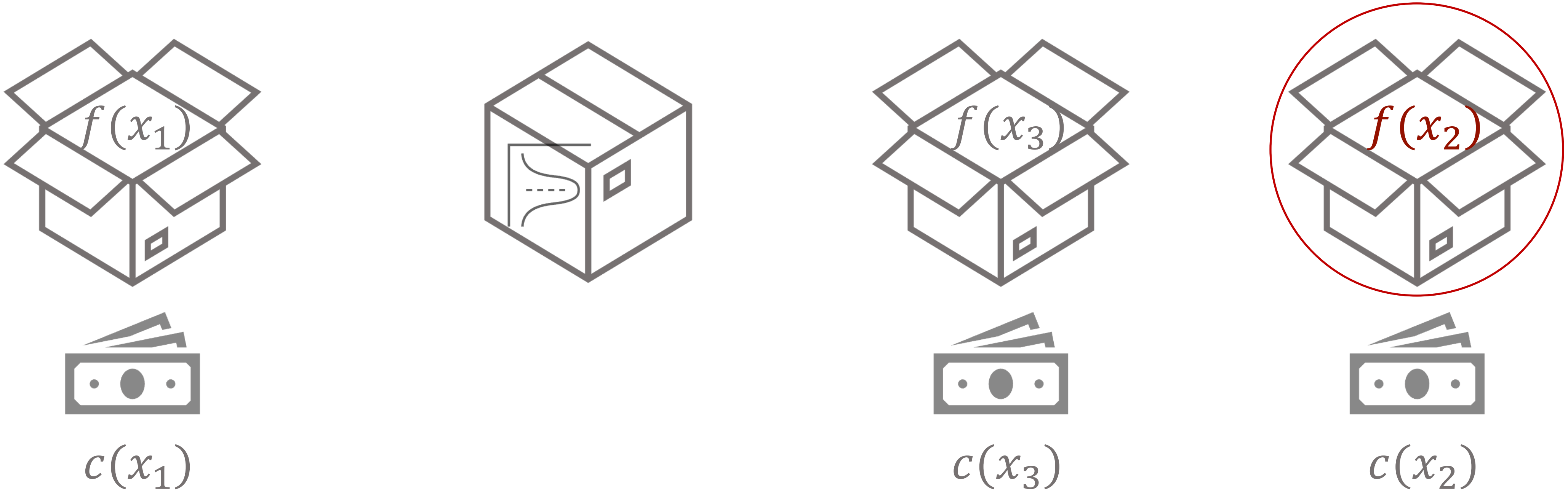


High-level goal: Choose $x_1, \ldots, x_T$ to maximize the expected utility

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

Pandora's Box

$t = T$, stop

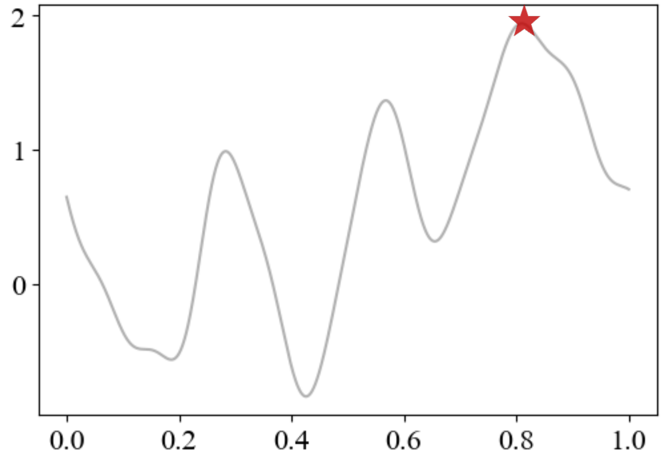


High-level goal: Choose $x_1, \ldots, x_T$ to maximize the expected utility

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

Bayesian Optimization

$f(x)$



Continuous

Correlated

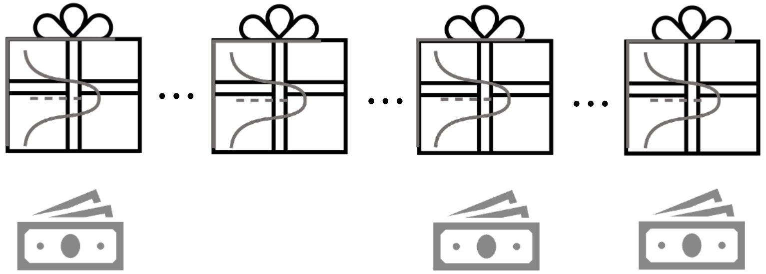
Fixed-iteration

Expected best-observed value

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

Pandora's Box

[Weitzman'79]



