

NeurIPS'24 & INFORMS Data
Mining Paper Competition Finalist

Cost-Aware Bayesian Optimization with Adaptive Stopping via Gittins Indices

Qian Xie 谢倩 (Cornell ORIE)

Joint work with Linda Cai (UC Berkeley), Raul Astudillo (MBZUAI), Theodore Brown (UCL), Peter Frazier, Alexander Terenin, Ziv Scully (Cornell), Yu Yu and Li Jin (SJTU)

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 →



non-analytical &
no gradient info

→ Performance metric $f(x)$

ML model training:

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



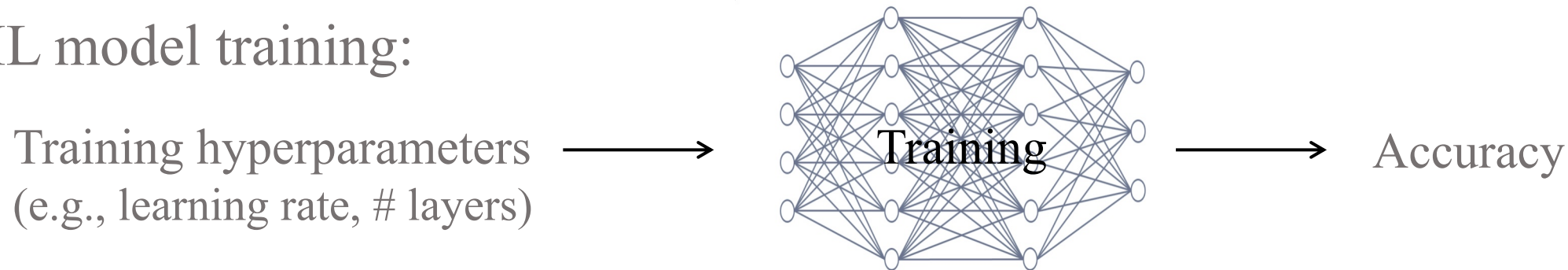
→ Accuracy

Optimization Under Uncertainty

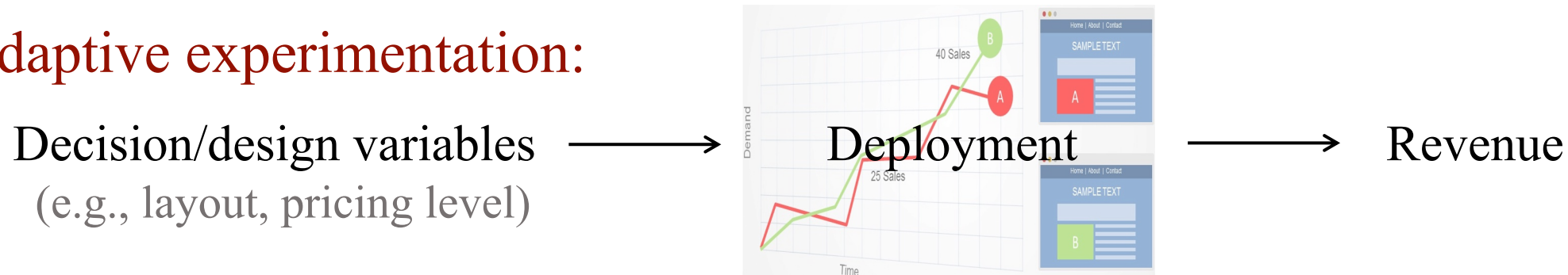
Black-box optimization:



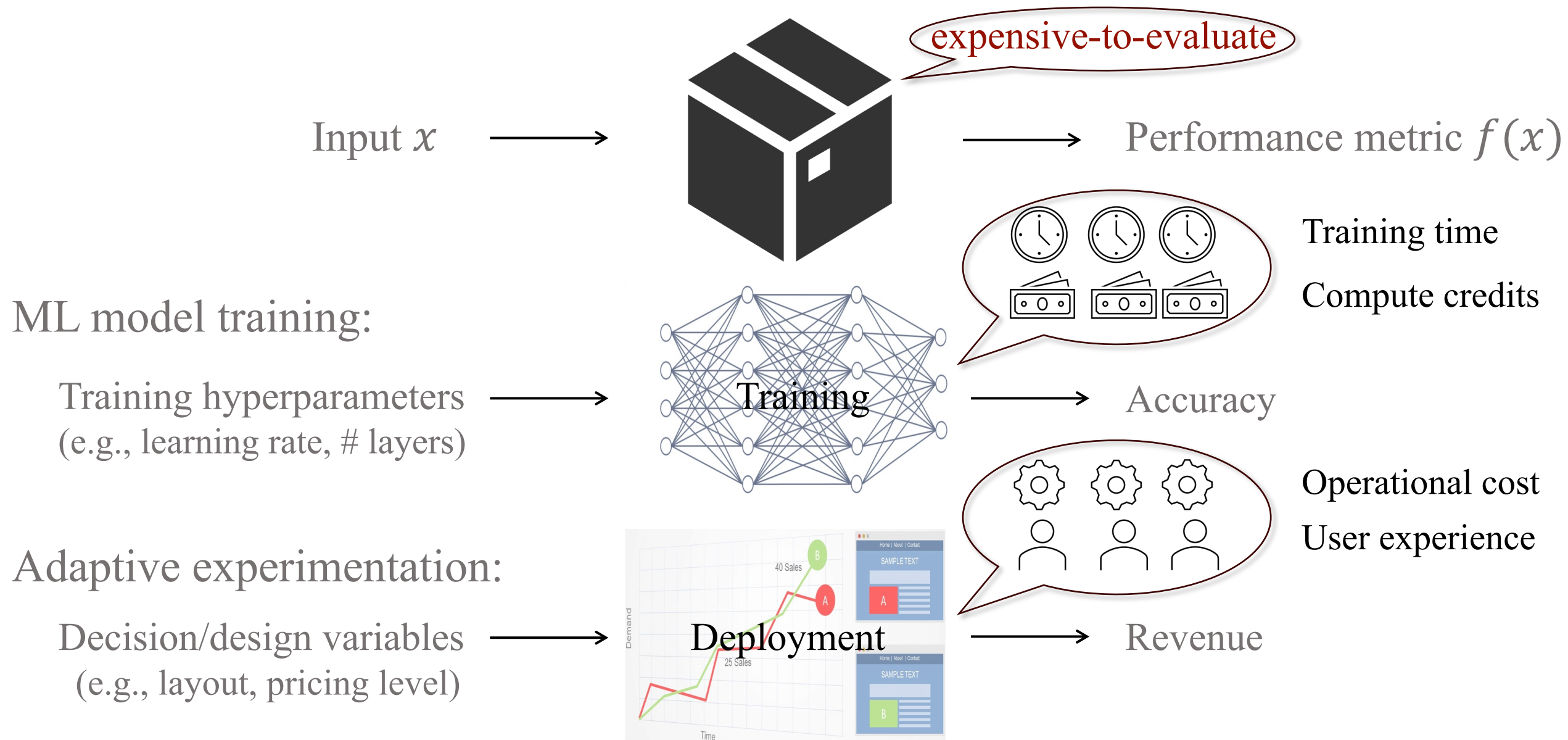
ML model training:



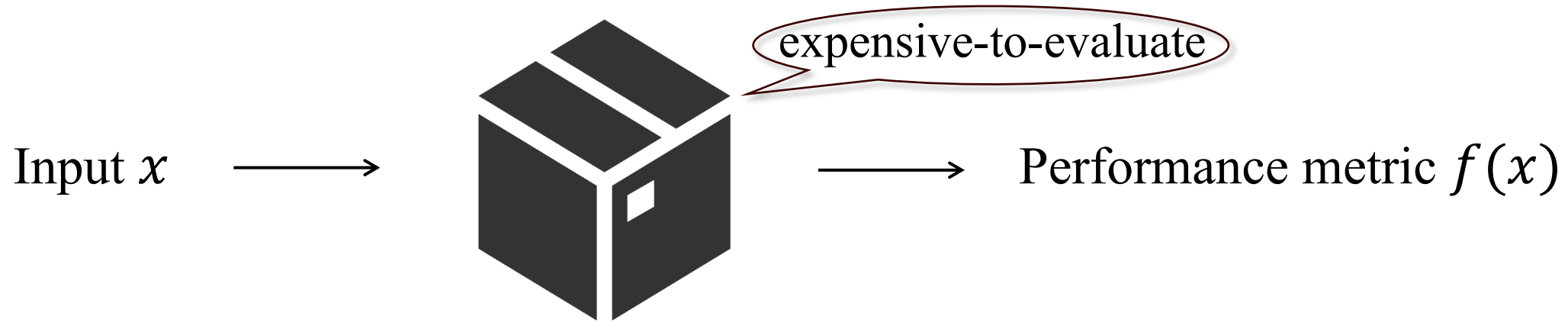
Adaptive experimentation:



Black-Box Optimization



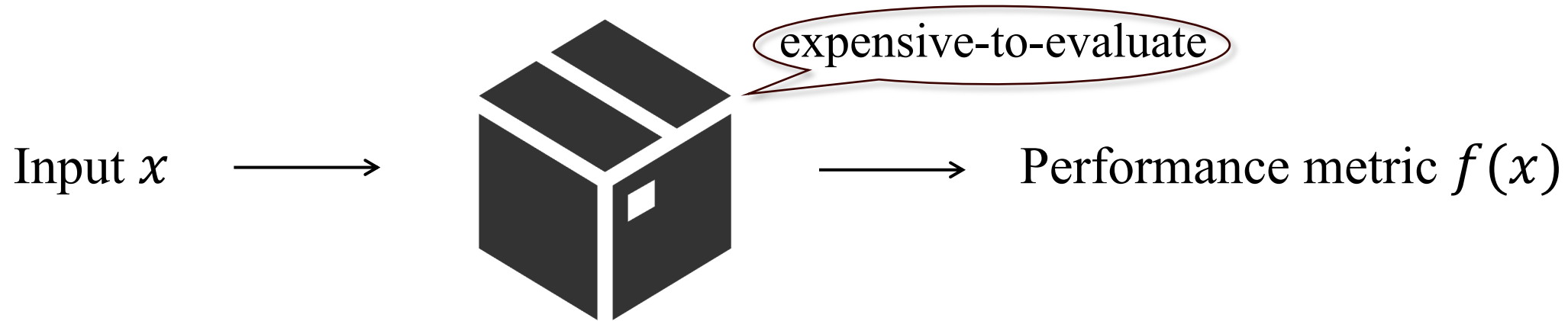
Black-Box Optimization



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

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

Data-Driven Black-Box Optimization



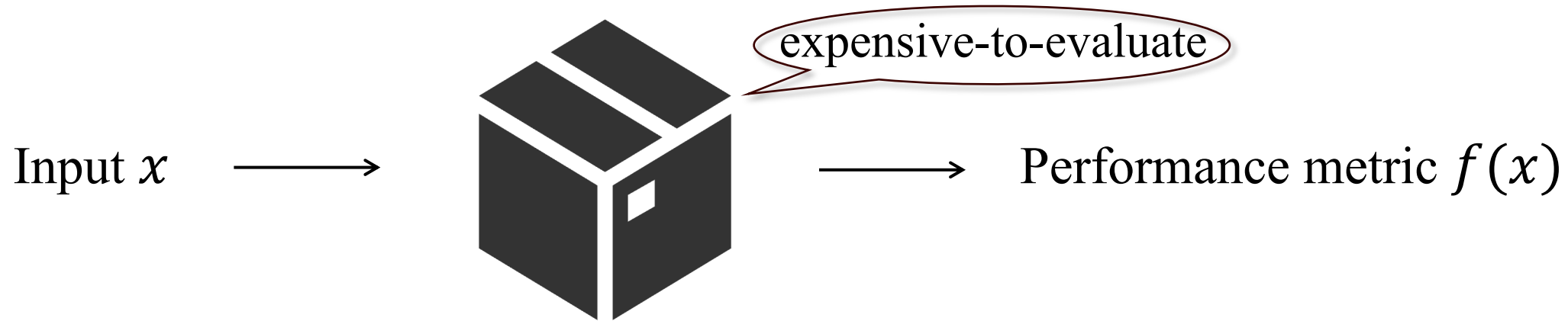
adaptively

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

Data-Driven Black-Box Optimization



adaptively

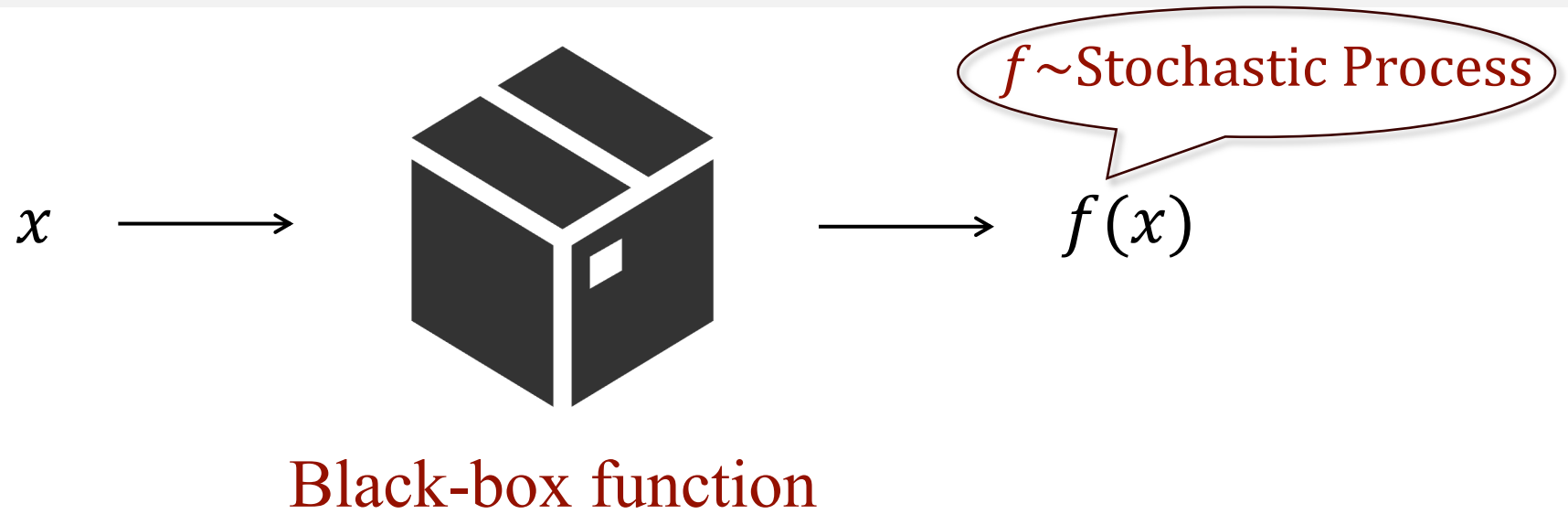
High-level goal: Choose x_1, \dots, x_T to maximize the expected best observed value

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Fewer #evaluations

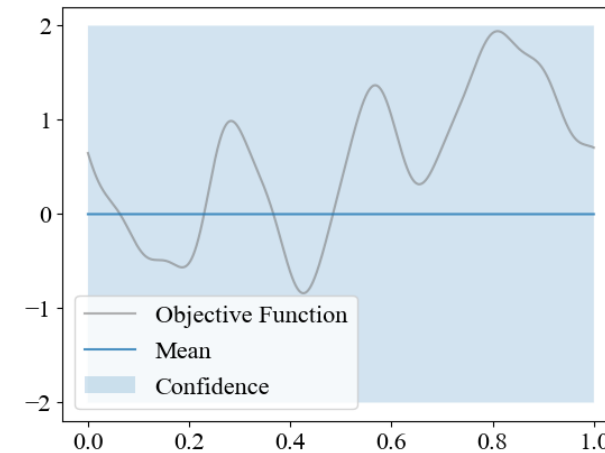
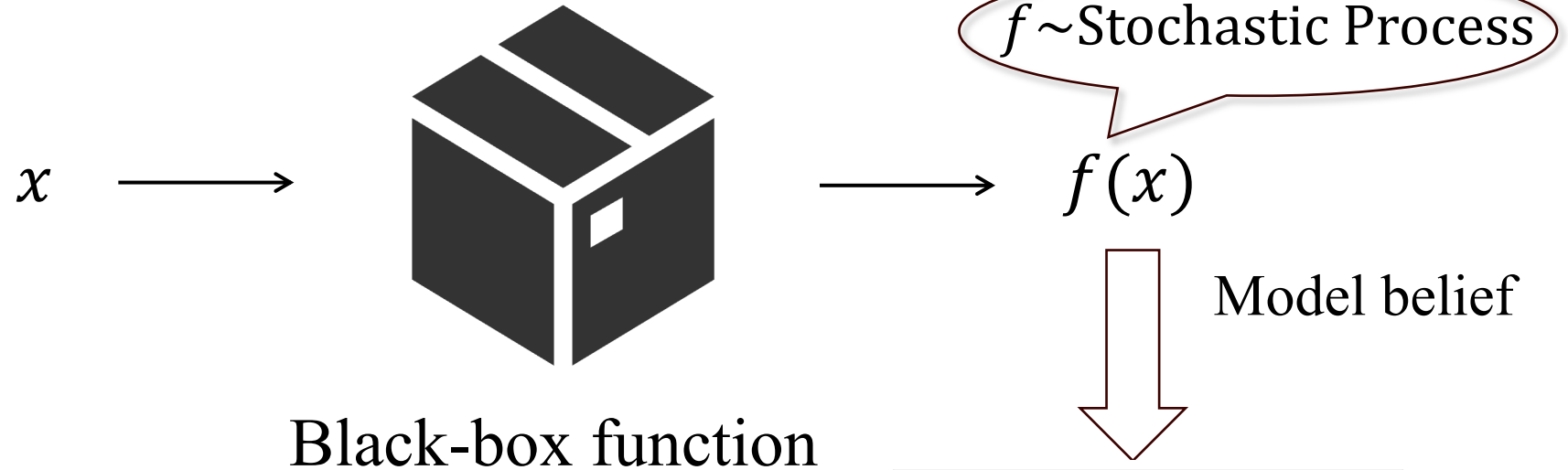
Efficient framework: Bayesian optimization

