

Cost-Aware Bayesian Optimization with Adaptive Stopping via Gittins Indices

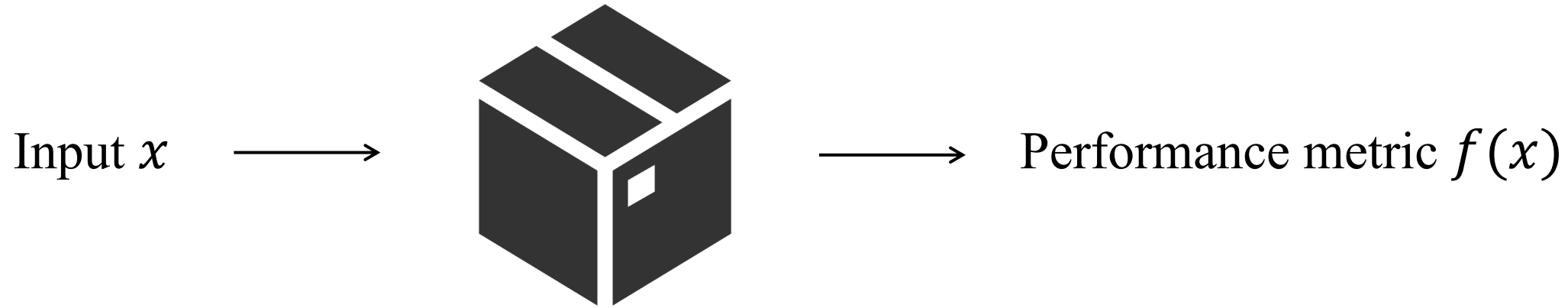
Qian Xie 谢倩 (Cornell ORIE)

INFORMS Annual Meeting 2025 Job Market Showcase

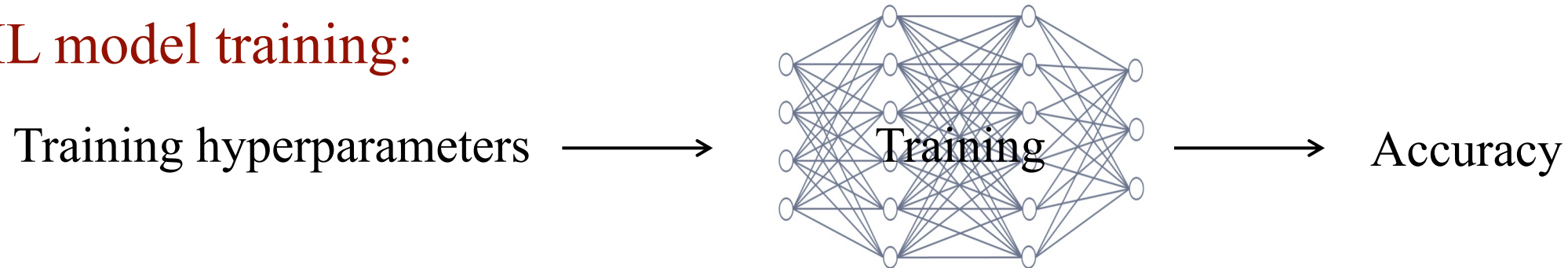
Black-Box Optimization



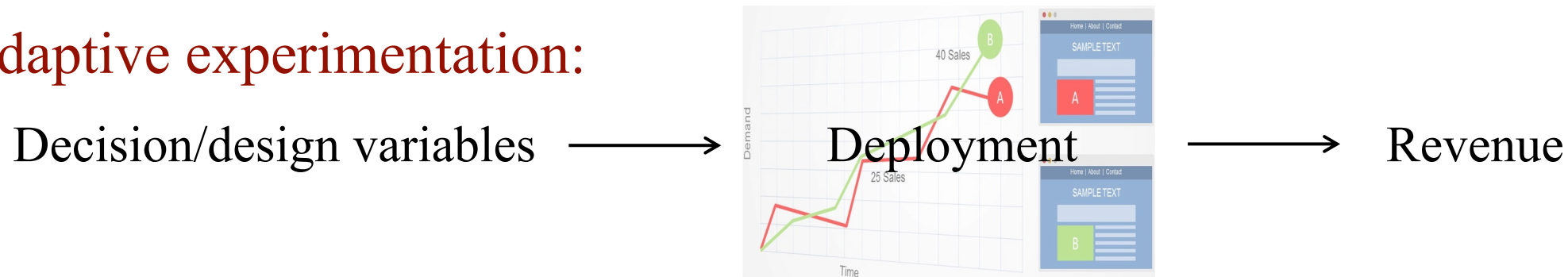
Black-Box Optimization



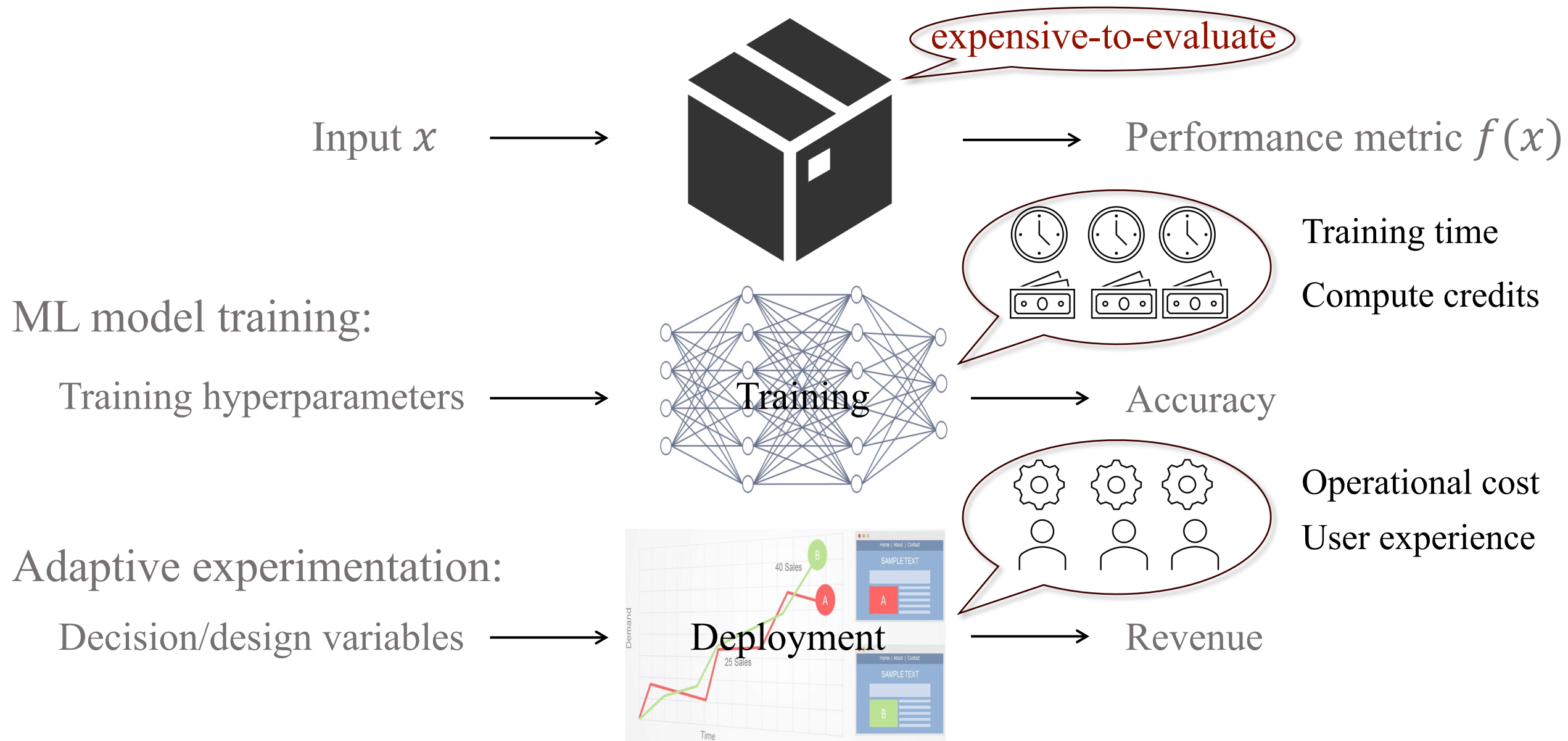
ML model training:



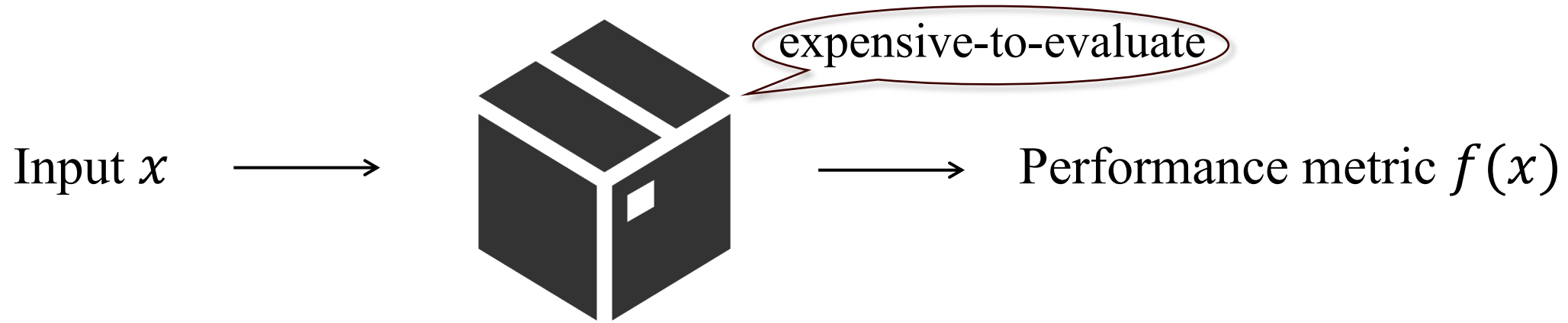
Adaptive experimentation:



Black-Box Optimization



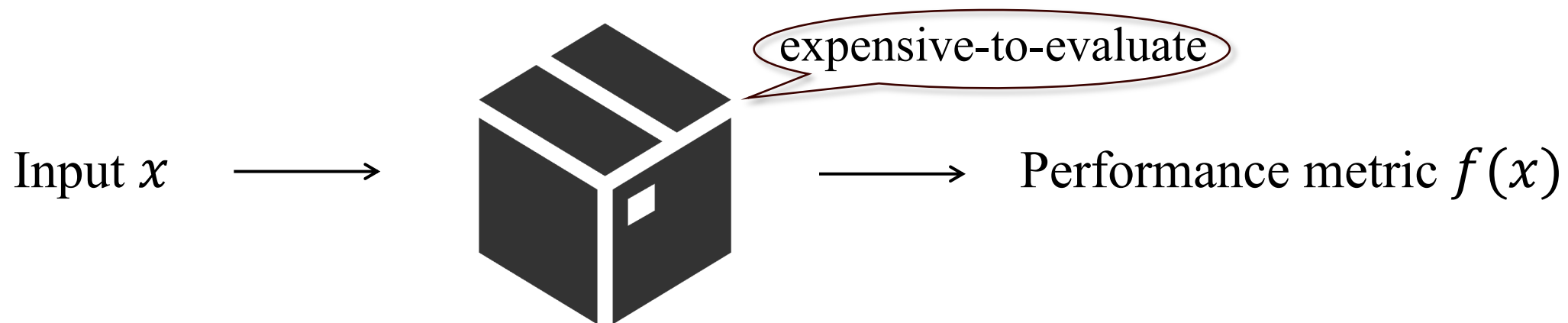
Black-Box Optimization



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

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

Black-Box Optimization



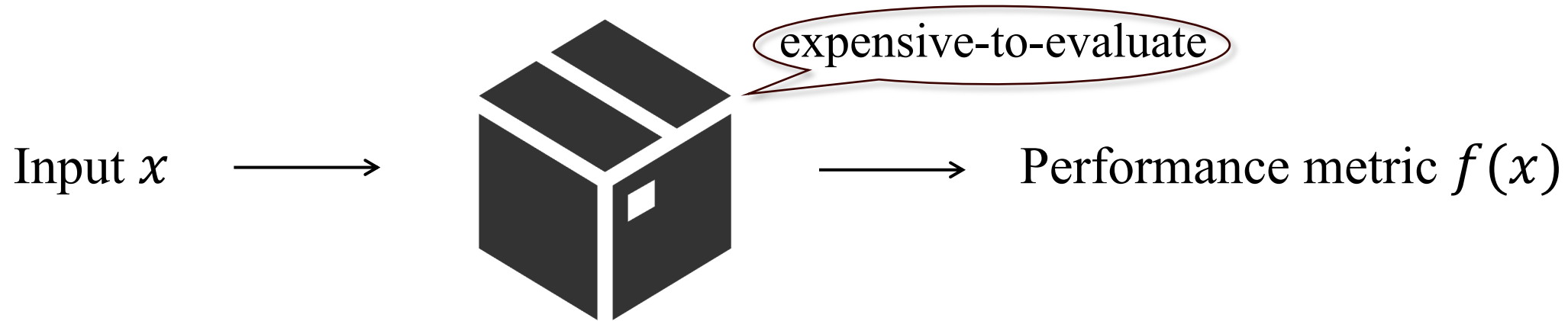
adaptively

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

Black-Box Optimization



adaptively

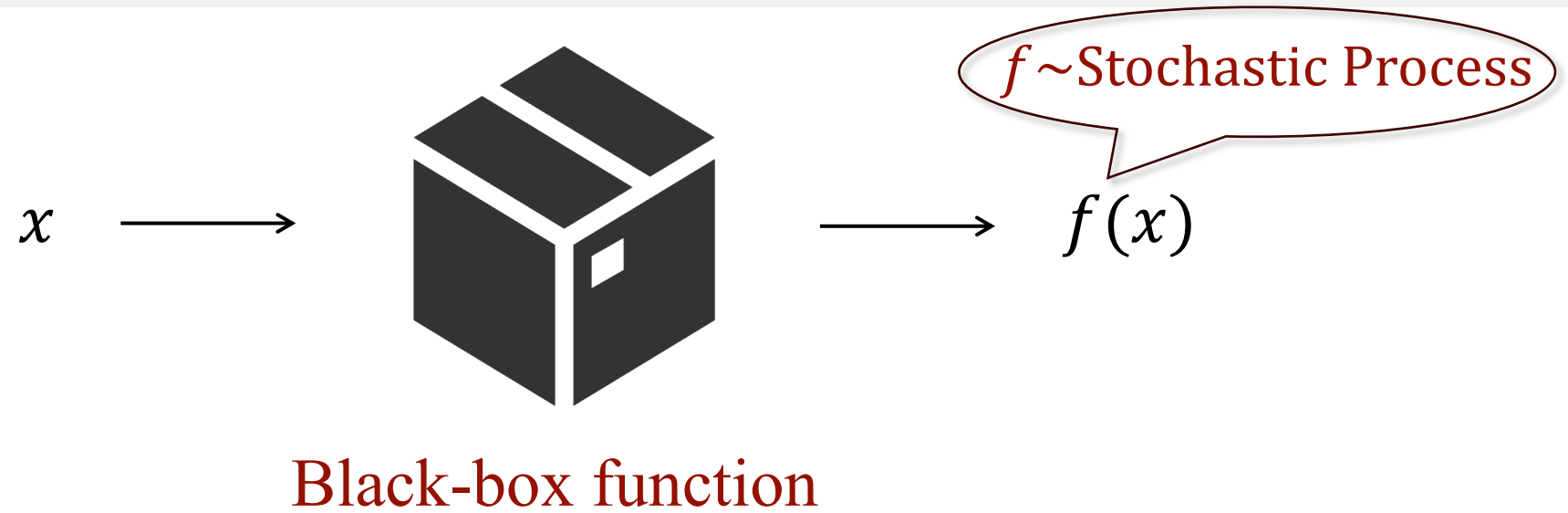
High-level goal: Choose x_1, \dots, x_T to maximize the expected best observed value

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

Fewer #evaluations

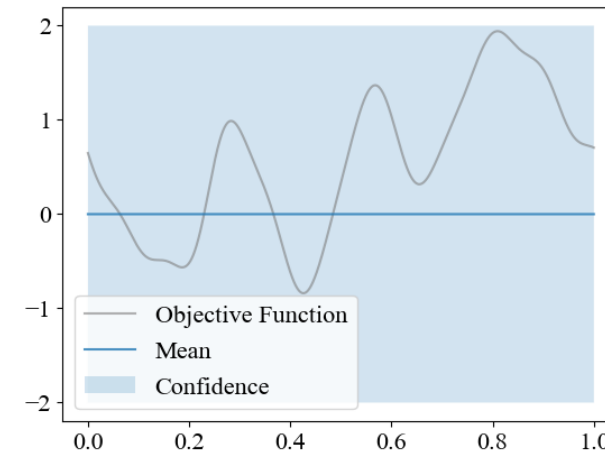
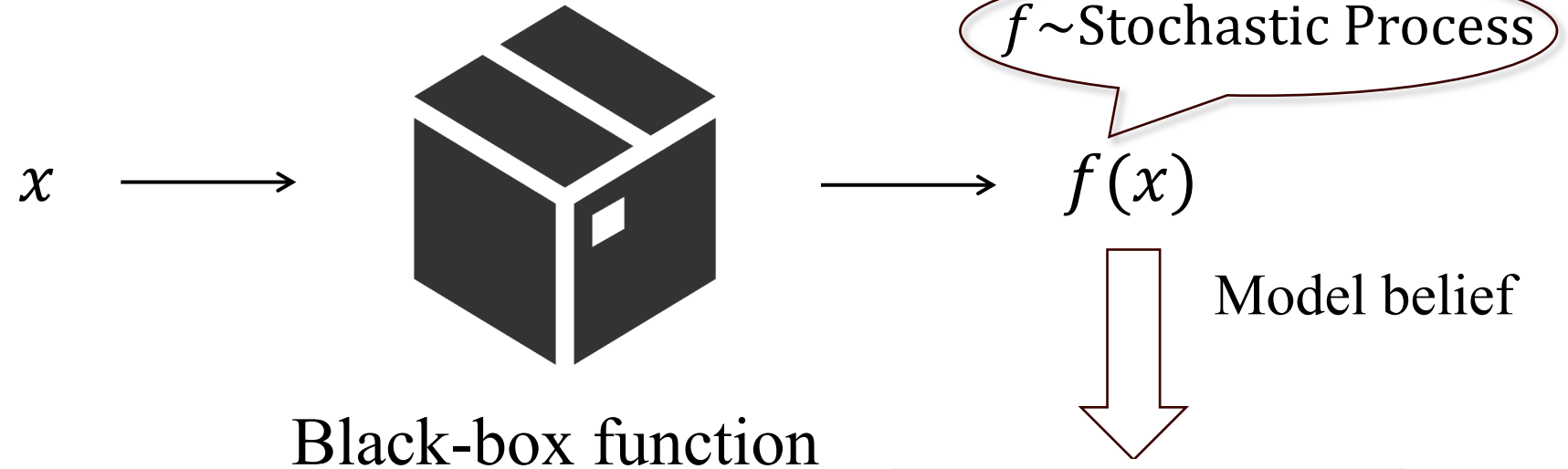
Efficient framework: Bayesian optimization

Bayesian Optimization



Bayesian Optimization

Time 0



Probabilistic model
(e.g., Gaussian process)

Bayesian Optimization

Time t

x_1, \dots, x_t



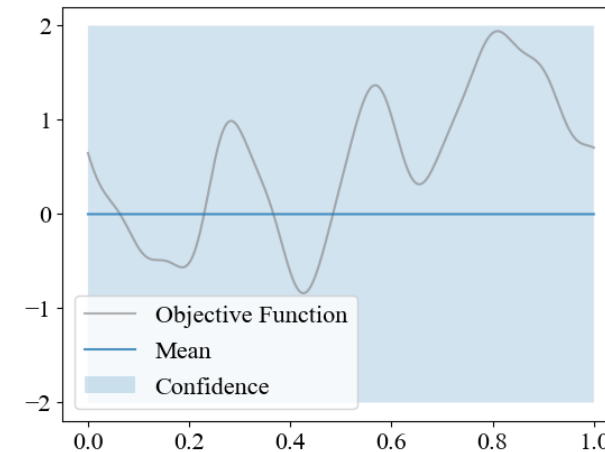
Black-box function



$f \sim \text{Stochastic Process}$

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

Model belief



Probabilistic model
(e.g., Gaussian process)