$f(x)$

$c(x)$

Discrete

Independent

Flexible-stopping

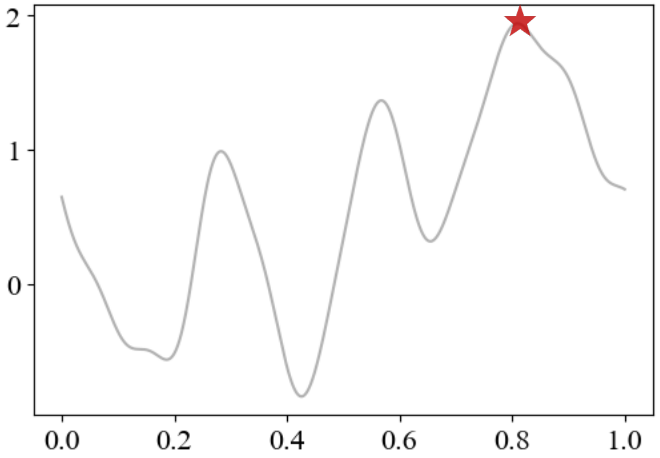
Expected utility

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

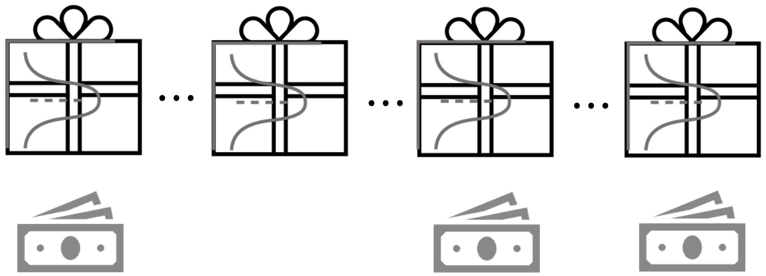
Fixed-iteration

Expected 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

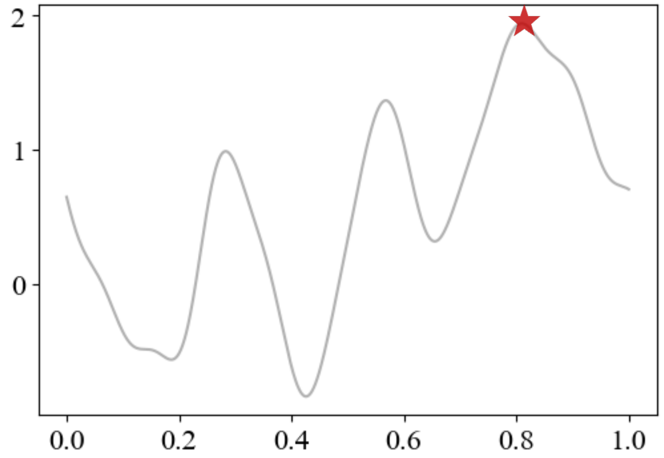
Expected utility

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

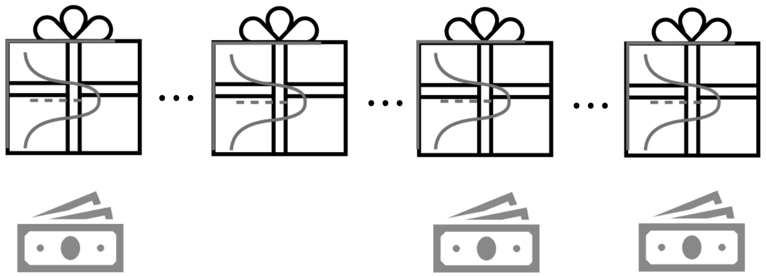
Fixed-iteration

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

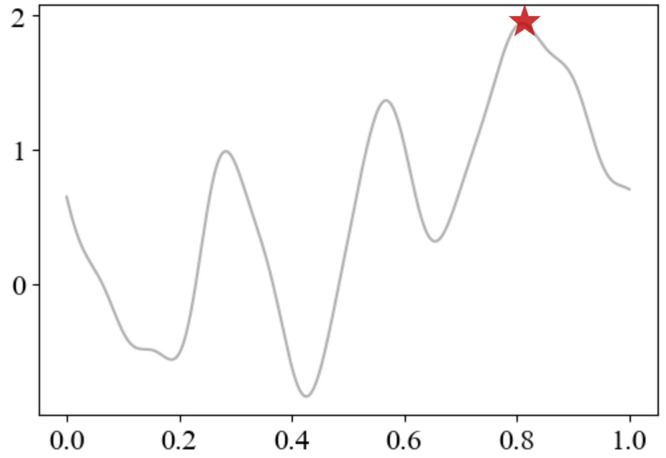
Expected utility

cumulative cost

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

Bayesian Optimization

$f(x)$



Continuous

Correlated

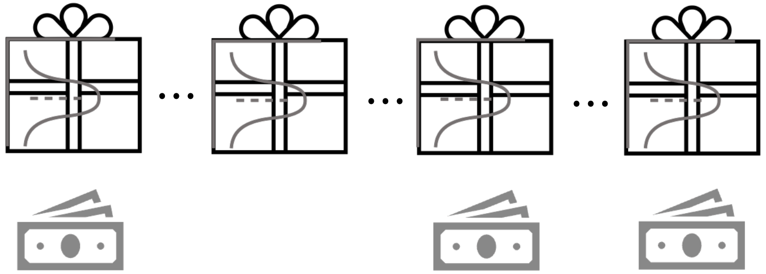
Fixed-iteration

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

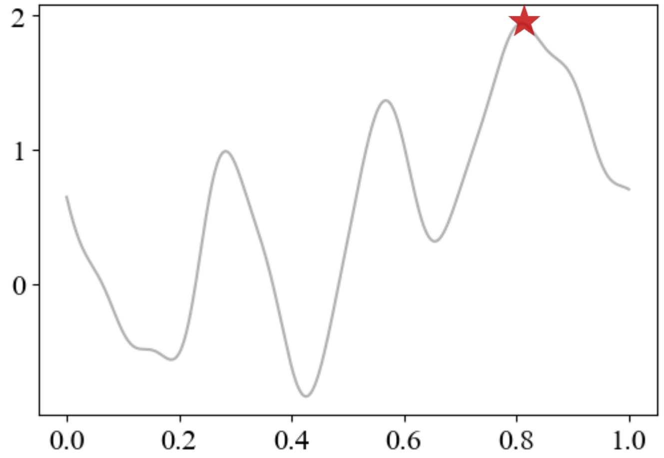
Expected cost-adjusted regret

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

cumulative cost

Bayesian Optimization

$f(x)$



Continuous

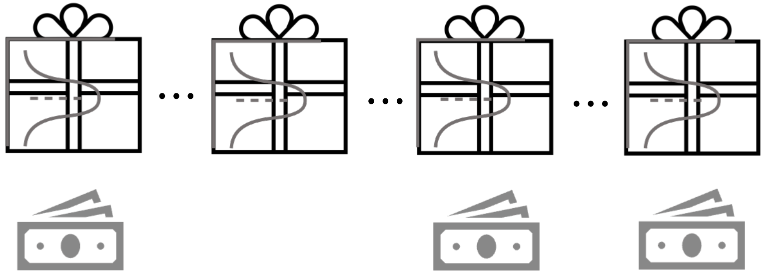
Correlated

Fixed-iteration

Expected regret

Pandora's Box

[Weitzman'79]