Bayesian Optimization



Bayesian Optimization

Time 0



Probabilistic model
(e.g., Gaussian process)

Bayesian Optimization

Time t

x_1, \dots, x_t



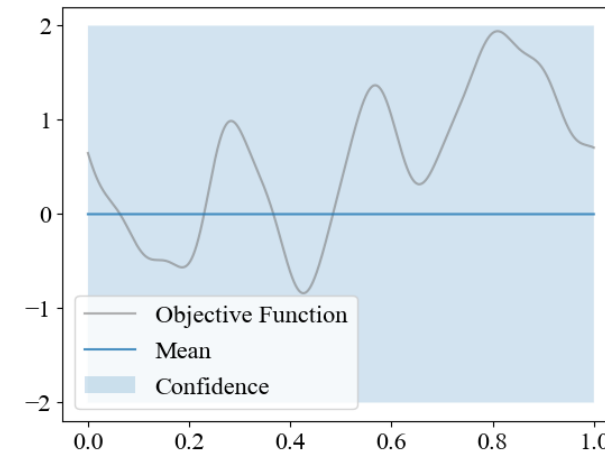
Black-box function



$f \sim \text{Stochastic Process}$

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

Model belief

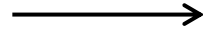


Probabilistic model
(e.g., Gaussian process)

Bayesian Optimization

Time t

x_1, \dots, x_t



Black-box function

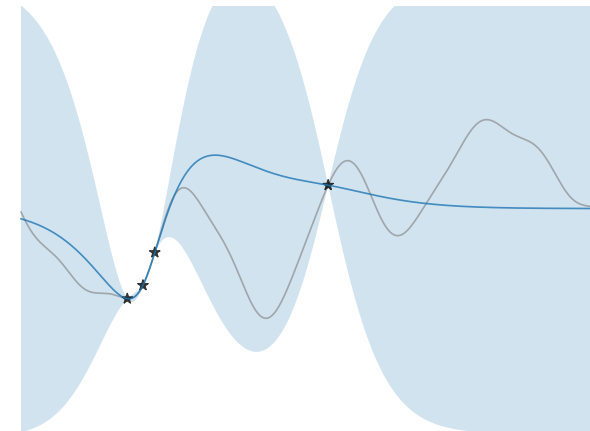


$f \sim \text{Stochastic Process}$

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



Update belief
(Bayes' rule)

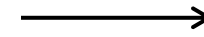


Probabilistic model
(e.g., Gaussian process)

Bayesian Optimization

Time t

x_1, \dots, x_t

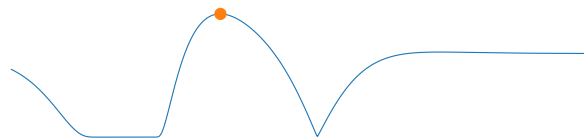


$f(x_1), \dots, f(x_t)$

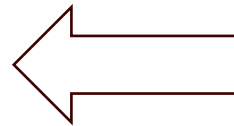


Update belief
(Bayes' rule)

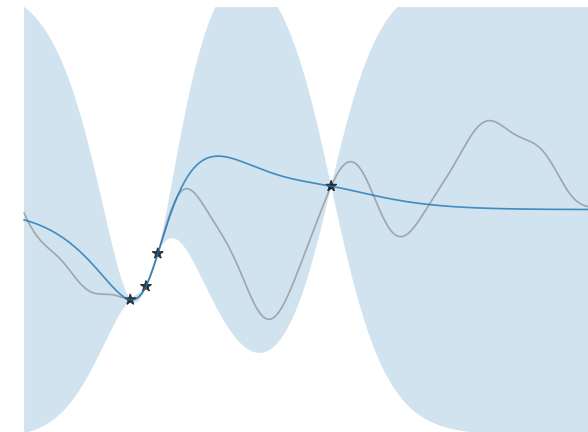
Black-box function



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



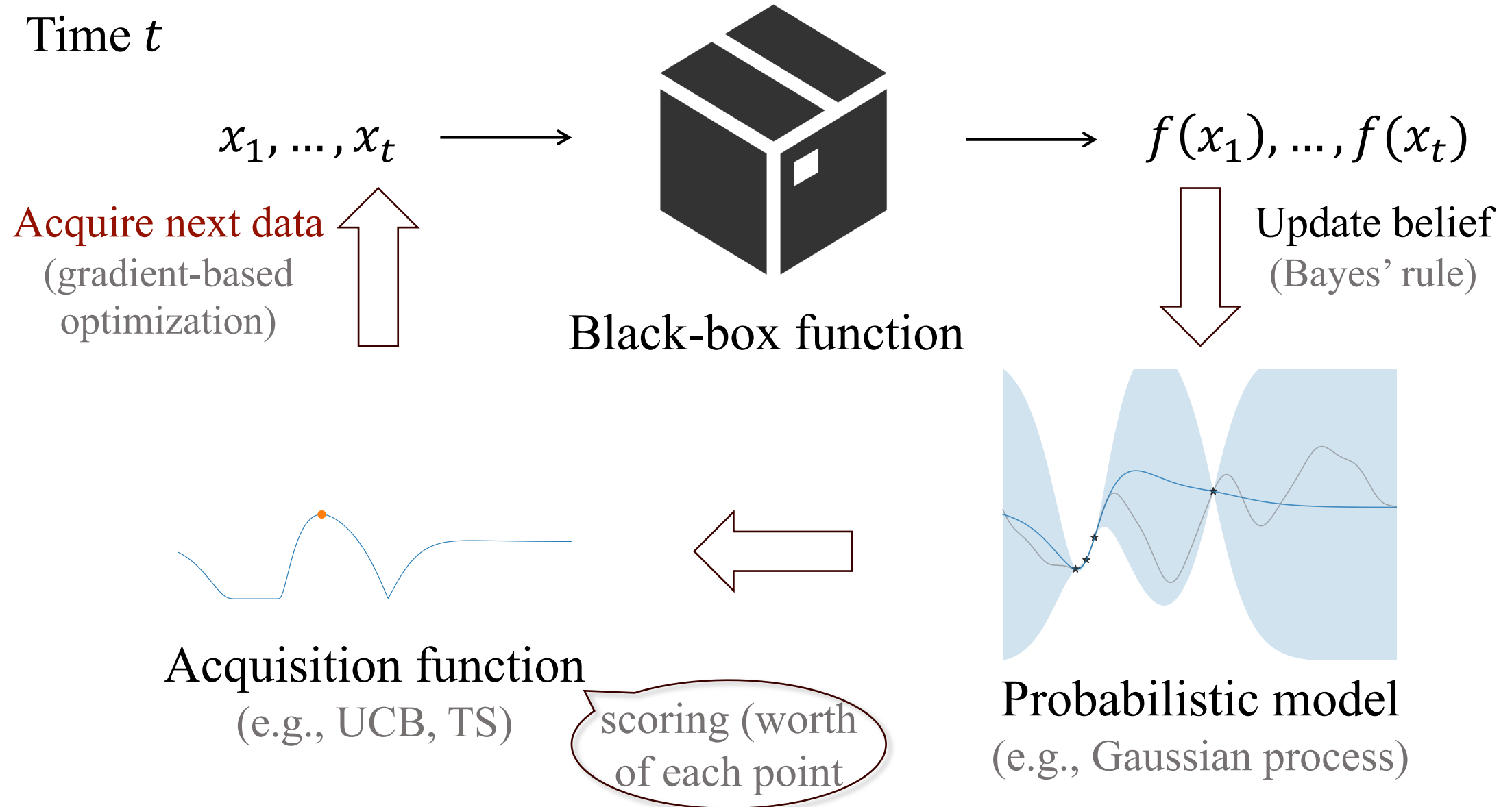
scoring (worth
of each point)



Probabilistic model
(e.g., Gaussian process)