Bayesian Optimization

Time t

x_1, \dots, x_t



Black-box function

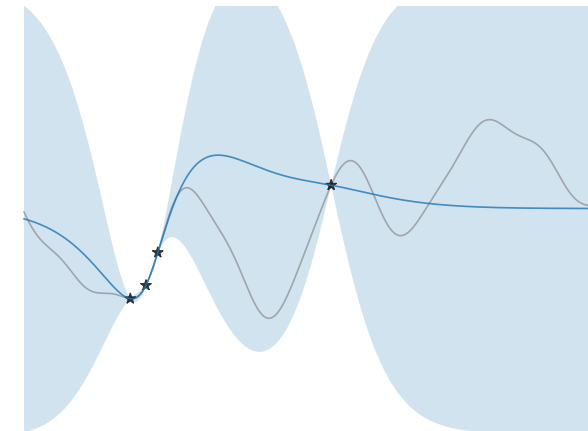


$f \sim \text{Stochastic Process}$

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



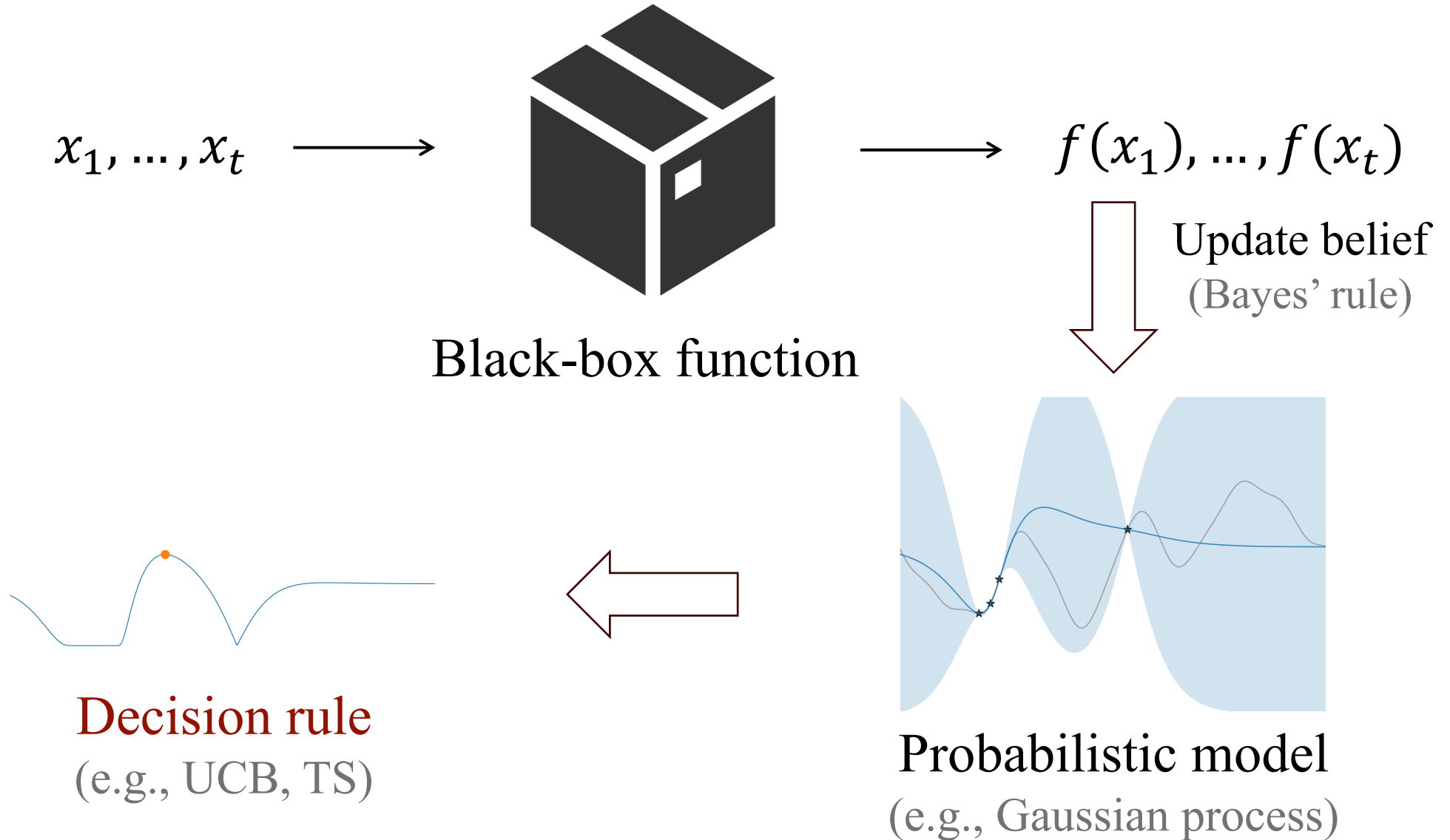
Update belief
(Bayes' rule)



Probabilistic model
(e.g., Gaussian process)