$f(x)$

$c(x)$

Discrete

Independent

Flexible-stopping

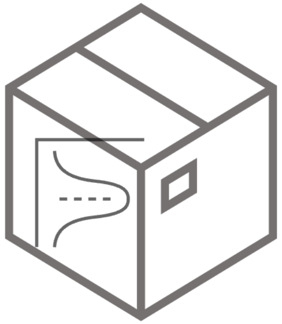
Expected cost-adjusted regret

Optimal policy: Gittins index

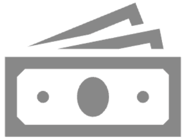
Optimal Policy: Gittins Index

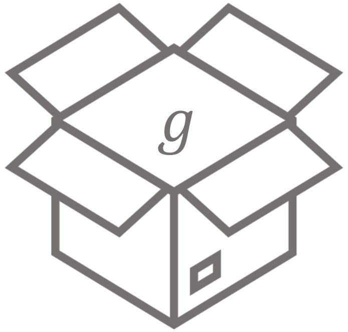
Step 1: Assign each box a Gittins index (higher is better)

$f(x)$



$c(x)$





$$\downarrow$$

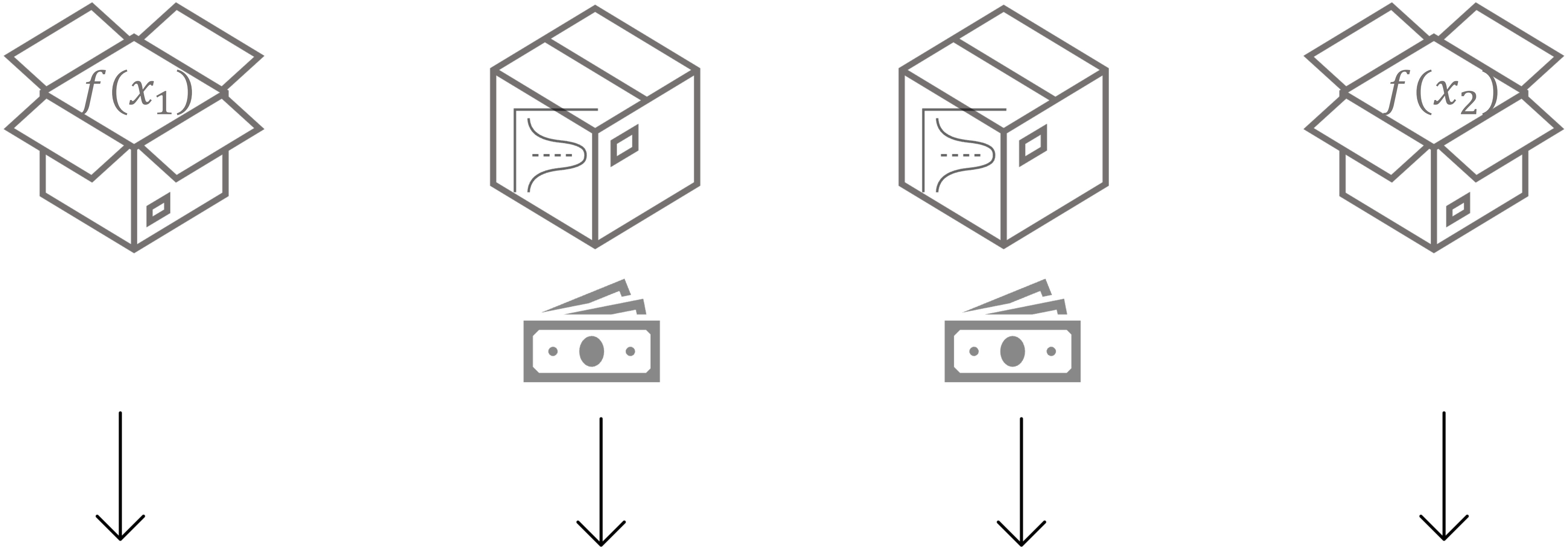
$$\mathrm{GI}_f(x; c(x))$$

$$\downarrow$$

$$g$$

Optimal Policy: Gittins Index

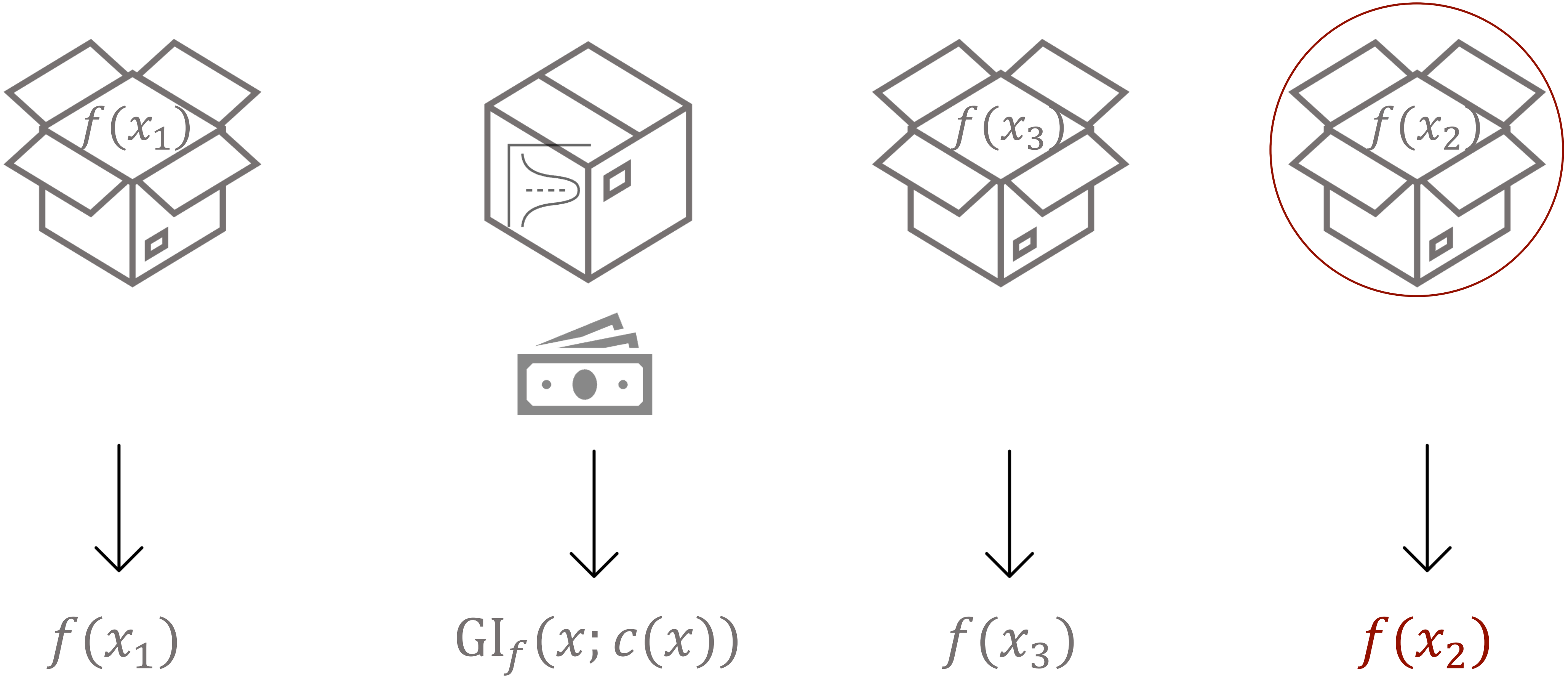
Step 2: Open the box with highest index if it is closed