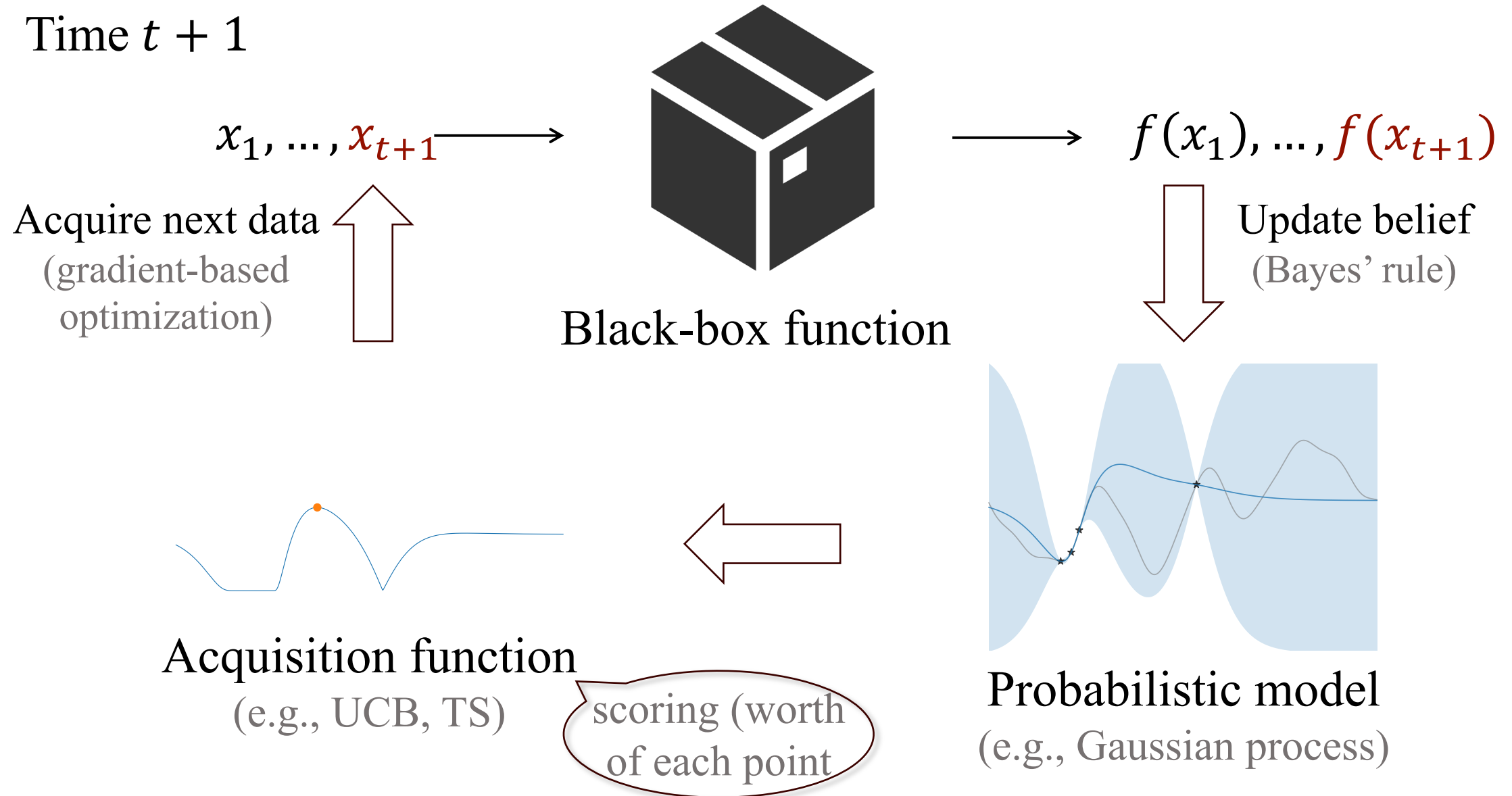
Bayesian Optimization

Time t

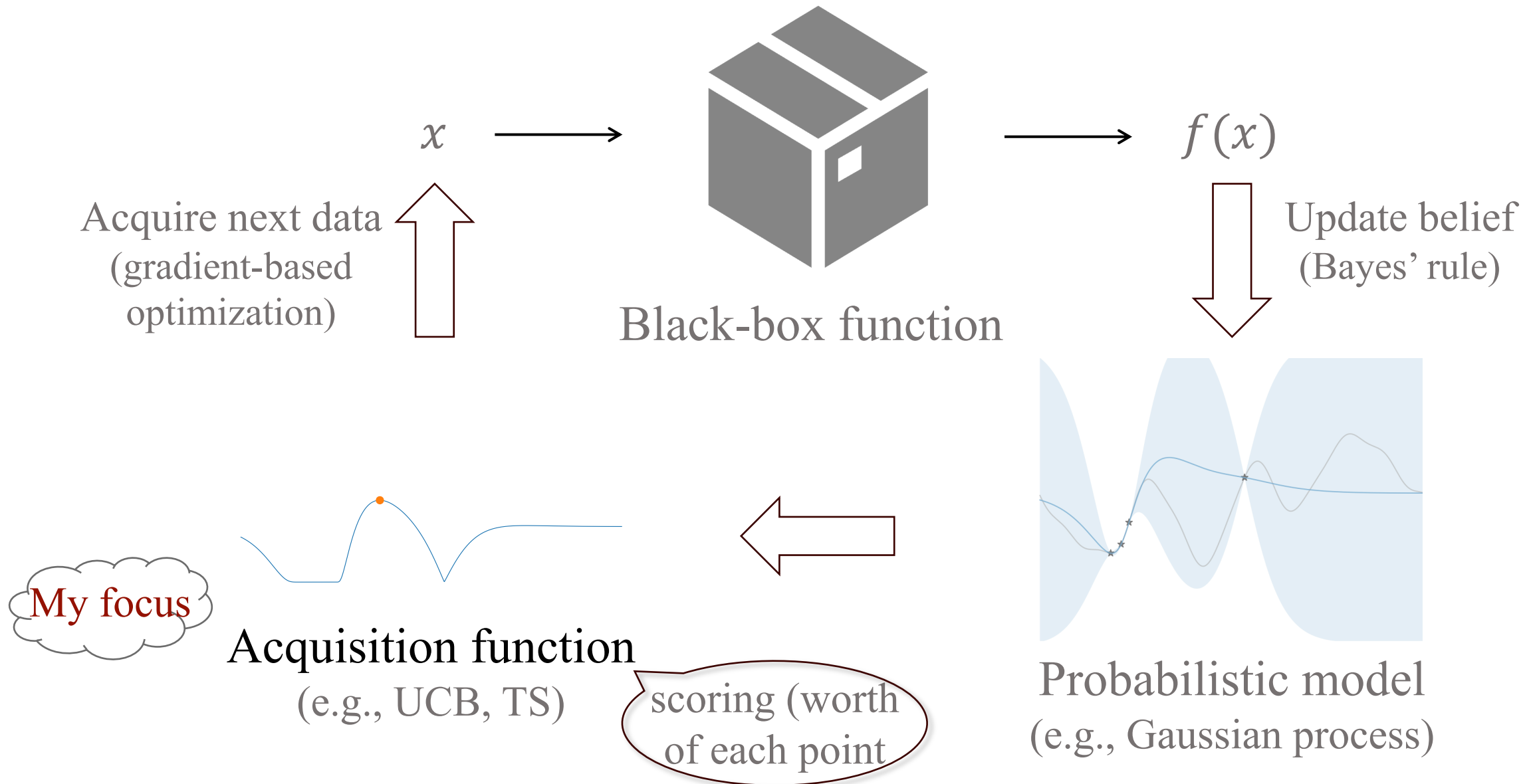


Bayesian Optimization

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 (TS)
- Gittins Index

New Design Principle: Gittins Index

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- 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

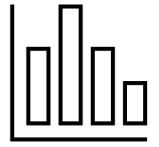
Our Contribution: Gittins Index Principle

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- Gittins Index

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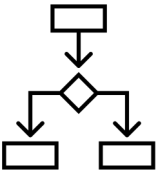
Under-explored Practical Considerations



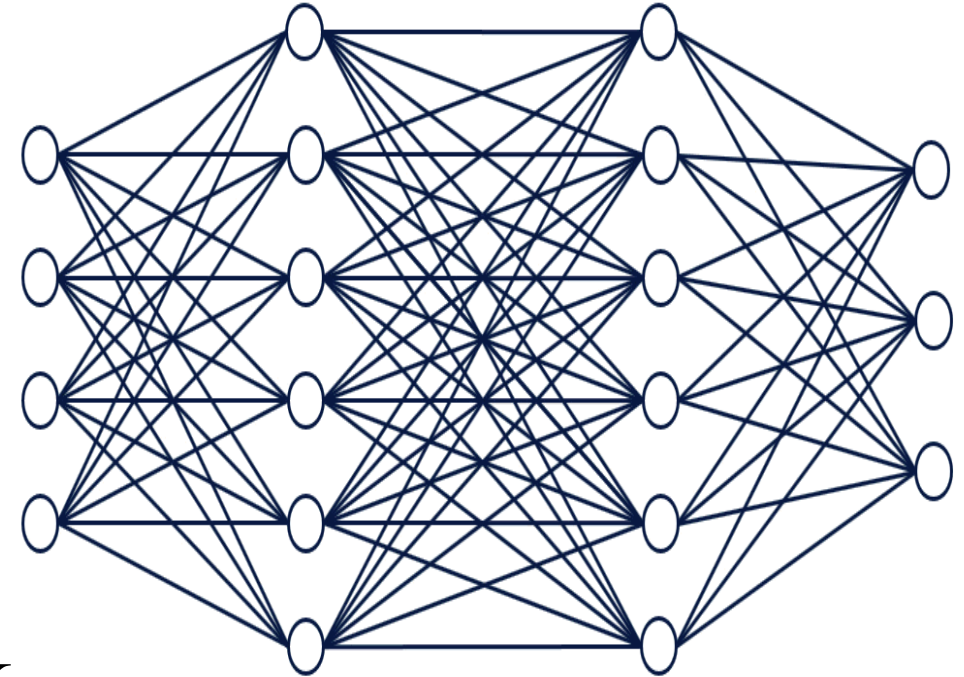
Varying evaluation costs



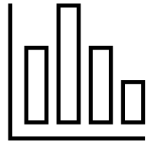
Smart stopping time



Observable multi-stage feedback



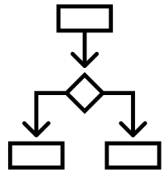
Under-explored Practical Considerations



Varying evaluation costs



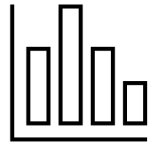
Smart stopping time



Observable multi-stage feedback

New design principle:
Gittins index

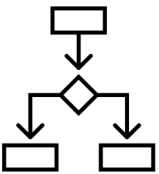
Why Gittins index?