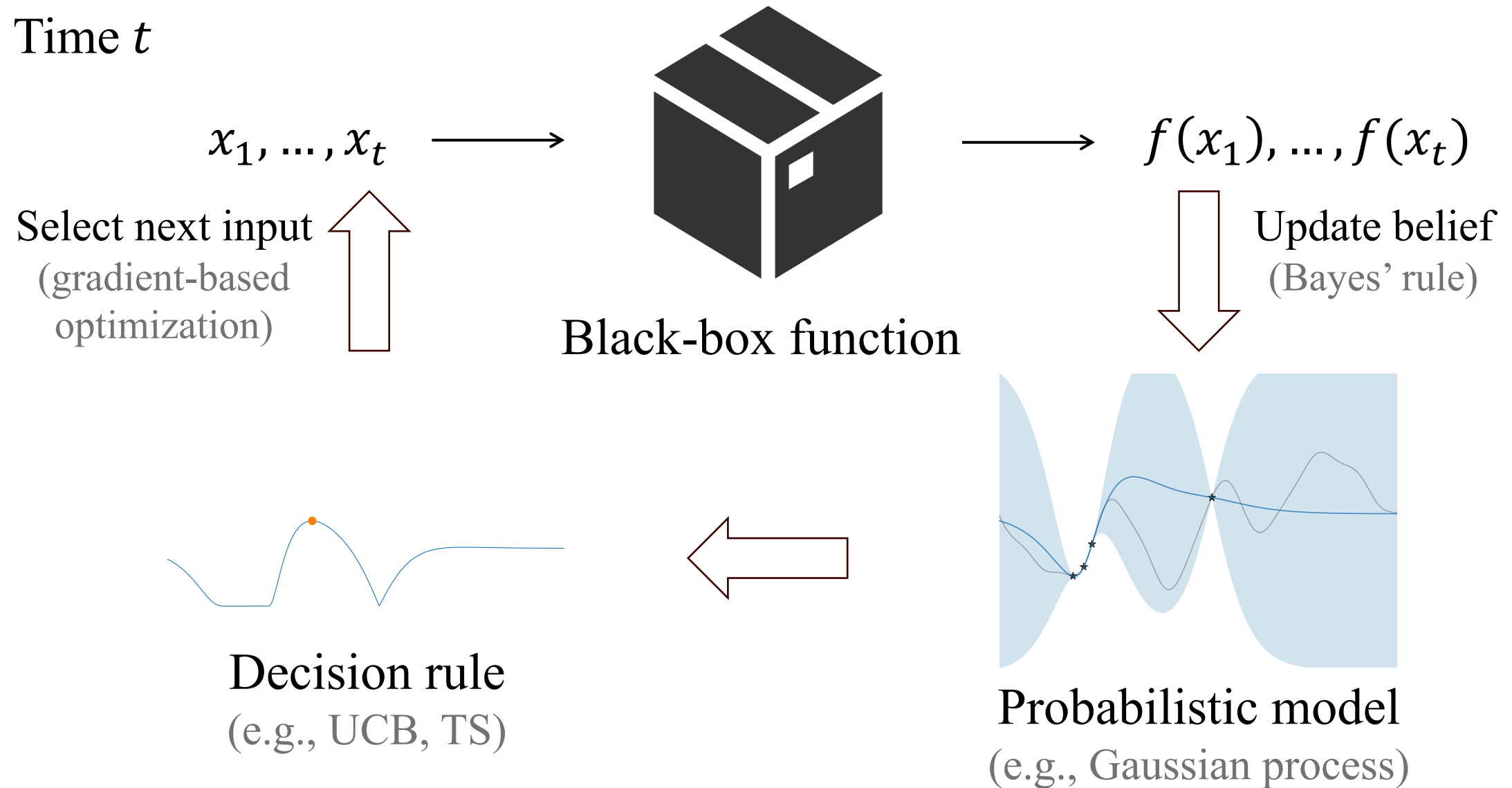
Bayesian Optimization

Time t



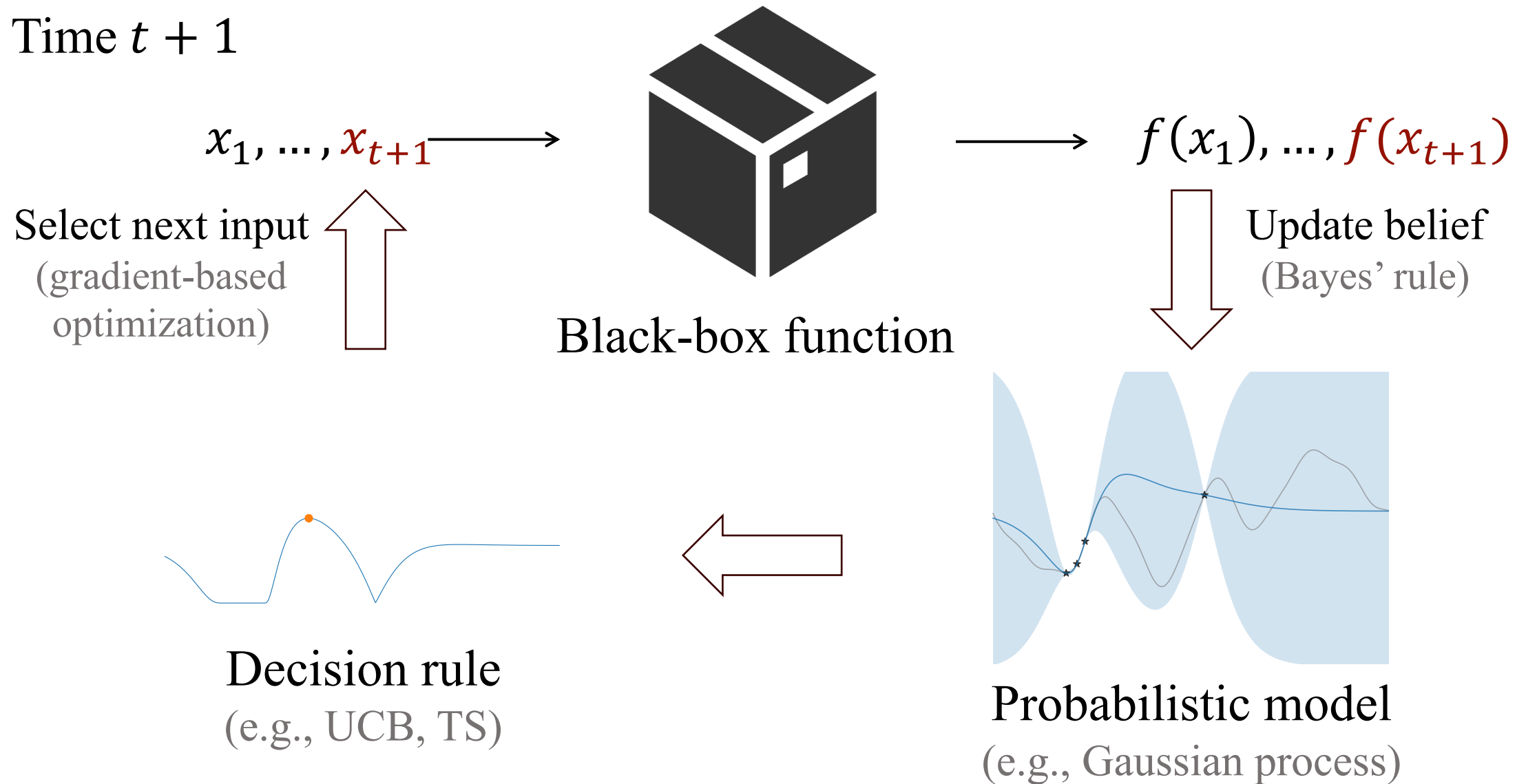
Bayesian Optimization

Time t

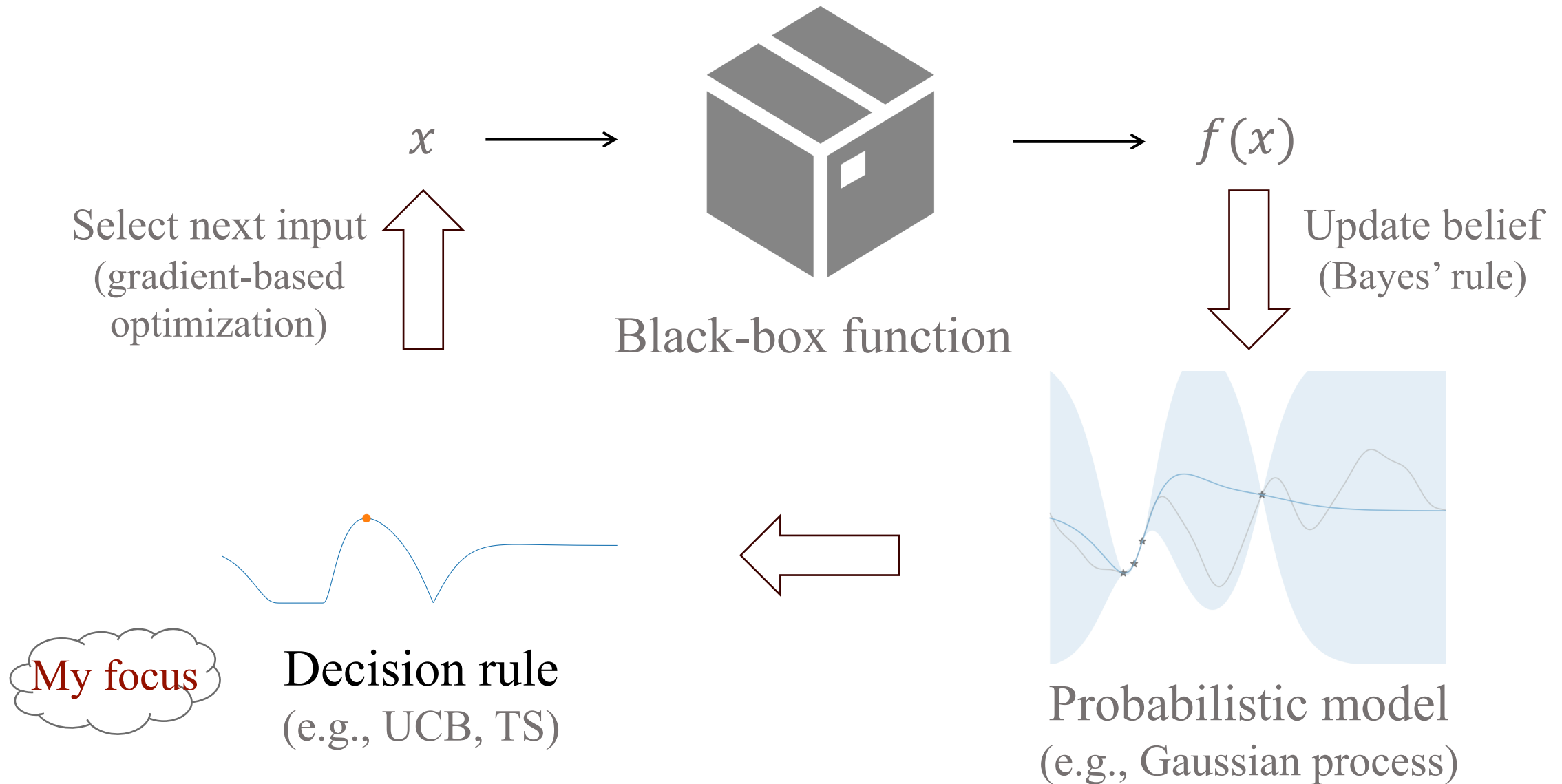


Bayesian Optimization

Time $t + 1$



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
- Gittins Index

New Design Principle: Gittins Index

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Why another principle?

New Design Principle: Gittins Index

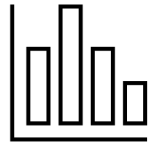
- Improvement-based
- Entropy-based
- Confidence bounds (UCB/LCB)
- Thompson sampling
- Gittins Index



Why another principle?

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

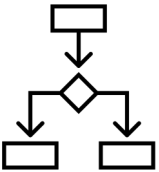
Under-explored Practical Considerations



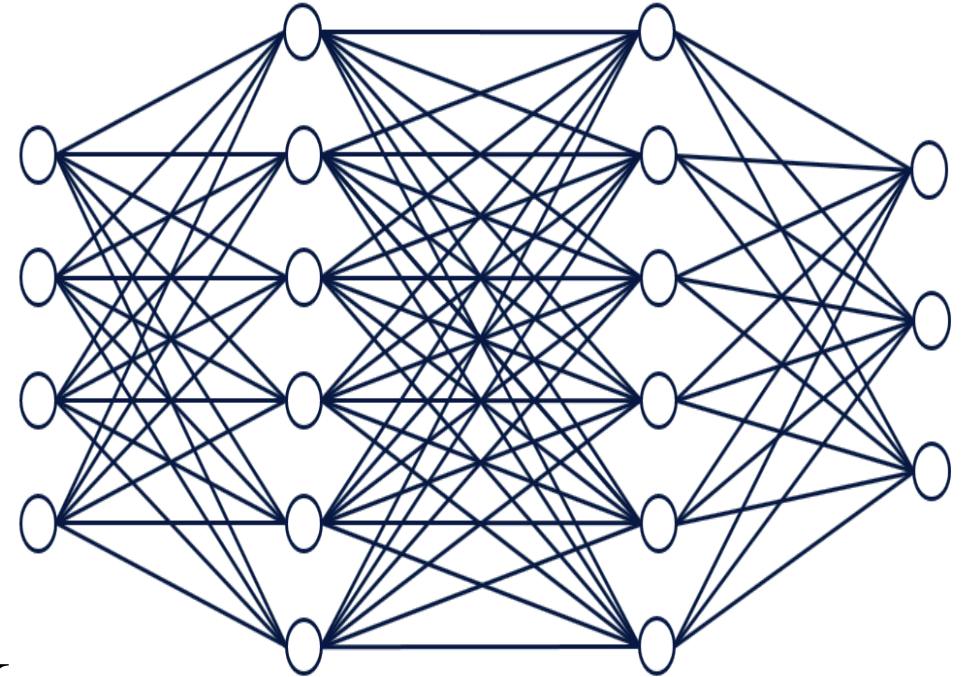
Varying evaluation costs



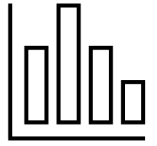
Smart stopping time



Observable multi-stage feedback



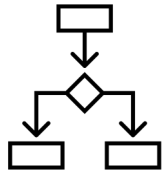
Under-explored Practical Considerations



Varying evaluation costs



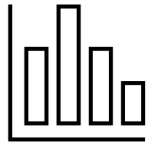
Smart stopping time



Observable multi-stage feedback

New design principle:
Gittins index

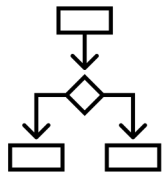
Why Gittins index?



Varying evaluation costs



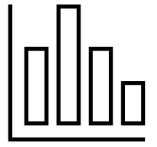
Smart stopping time



Observable multi-stage feedback

New design principle:
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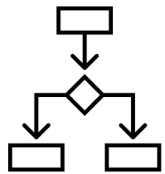
Why Gittins index?



Varying evaluation costs



Smart stopping time

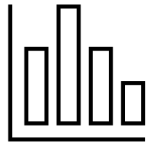


Observable multi-stage feedback

New design principle:
Gittins index

Optimal in related sequential
decision problems

Why Gittins index?



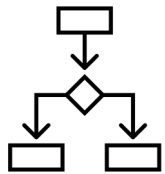
Varying evaluation costs

Features in Pandora's box



Smart stopping time

Features in Pandora's box

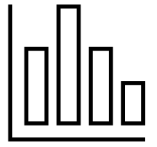


Observable multi-stage feedback

New design principle:
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Optimal in related sequential
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Why Gittins index?



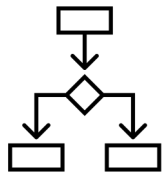
Varying evaluation costs

Features in Pandora's box



Smart stopping time

Features in Pandora's box



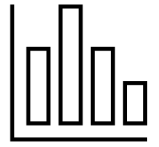
Observable multi-stage feedback

Features in **Markovian bandits**

New design principle:
Gittins index

Optimal in related sequential
decision problems

What is Pandora's Box?



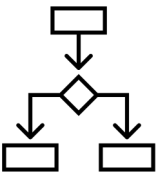
Varying evaluation costs

Features in Pandora's box



Smart stopping time

Features in Pandora's box

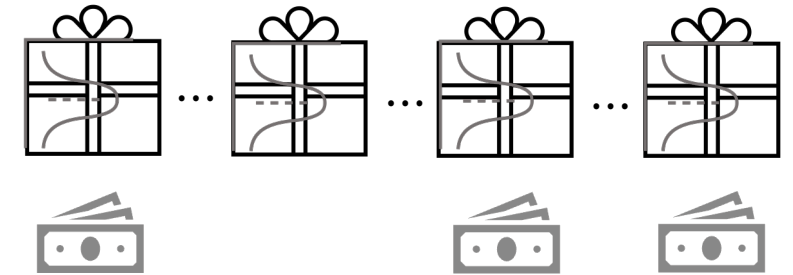


Observable multi-stage feedback

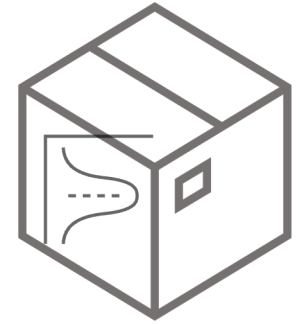
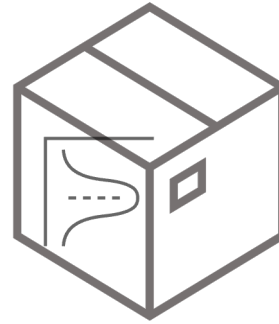
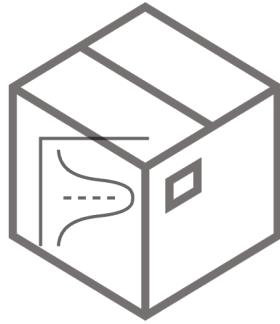
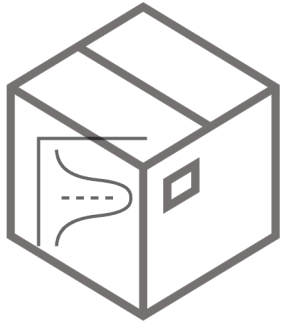
Features in Markovian bandits