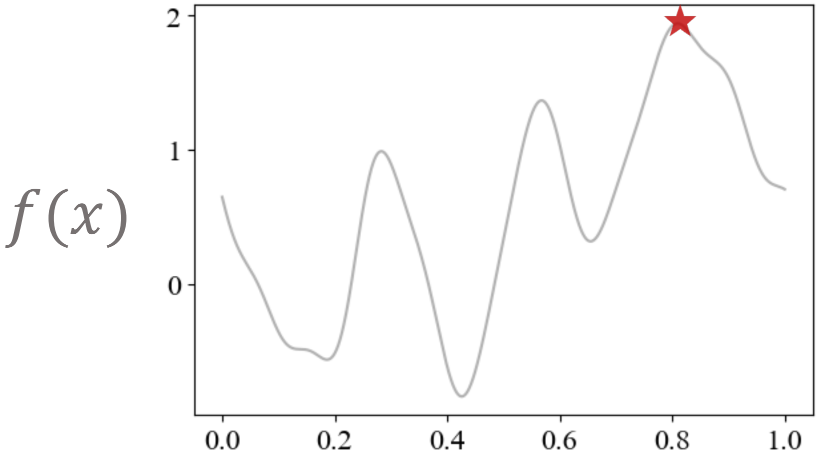
$f(x_1)$ $\mathrm{GI}_f(x; c(x))$ $\mathrm{GI}_f(x'; c(x'))$ $f(x_2)$

Optimal Policy: Gittins Index

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



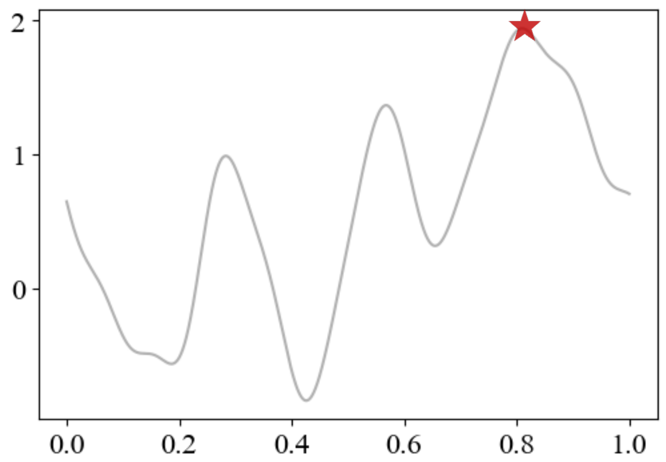
Bayesian Optimization	Pandora's Box
	[Weitzman'79]



Continuous	Discrete
Correlated	Independent
Fixed-iteration	Flexible-stopping
Expected regret	Expected cost-adjusted regret
Is Gittins index good?	Gittins index is optimal