Varying evaluation costs



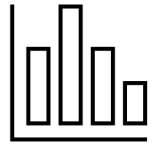
Smart stopping time



Observable multi-stage feedback

New design principle:
Gittins index

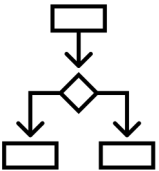
Why Gittins index?



Varying evaluation costs



Smart stopping time

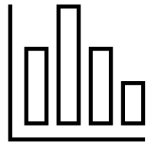


Observable multi-stage feedback

New design principle:
Gittins index

Optimal in related sequential
decision problems

Why Gittins index?



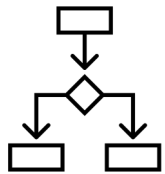
Varying evaluation costs

Features in Pandora's box



Smart stopping time

Features in Pandora's box

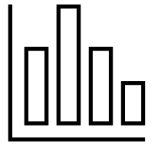


Observable multi-stage feedback

New design principle:
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Why Gittins index?



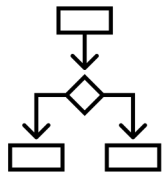
Varying evaluation costs

Features in Pandora's box



Smart stopping time

Features in Pandora's box



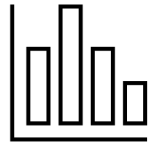
Observable multi-stage feedback

Features in **Markovian bandits**

New design principle:
Gittins index

Optimal in related sequential
decision problems

What is Pandora's Box?



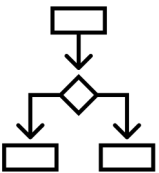
Varying evaluation costs

Features in Pandora's box



Smart stopping time

Features in Pandora's box

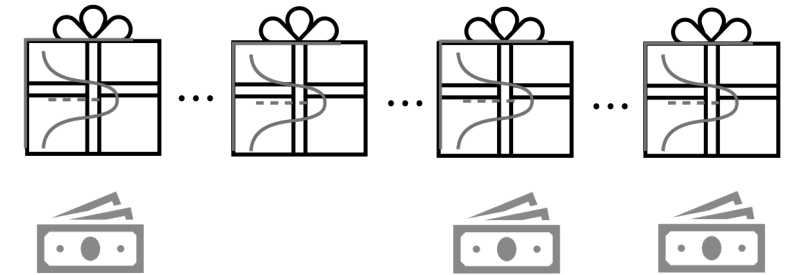


Observable multi-stage feedback

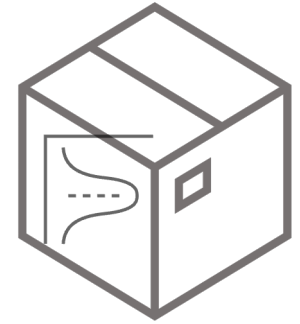
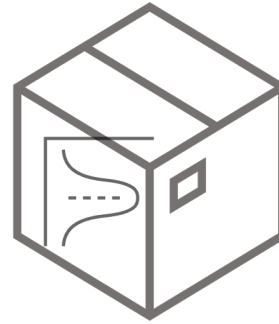
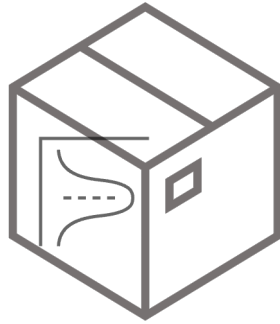
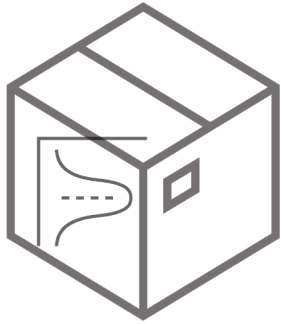
Features in Markovian bandits

New design principle:
Gittins index

Optimal in related sequential
decision problems



Pandora's Box



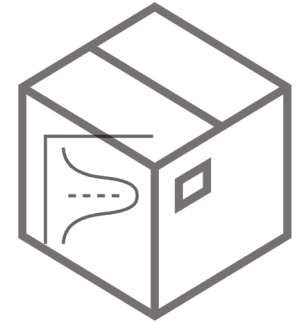
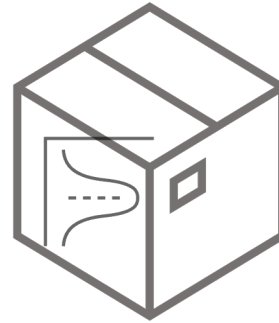
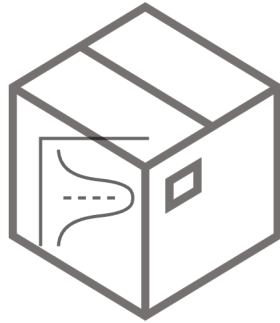
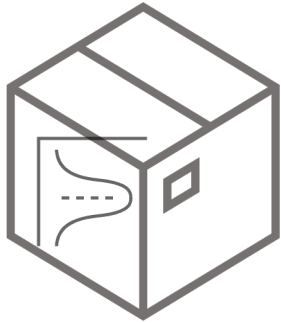
High-level goal: Choose x_1, \dots, x_T to maximize the expected utility

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

Flexible stopping time

Pandora's Box

$t = 0$

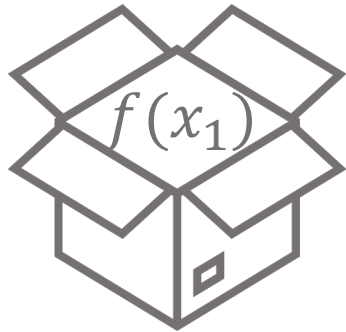


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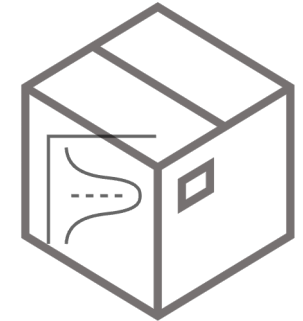
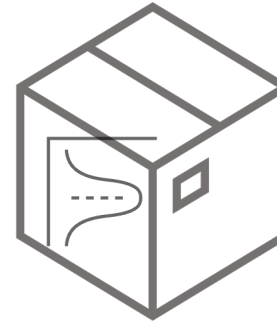
$$\mathbb{E} \max_{t=1,2,\dots,T} f(x_t) - \mathbb{E} \sum_{t=1}^T c(x_t)$$

Pandora's Box

$t = 1$



$c(x_1)$

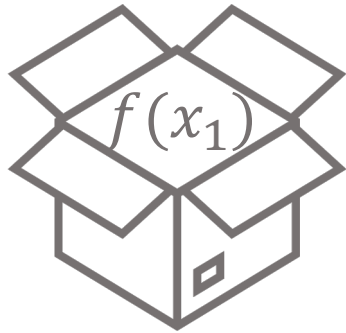


High-level goal: Choose x_1, \dots, x_T to maximize the expected utility

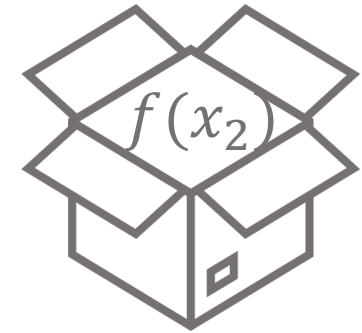
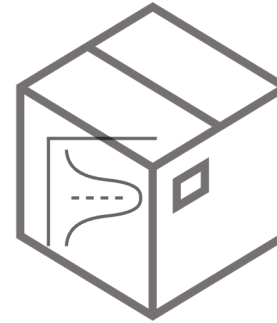
$$\mathbb{E} \max_{t=1,2,\dots,T} f(x_t) - \mathbb{E} \sum_{t=1}^T c(x_t)$$

Pandora's Box

$t = 2$



$c(x_1)$



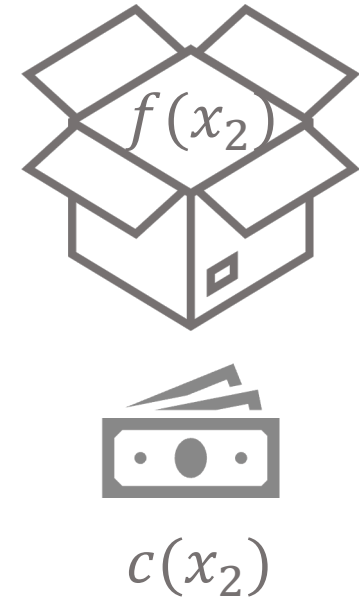
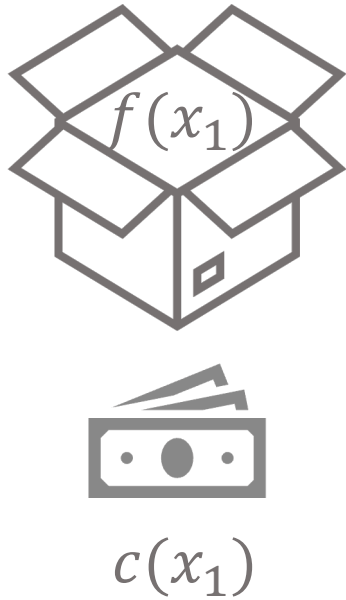
$c(x_2)$