New design principle:
Gittins index

Optimal in related sequential
decision problems



Pandora's Box



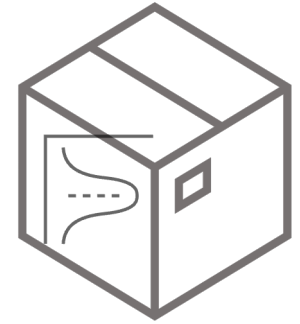
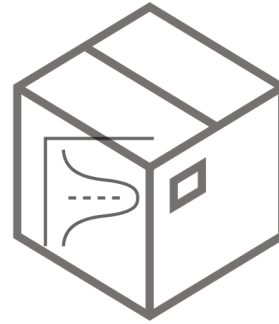
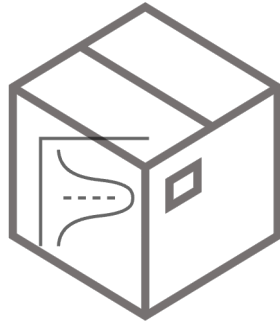
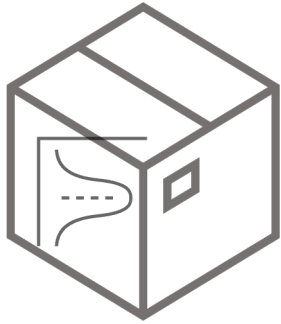
High-level goal: Choose x_1, \dots, x_T to maximize the expected utility

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

Flexible stopping time

Pandora's Box

$t = 0$

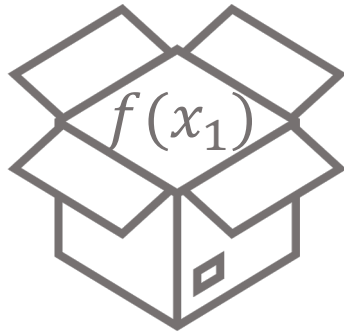


High-level goal: Choose x_1, \dots, x_T to maximize the expected utility

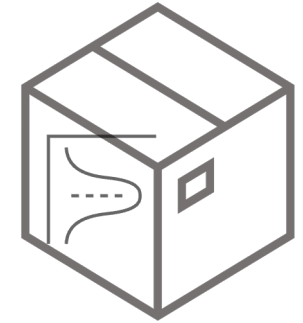
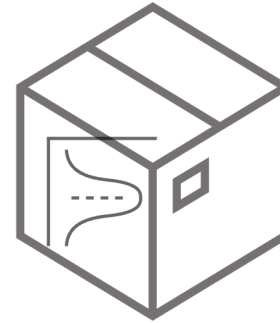
$$\mathbb{E} \max_{t=1,2,\dots,T} f(x_t) - \mathbb{E} \sum_{t=1}^T c(x_t)$$

Pandora's Box

$t = 1$



$c(x_1)$

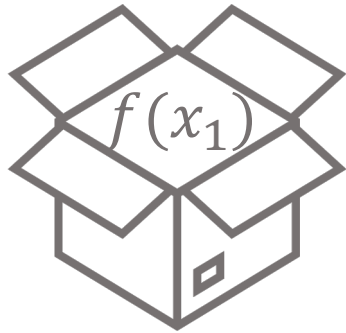


High-level goal: Choose x_1, \dots, x_T to maximize the expected utility

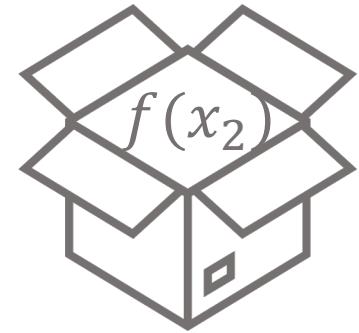
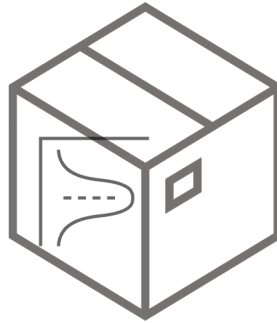
$$\mathbb{E} \max_{t=1,2,\dots,T} f(x_t) - \mathbb{E} \sum_{t=1}^T c(x_t)$$

Pandora's Box

$t = 2$



$c(x_1)$



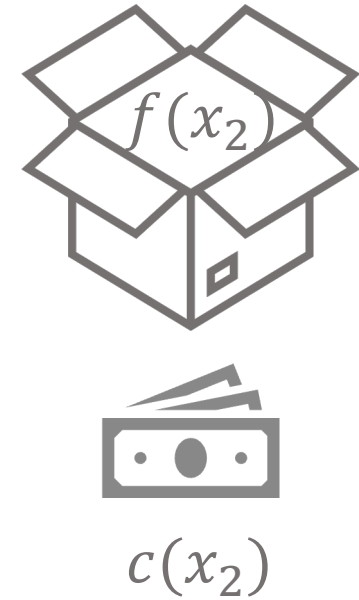
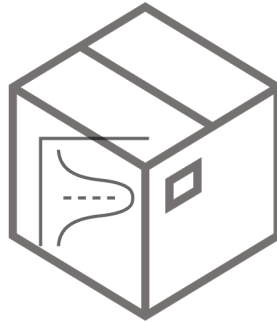
$c(x_2)$

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

$t = 3$

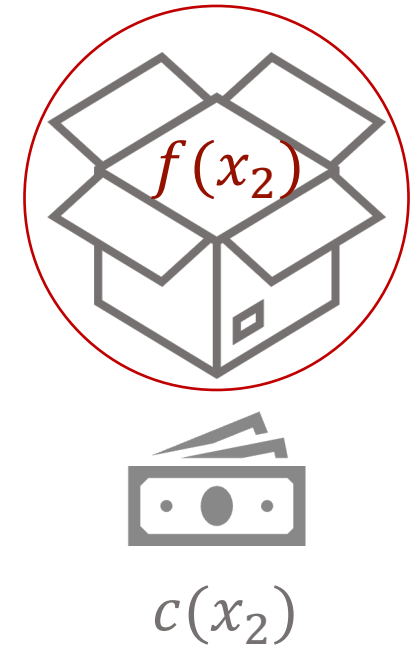
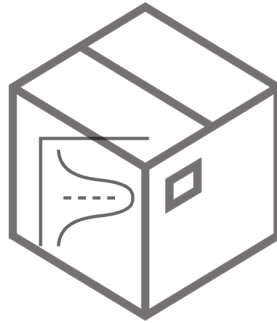
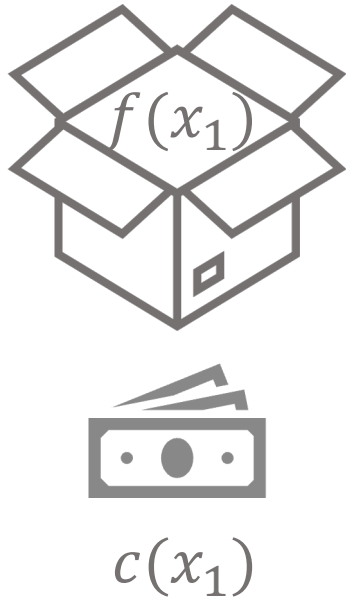


High-level goal: Choose x_1, \dots, x_T to maximize the expected utility

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

Pandora's Box

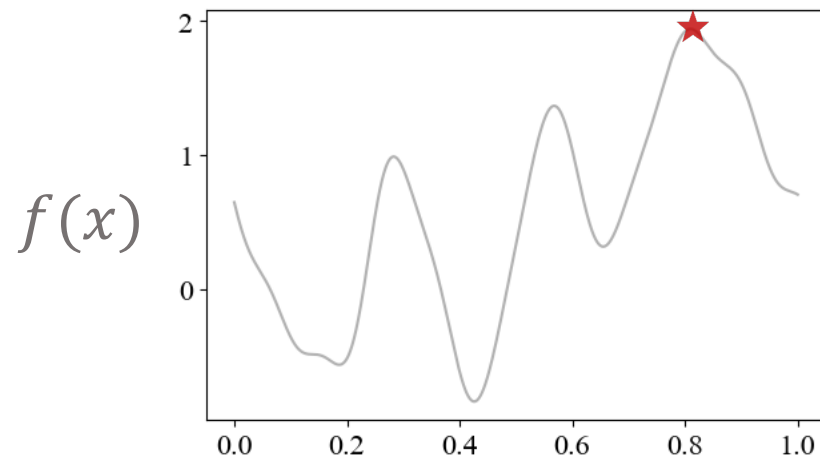
$t = T$, stop



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



Continuous

Correlated

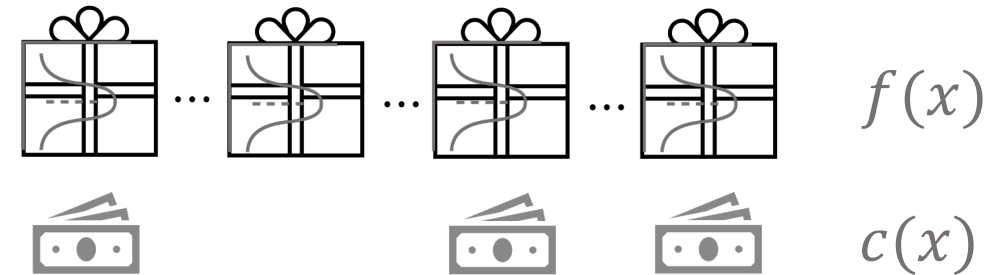
Fixed-iteration

Expected best-observed value

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

Pandora's Box

[Weitzman'79]



Discrete

Independent

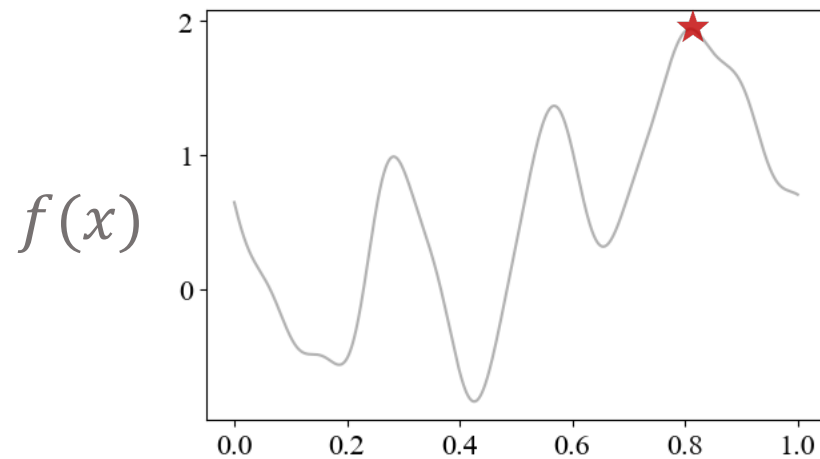
Flexible-stopping

Expected utility

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

cumulative cost

Bayesian Optimization



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]