Bayesian Optimization

$f(x)$



Continuous

Correlated

Fixed-iteration

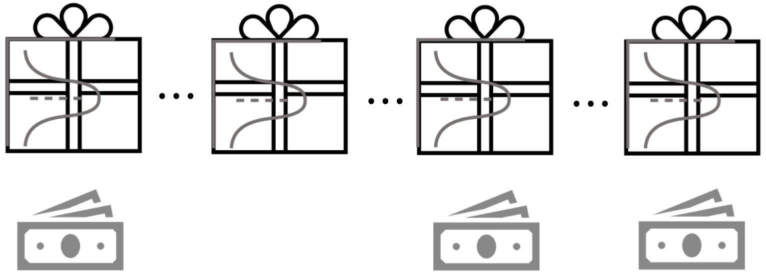
Expected regret

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

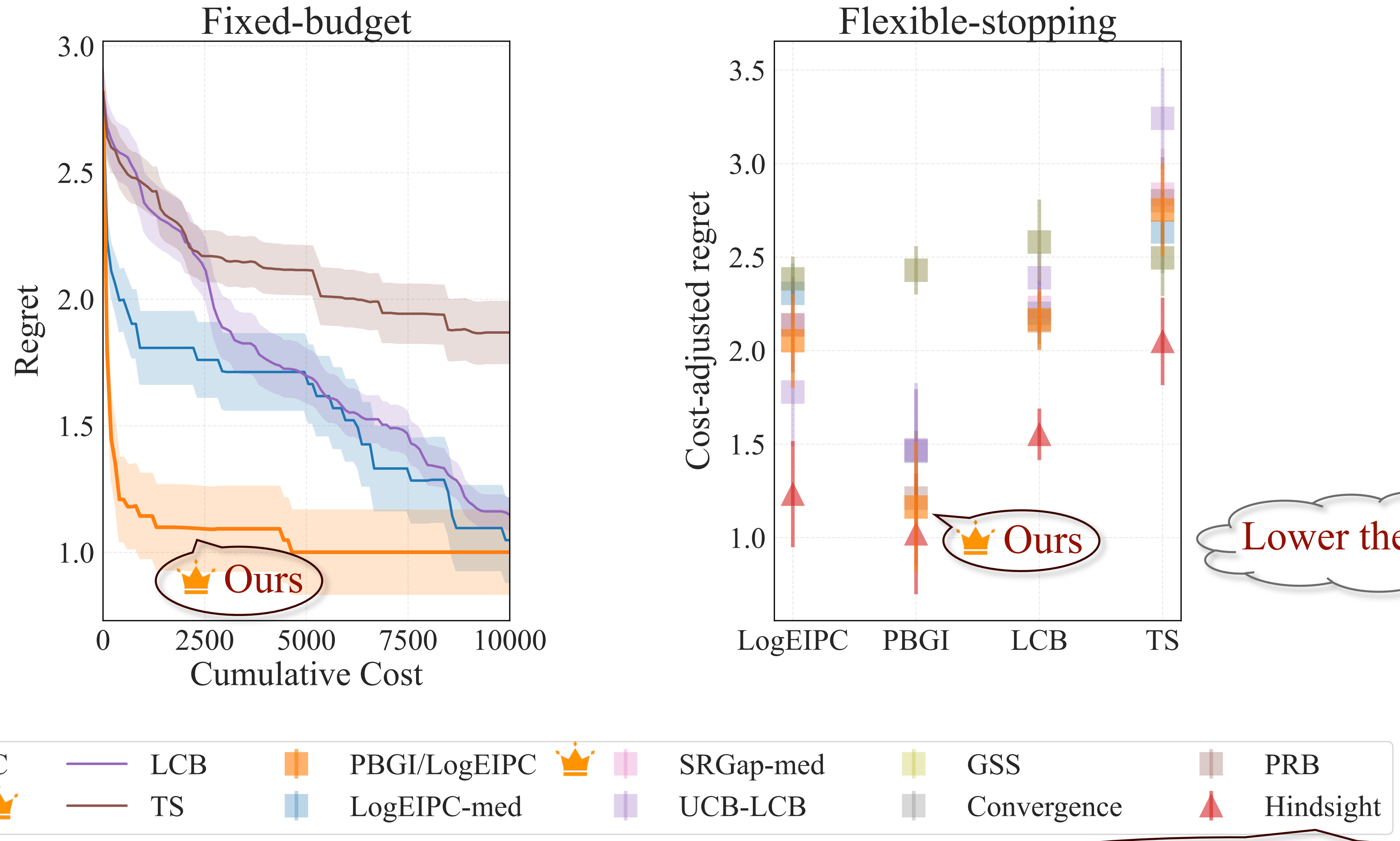
New Design Principle: Gittins Index

- 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

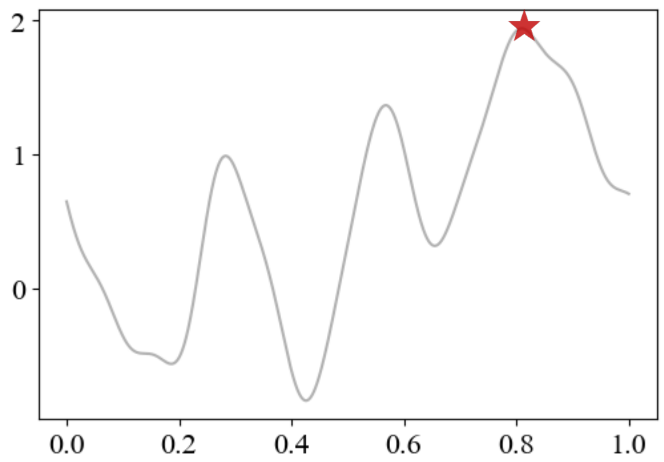


Lower the better

Bound on achievable performance

Bayesian Optimization

$f(x)$



Continuous

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Expected regret

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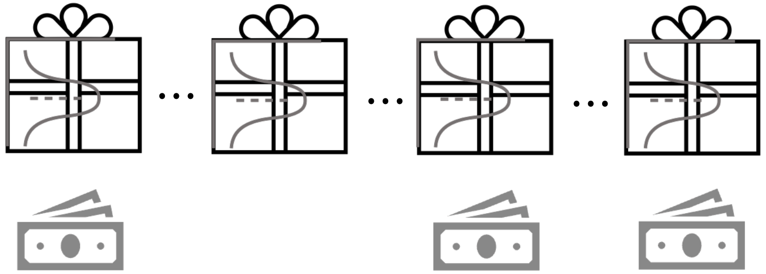

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- **Gittins Index**

? Why another principle?

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Theoretical Guarantee and Empirical Validation

Theorem (No worse than stopping-immediately)