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

$t = 3$

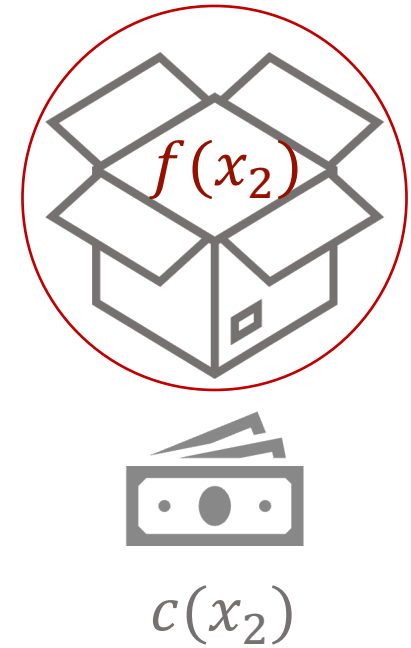
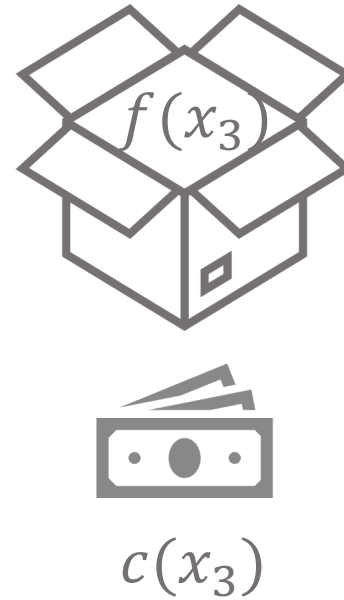
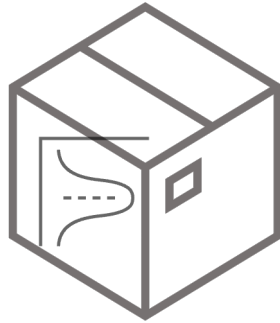
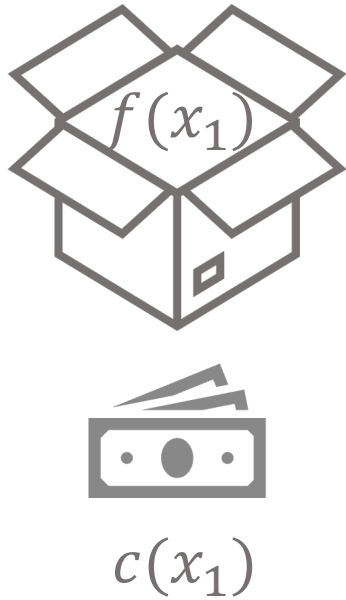


High-level goal: Choose x_1, \dots, x_T to maximize the expected utility

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

Pandora's Box

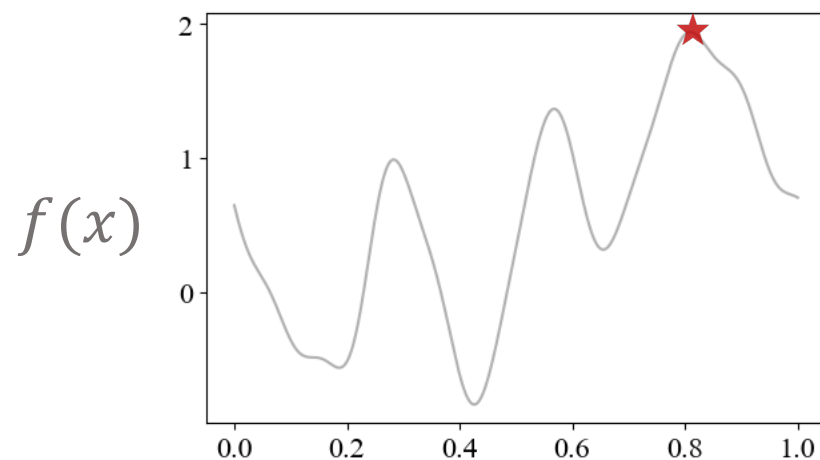
$t = T$, stop



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

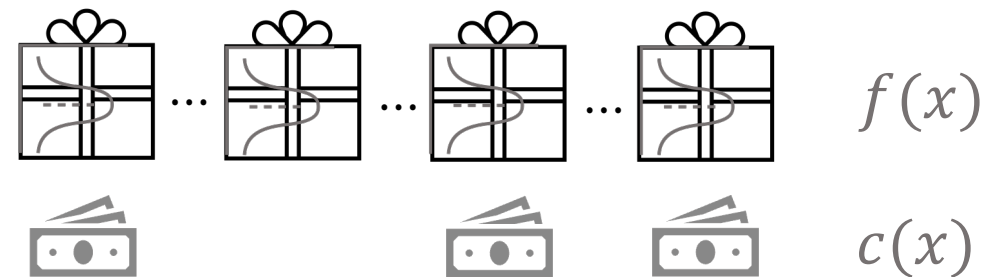
Fixed-iteration

Expected best-observed value

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

Pandora's Box

[Weitzman'79]



Discrete

Independent

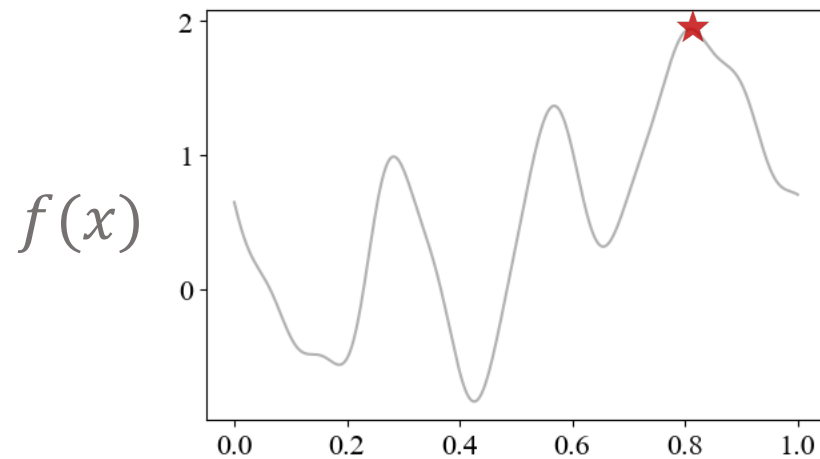
Flexible-stopping

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 best-observed value

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

Pandora's Box

[Weitzman'79]