Discrete

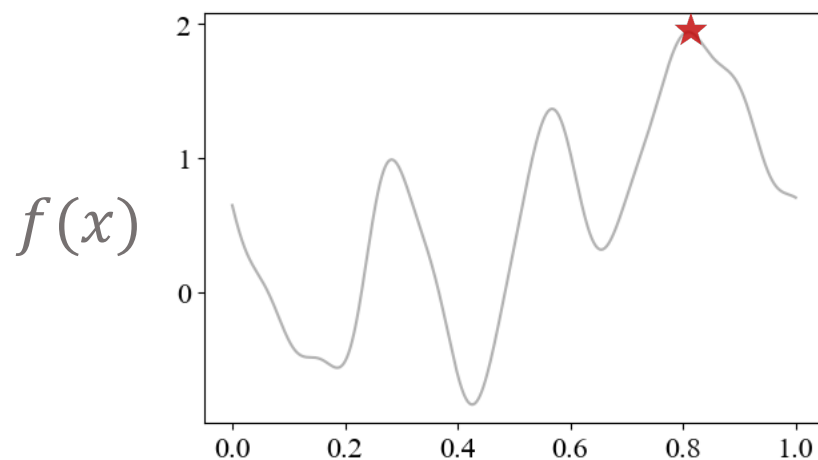
Independent

Flexible-stopping

Expected cost-adjusted regret

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

Bayesian Optimization



Continuous

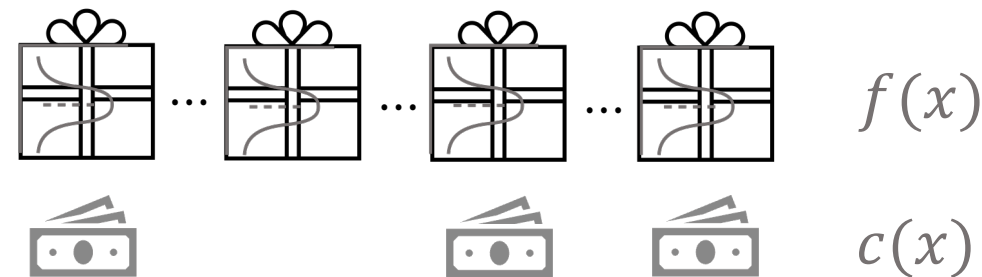
Correlated

Fixed-iteration

Expected regret

Pandora's Box

[Weitzman'79]



Discrete

Independent

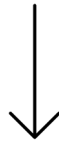
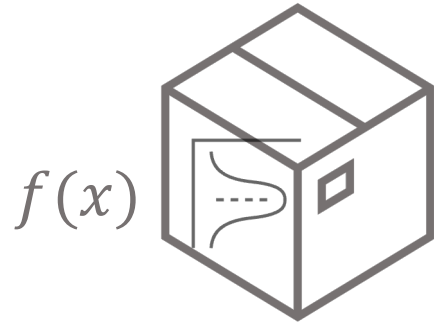
Flexible-stopping

Expected cost-adjusted regret

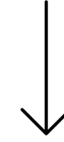
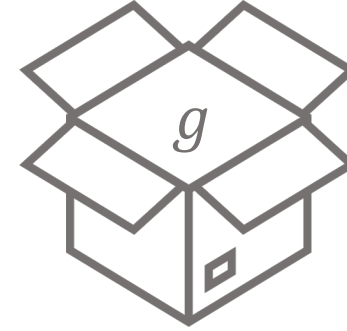
Optimal policy: Gittins index

Optimal Policy: Gittins Index

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



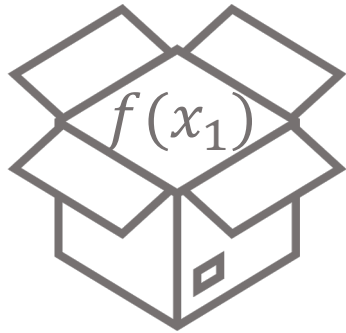
$GI_f(x; c(x))$



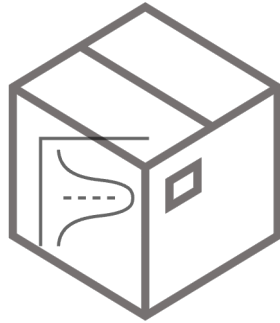
g

Optimal Policy: Gittins Index

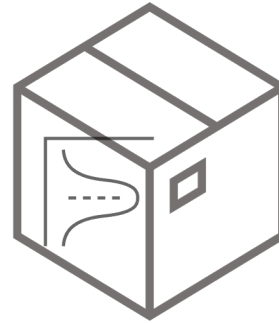
Step 2: **Open** the box with highest index if it is closed



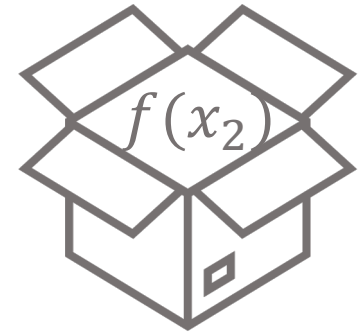
↓
 $f(x_1)$



↓
 $GI_f(x; c(x))$



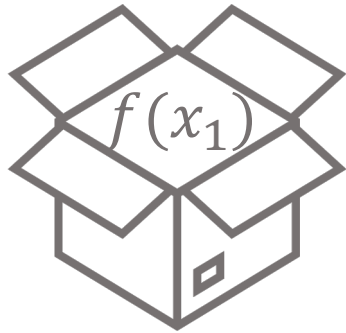
↓
 $GI_f(x'; c(x'))$



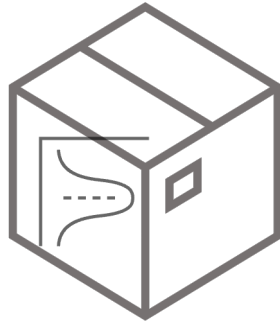
↓
 $f(x_2)$

Optimal Policy: Gittins Index

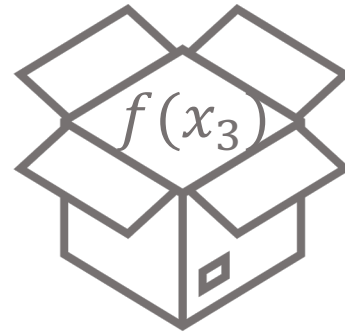
Step 2': **Select** the box with highest index if it is opened and **stop**



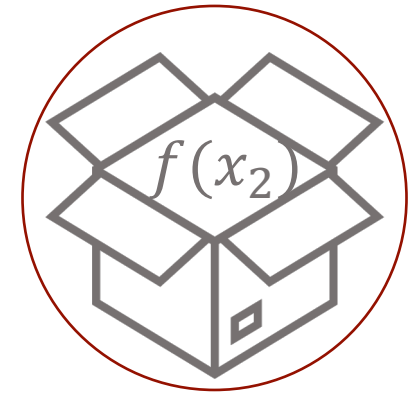
↓
 $f(x_1)$



↓
 $GI_f(x; c(x))$

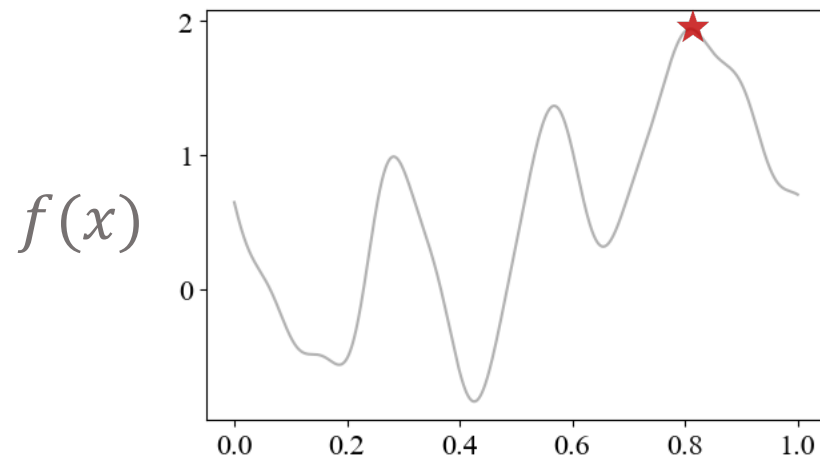


↓
 $f(x_3)$



↓
 $f(x_2)$

Bayesian Optimization



Continuous

Correlated

Fixed-iteration

Expected regret

Is Gittins index good?

Pandora's Box

[Weitzman'79]



Discrete

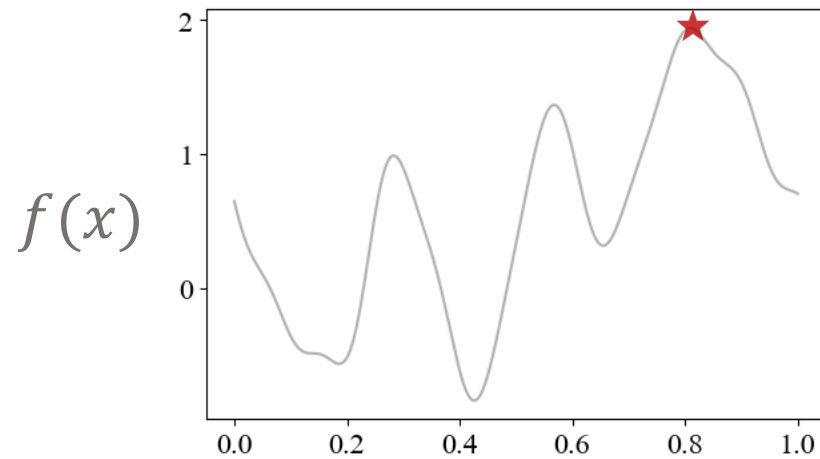
Independent

Flexible-stopping

Expected cost-adjusted regret

Gittins index is optimal

Bayesian Optimization



Continuous

Correlated

Fixed-iteration

Expected regret

Is Gittins index good?

empirically

Pandora's Box

[Weitzman'79]