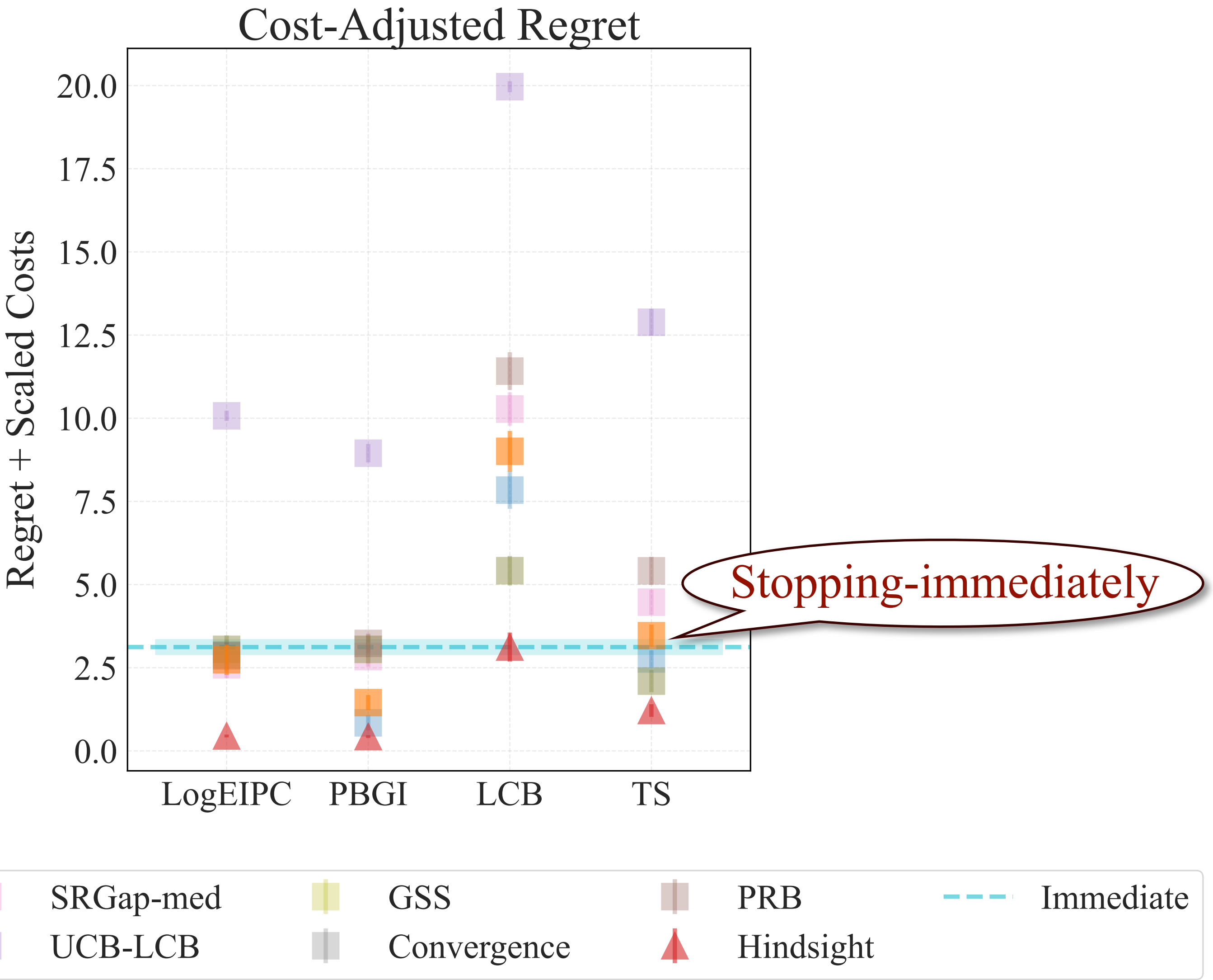
$\mathbb{E}[R(\text{ours; PBGI})] \leq R[\text{stopping immediately}]$

or LogEIPC

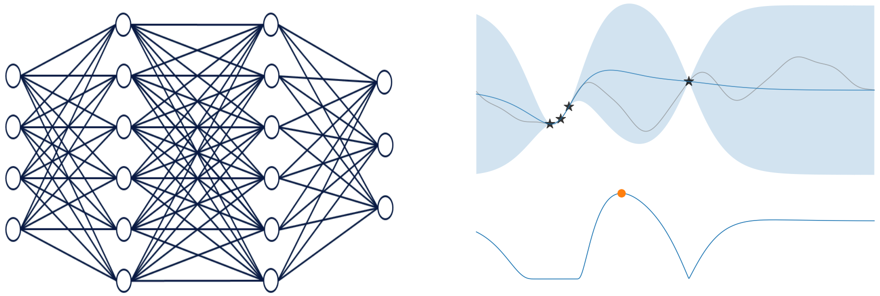
cost-adjusted regret

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.