Discrete

Independent

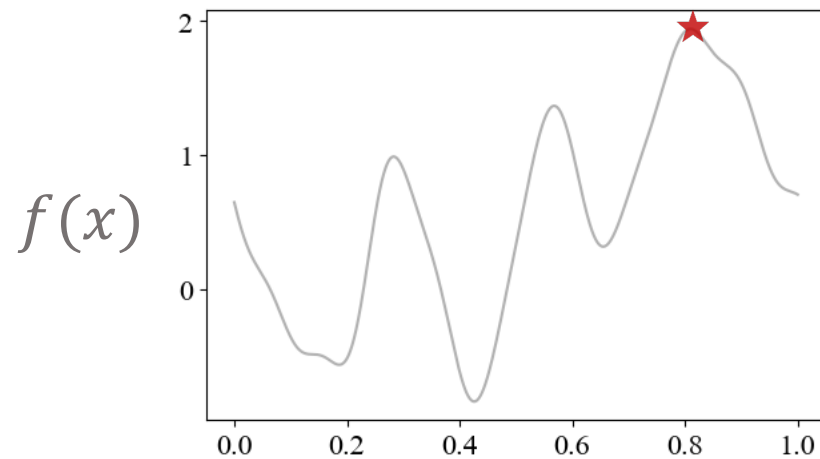
Flexible-stopping

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

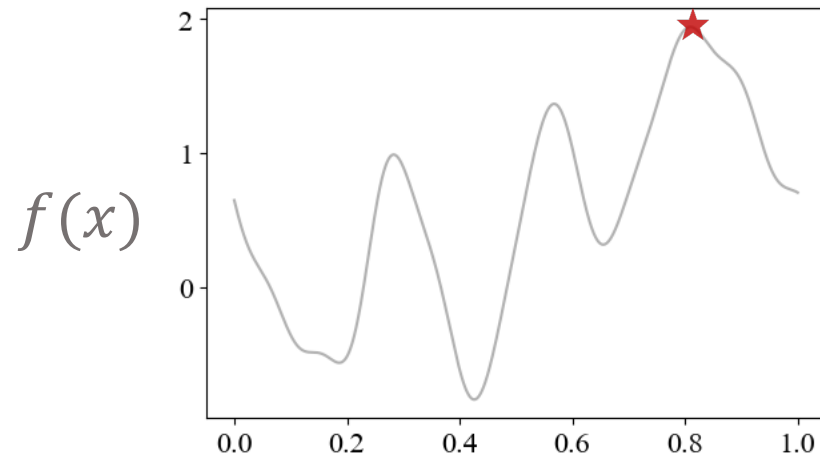
Flexible-stopping

Expected 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

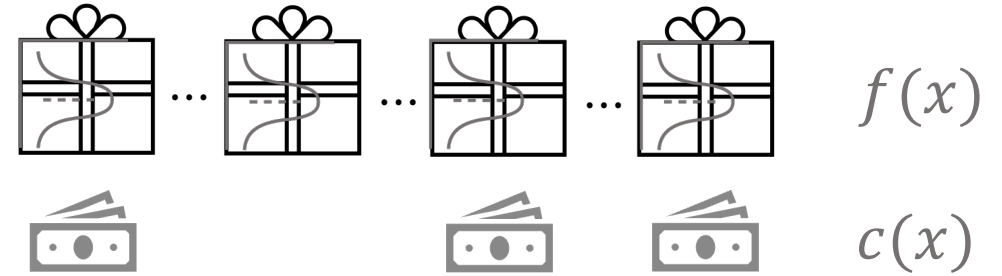
Fixed-iteration

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

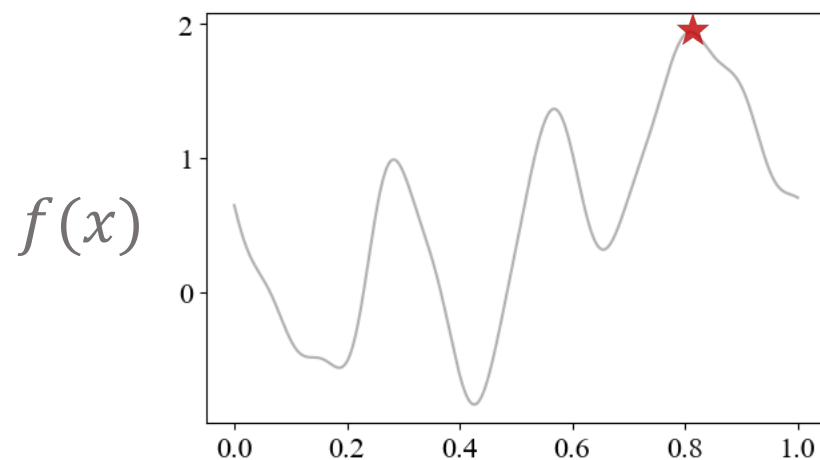
Independent

Flexible-stopping

Expected cost-adjusted regret

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

Bayesian Optimization



Continuous

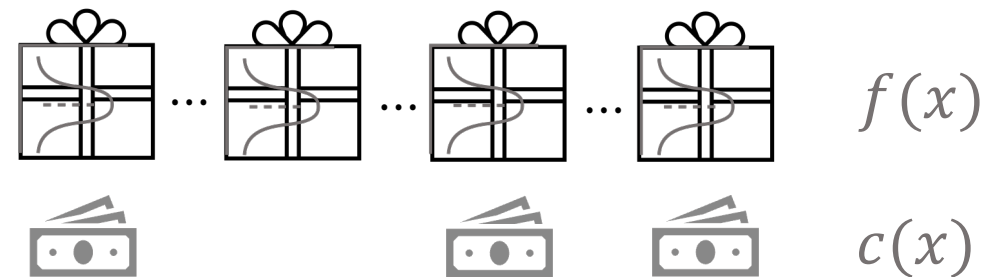
Correlated

Fixed-budget / Flexible-stopping

Expected (cost-adjusted) regret

Pandora's Box

[Weitzman'79]



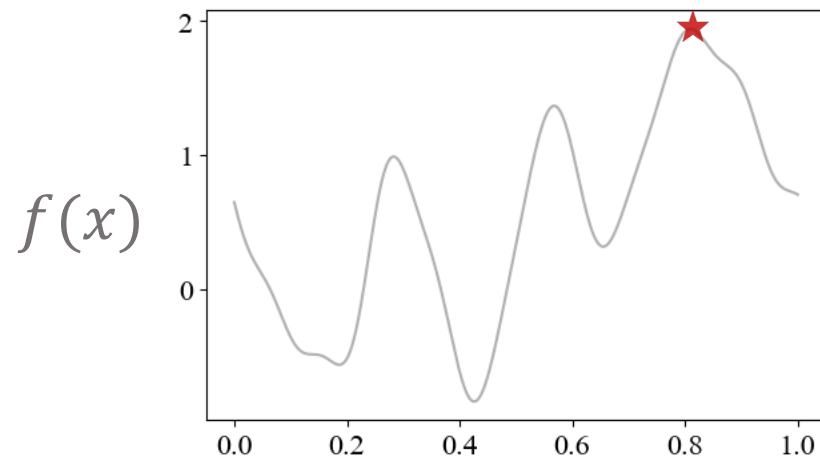
Discrete

Independent

Flexible-stopping

Expected cost-adjusted regret

Bayesian Optimization



Continuous

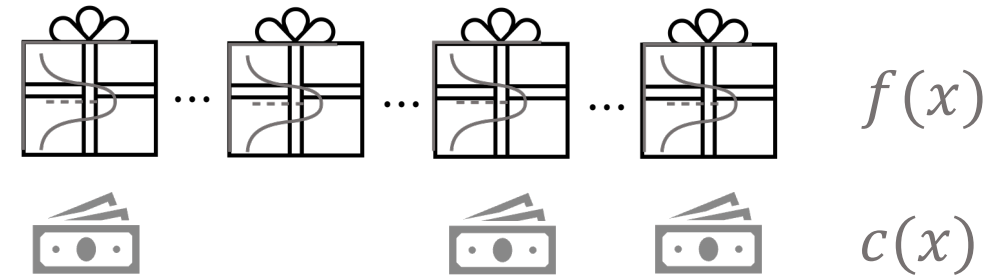
Correlated

Fixed-budget / Flexible-stopping

Expected (cost-adjusted) regret

Pandora's Box

[Weitzman'79]



Discrete

Independent

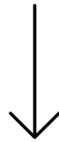
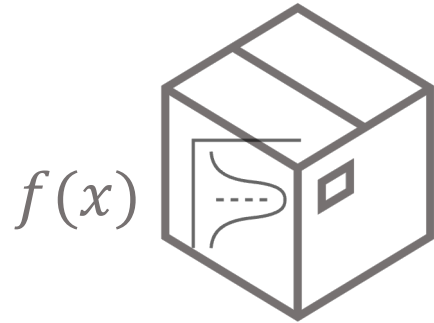
Flexible-stopping

Expected cost-adjusted regret

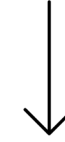
Optimal policy: Gittins index

Optimal Policy: Gittins Index

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



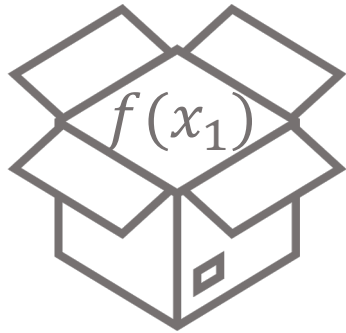
$$GI_f(x; c(x))$$



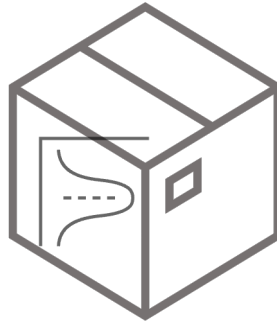
$$g$$

Optimal Policy: Gittins Index

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



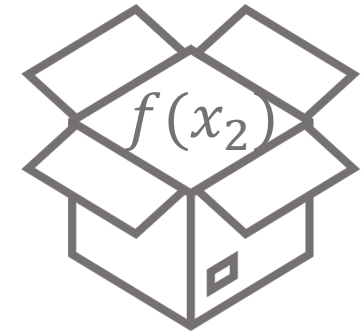
↓
 $f(x_1)$



↓
 $GI_f(x; c(x))$



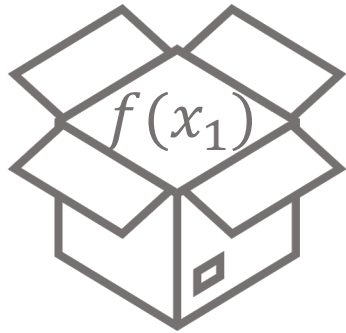
↓
 $GI_f(x'; c(x'))$



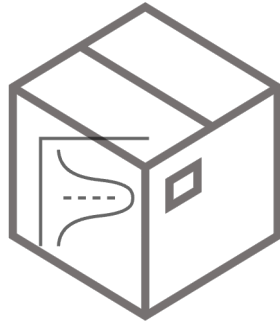
↓
 $f(x_2)$

Optimal Policy: Gittins Index

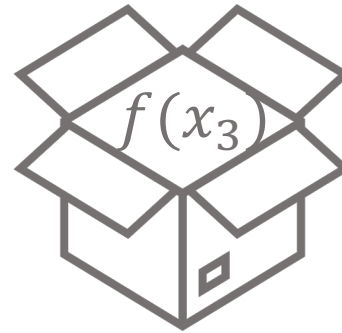
Step 2': **Select** the box with highest index if it is opened and **stop**