Discrete

Independent

Flexible-stopping

Expected cost-adjusted regret

Gittins index is optimal

New Design Principle: Gittins Index

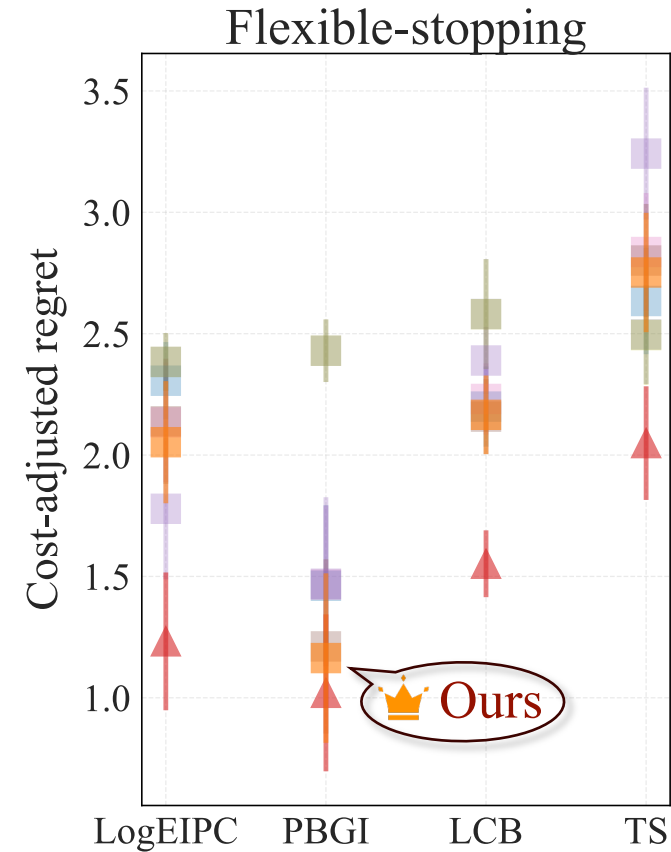
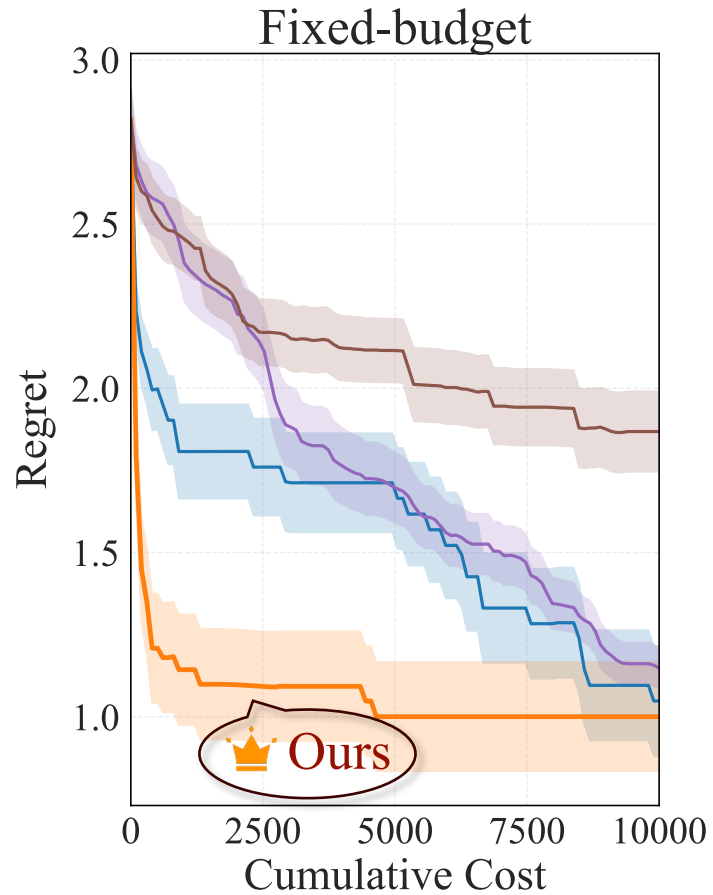
- Improvement-based (e.g., LogEIPC)
- Entropy-based
- Confidence bounds (UCB/LCB)
- Thompson sampling (TS)
- Gittins Index (PBGI)



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

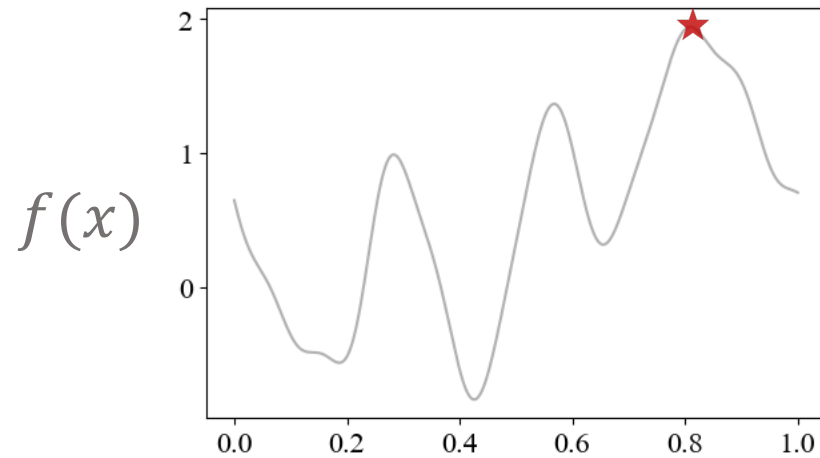


Lower the better



Bound on achievable performance

Bayesian Optimization



Continuous

Correlated

Fixed-iteration

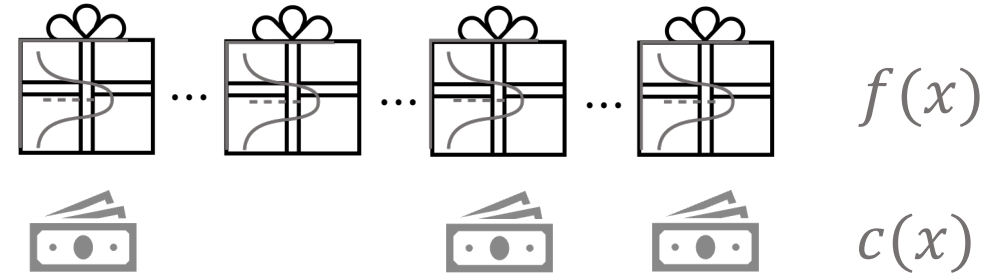
Expected regret

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theoretically

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[Weitzman'79]



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
- Thompson sampling
- **Gittins Index**



Why another principle?

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

Theoretical Guarantee and Empirical Validation

Theorem (No worse than stopping-immediately)

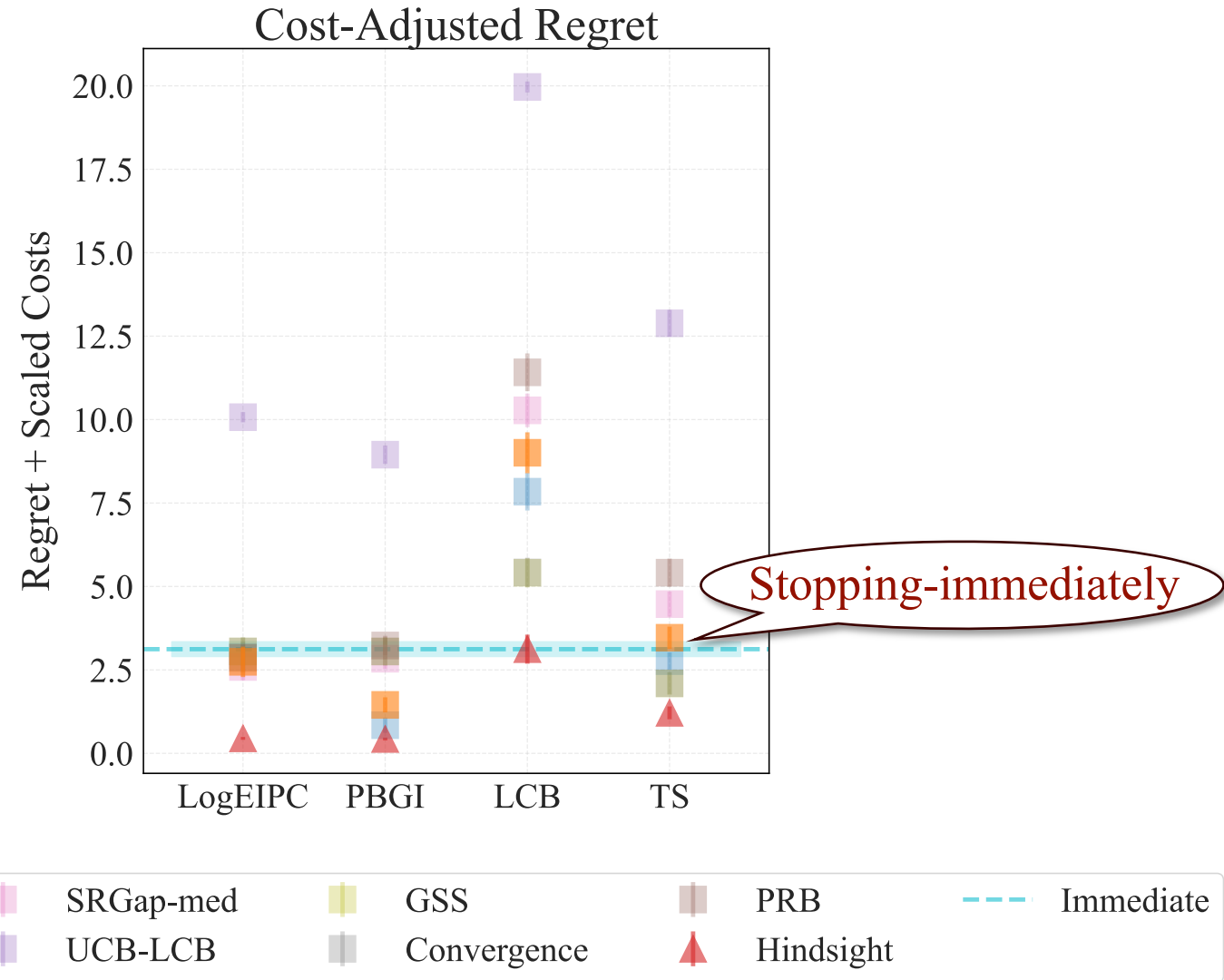
$$\mathbb{E}[R(\text{ours}; \text{PBGI})] \leq R[\text{stopping immediately}]$$

or LogEIPC

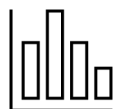
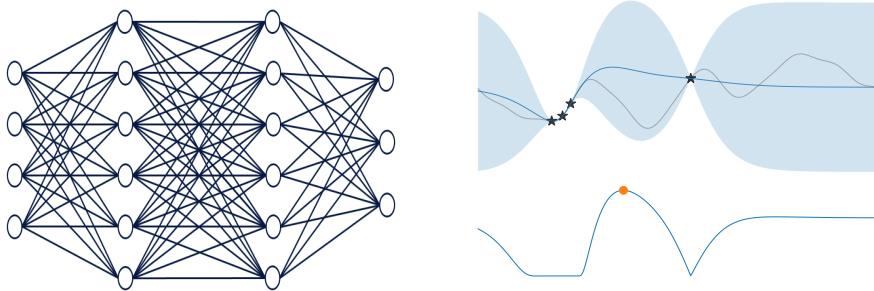
cost-adjusted regret