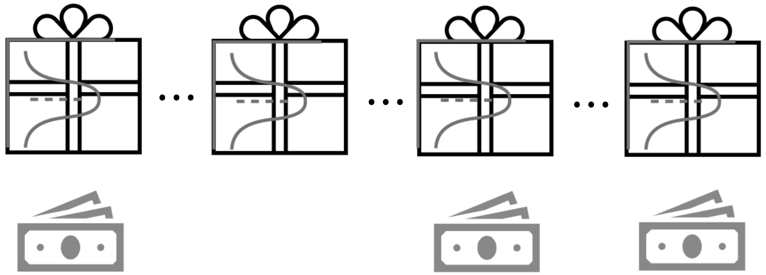
Studied problem



Varying evaluation costs

Adaptive stopping time

Key idea



Link to Pandora’s Box problem & Gittins index theory

Impact

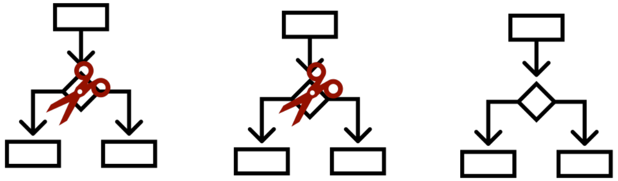
Meta

BoTorch Ax

Competitive empirical performance & interests from practitioners

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

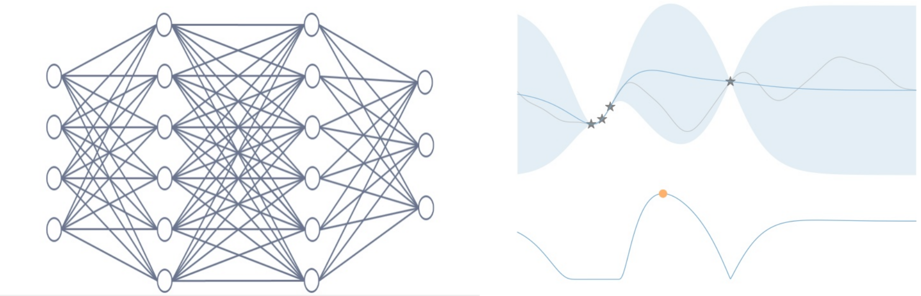
Ongoing work



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

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

Studied problem



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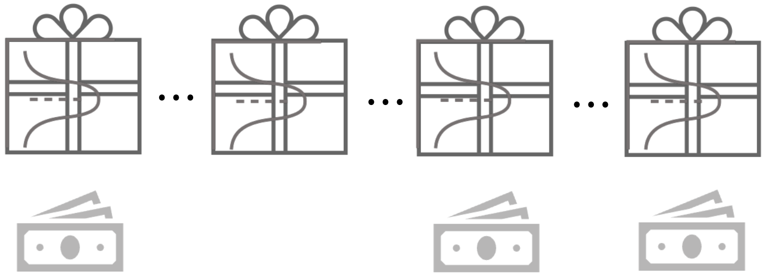