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

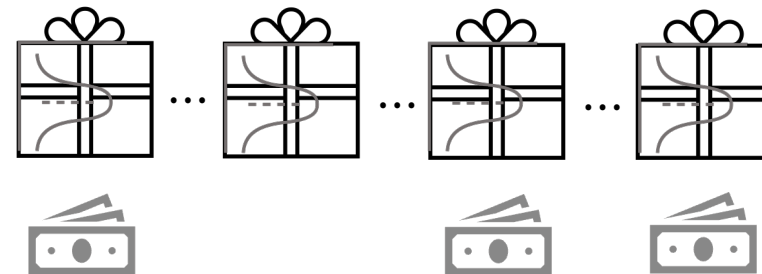


Varying evaluation costs



Adaptive stopping time

Key idea



Link to Pandora's Box problem
& Gittins index theory

Impact

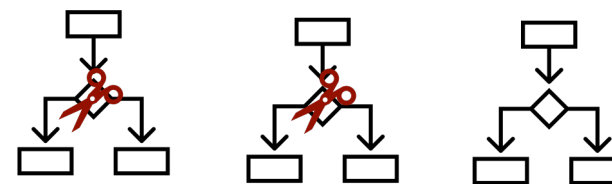


Competitive empirical performance &
interests from practitioners



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

Ongoing work

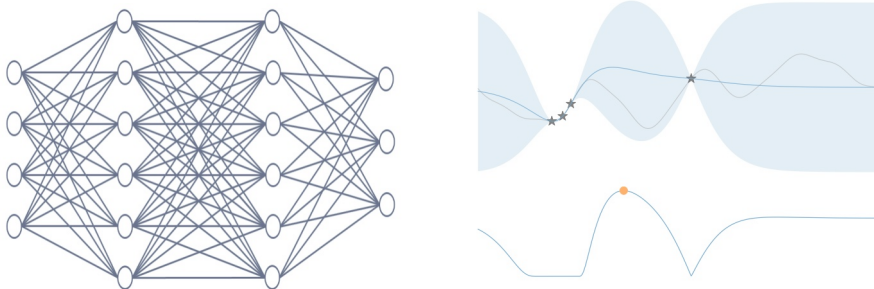


Sharper theoretical guarantees & black-
box optimization w/ multi-stage feedback



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

Studied problem

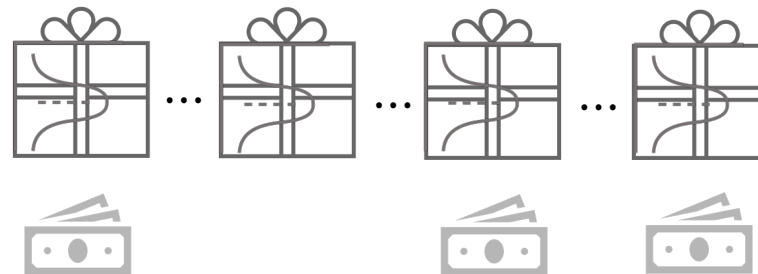


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Competitive empirical performance &
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Ongoing work



ChatGPT



Gemini



deepseek



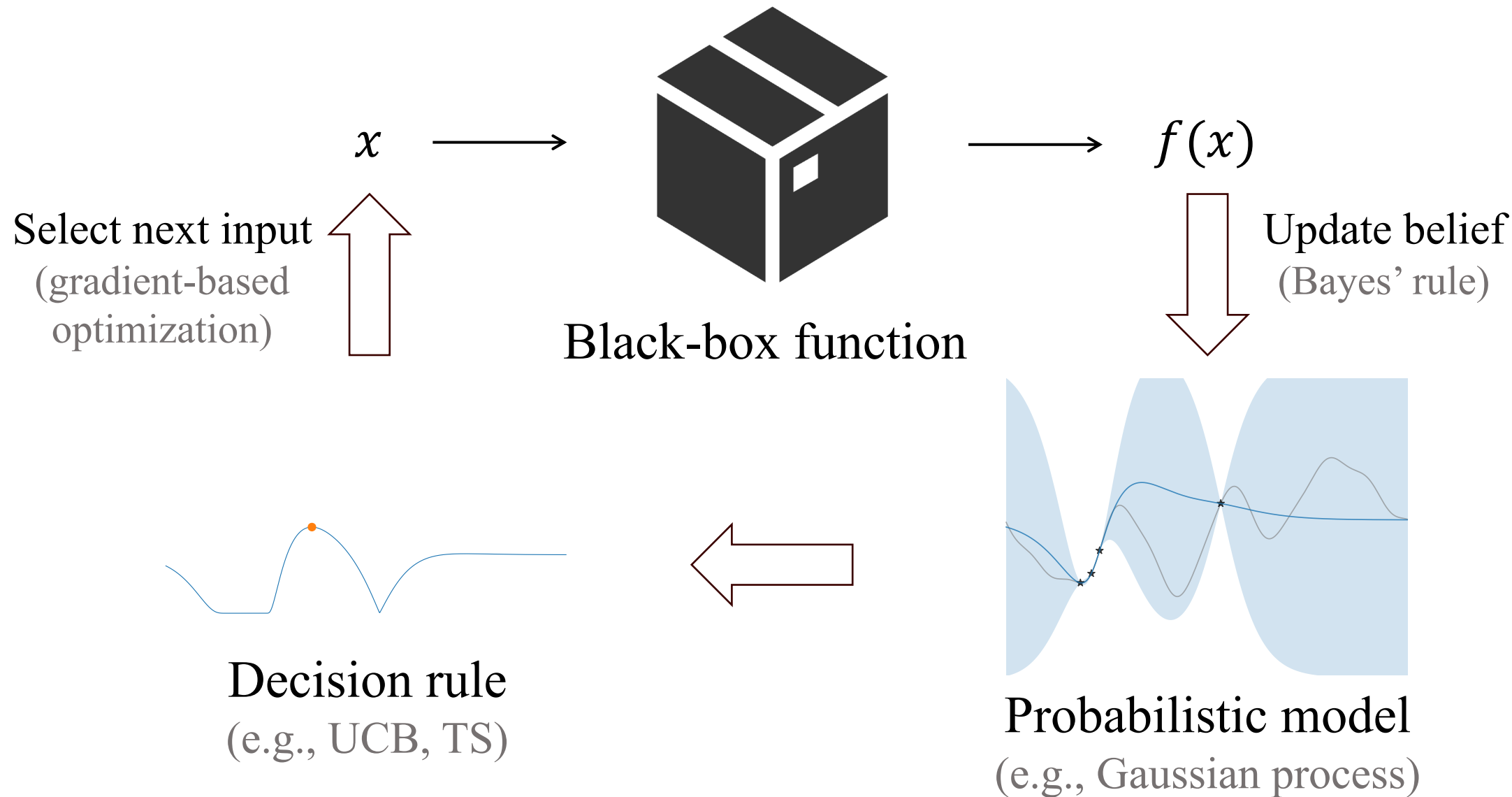
Claude

LLM-driven black-box optimization

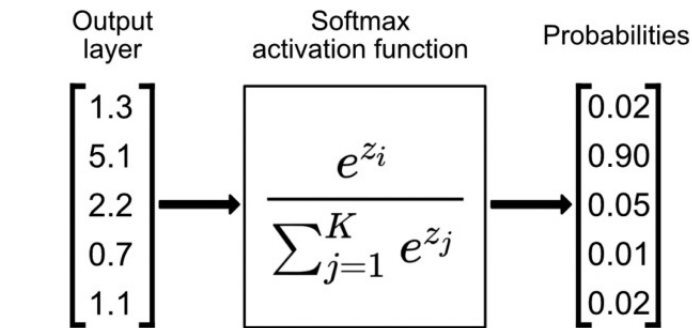
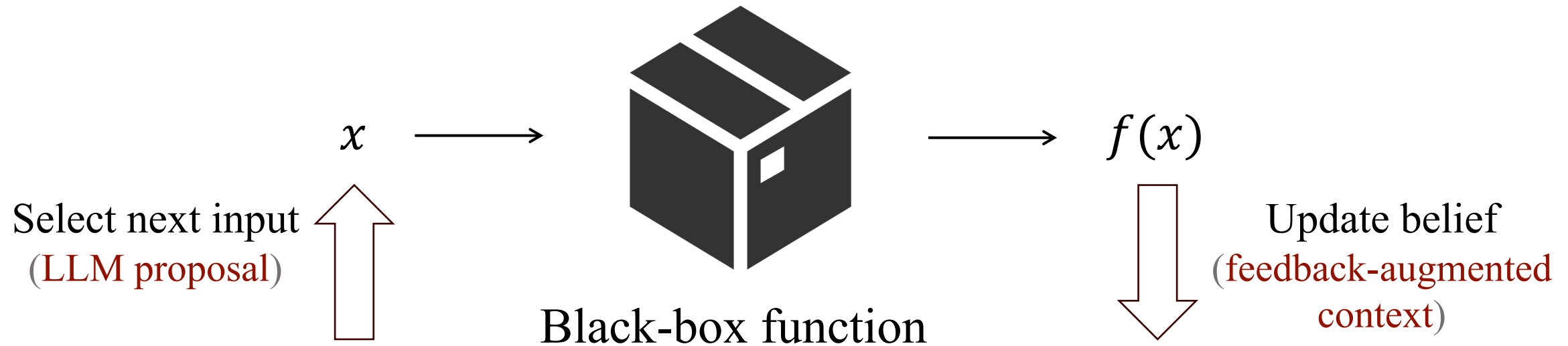


"Cost-aware Stopping for Bayesian
Optimization." Under review.

Recap: Bayesian Optimization



Ongoing: LLM-Driven Black-Box Optimization



Decision rule
(e.g., **Softmax sampling**)



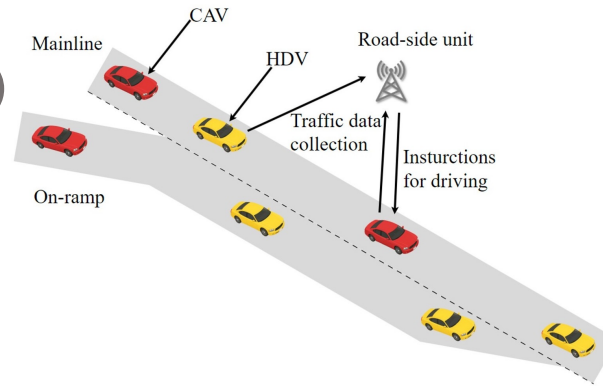
Probabilistic model
(**large language model**)

Ongoing: LLM-Driven RL Training Optimization

Mixed-autonomy traffic control:

(e.g., Transformer config)

x

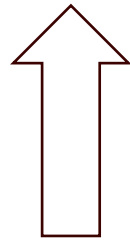


(e.g., average speed)



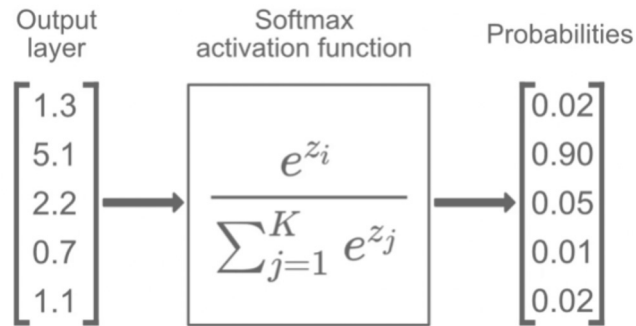
$f(x)$

Select next input
(LLM proposal)

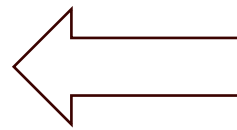


Black-box function
(RL training & evaluation)

Update belief
(feedback-augmented context)



Decision rule
(e.g., Softmax sampling)



Probabilistic model
(large language model)