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Ongoing work

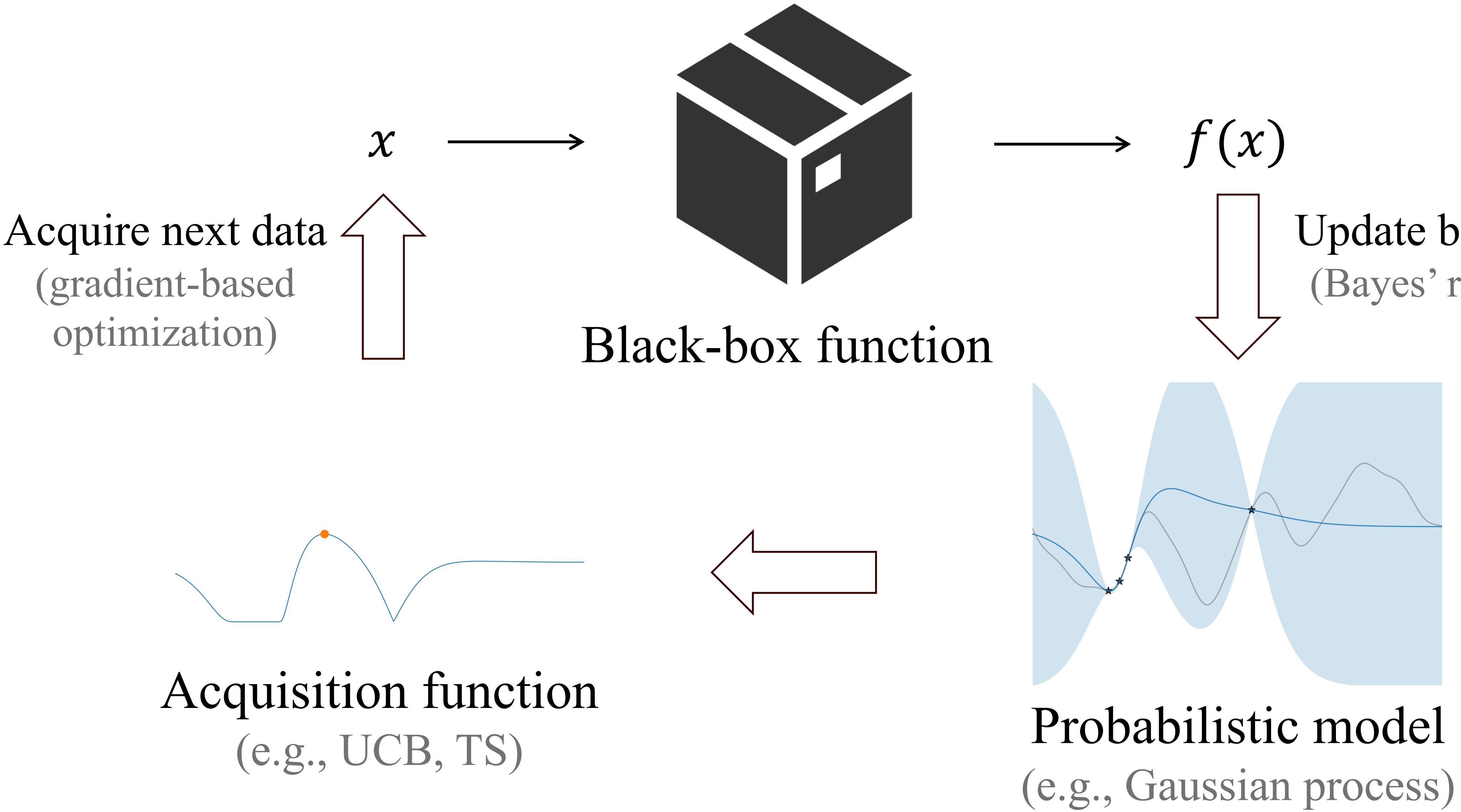
ChatGPT Gemini

deepseek Claude

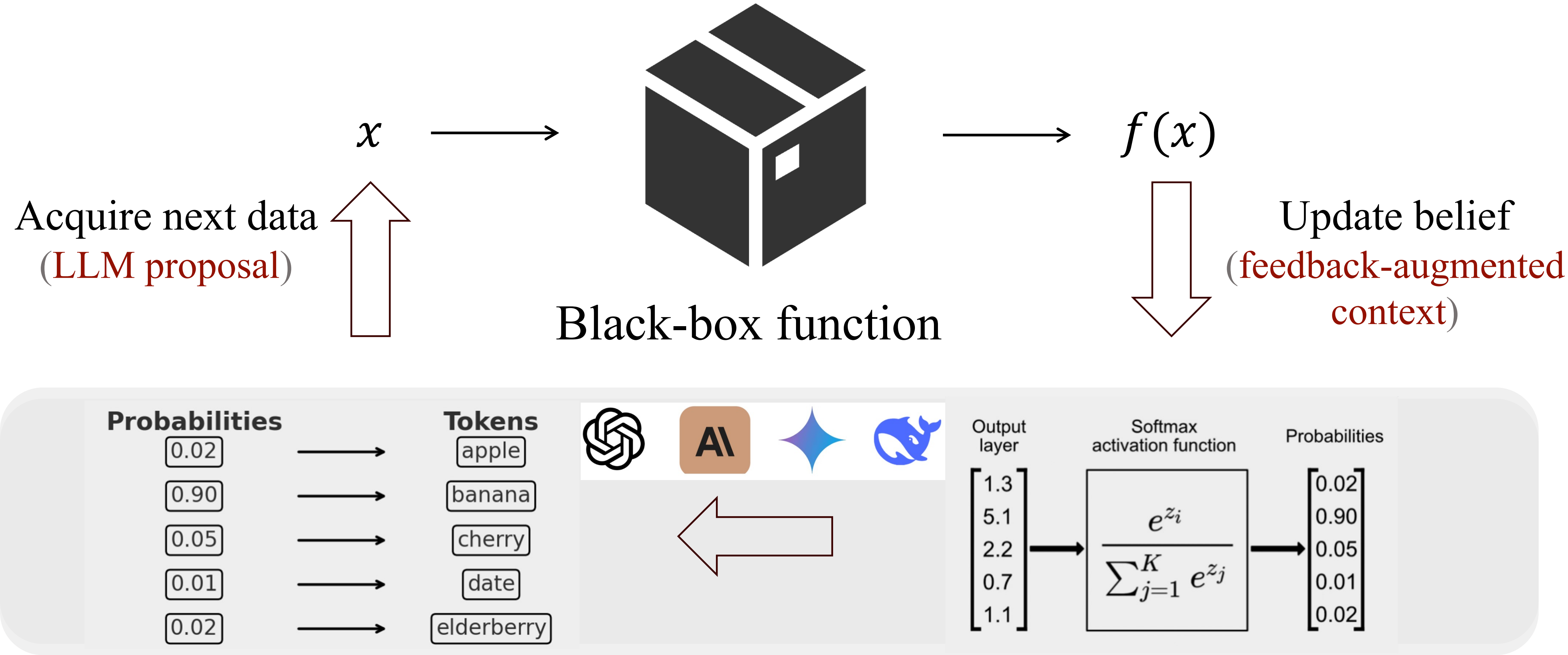
LLM-driven black-box optimization

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

Recap: Bayesian Optimization



Ongoing: LLM-Driven Black-Box Optimization



Acquisition function
(e.g., Softmax sampling)

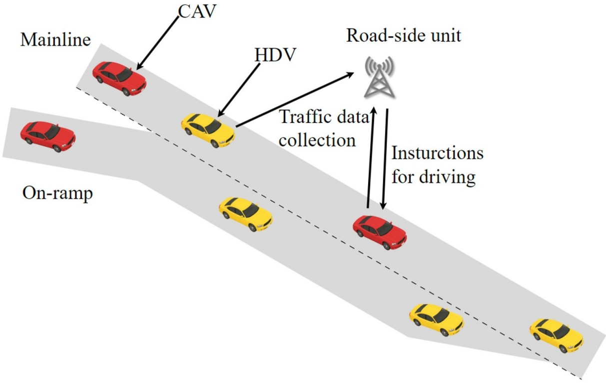
Probabilistic model
(e.g., autoregressive model)

Ongoing: LLM-Driven RL Training Optimization

Mixed-autonomy traffic control:

(e.g., Transformer config)

x



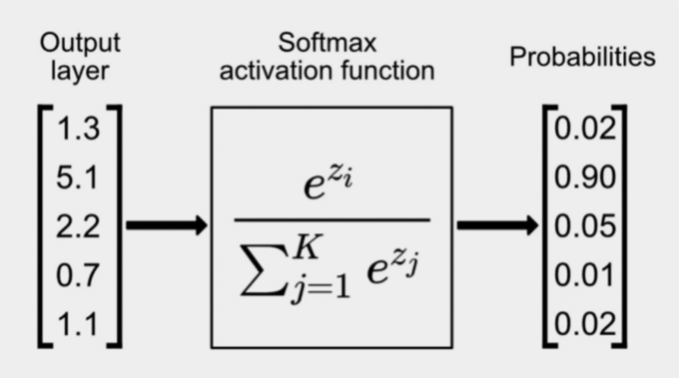
(e.g., average speed)

$f(x)$

Acquire next data
(LLM proposal)

Update belief
(feedback-augmented context)

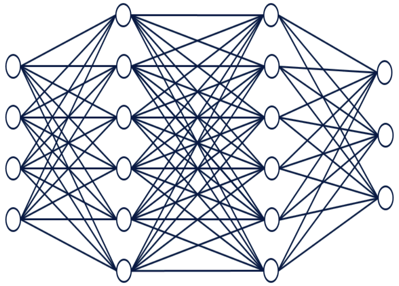
Black-box function
(RL training & evaluation)

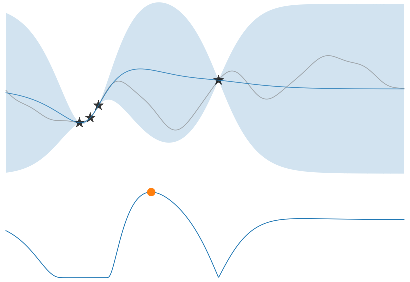


Acquisition function
(e.g., Softmax sampling)

Probabilistic model
(large language model)

Studied problem





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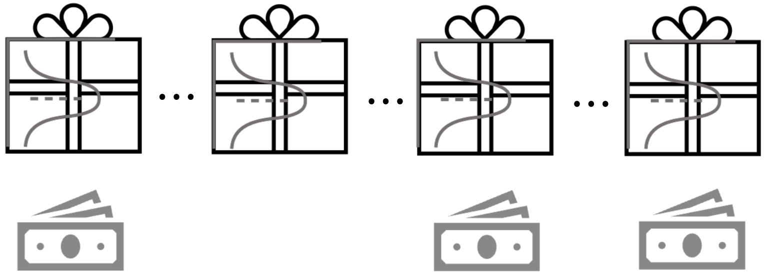

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