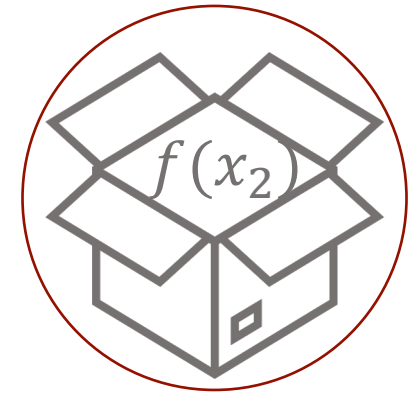
↓
 $f(x_1)$



↓
 $GI_f(x; c(x))$

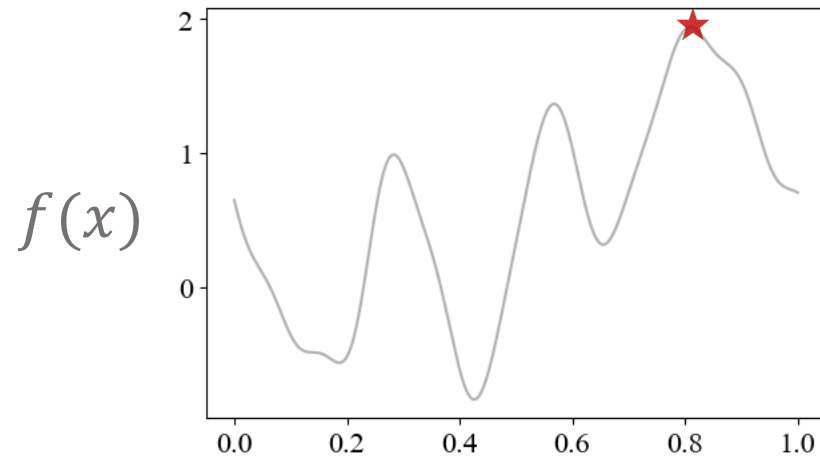


↓
 $f(x_3)$



↓
 $f(x_2)$

Bayesian Optimization



Continuous

Correlated

Fixed-budget / Flexible-stopping

Expected (cost-adjusted) regret

Is Gittins index good?

Pandora's Box

[Weitzman'79]



Discrete

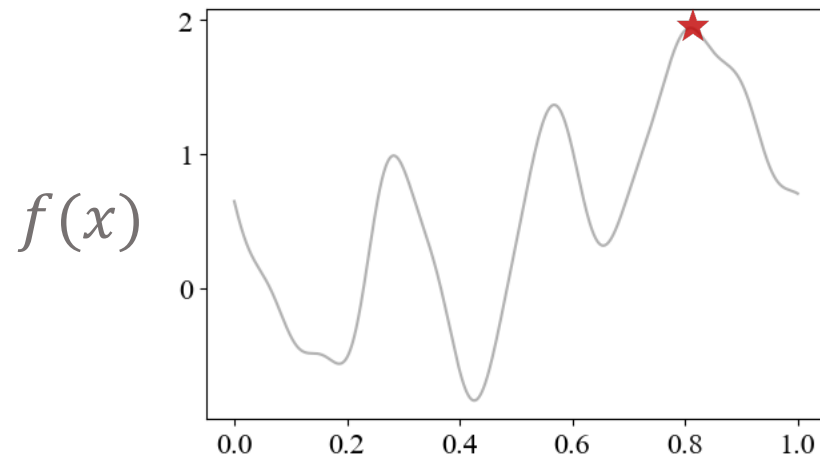
Independent

Flexible-stopping

Expected cost-adjusted regret

Gittins index is optimal

Bayesian Optimization



Continuous

Correlated

Fixed-budget / Flexible-stopping

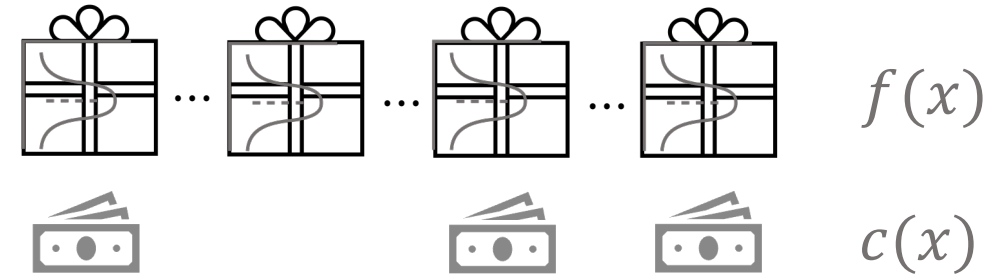
Expected (cost-adjusted) regret

Is Gittins index good?

empirically

Pandora's Box

[Weitzman'79]



Discrete

Independent

Flexible-stopping

Expected cost-adjusted regret

Gittins index is optimal

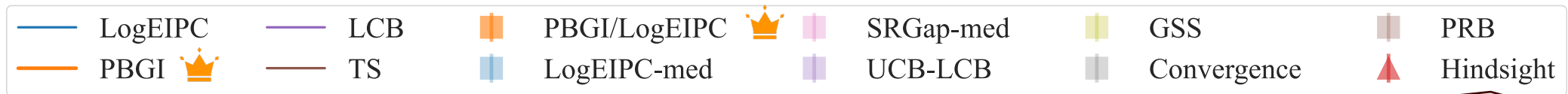
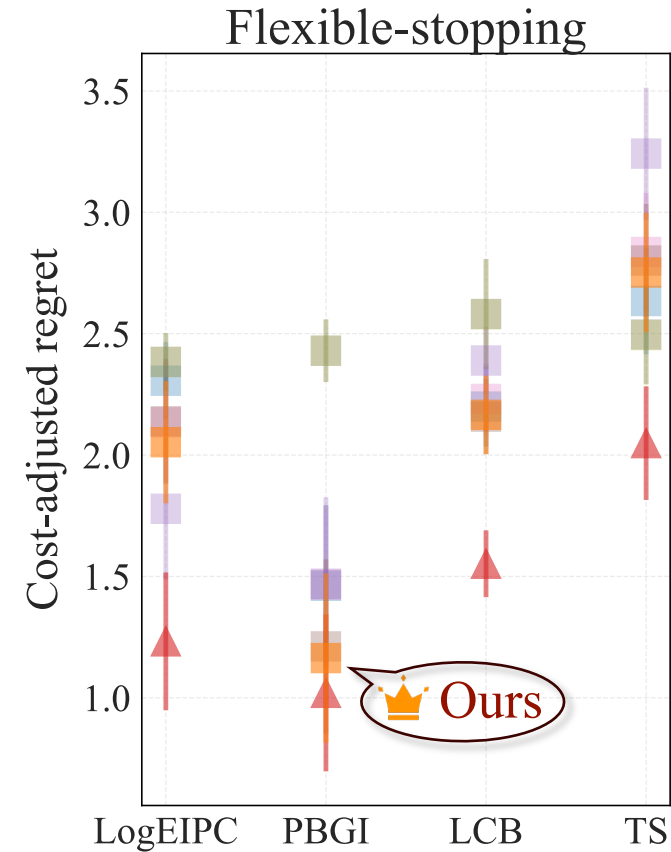
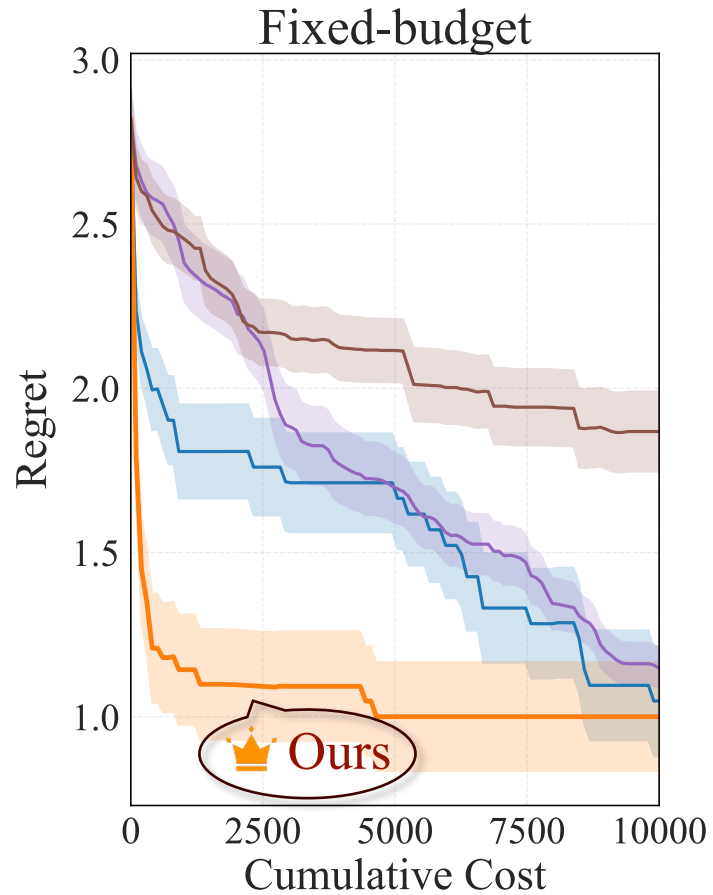
Our Contribution: Gittins Index Principle

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

 Why another principle?

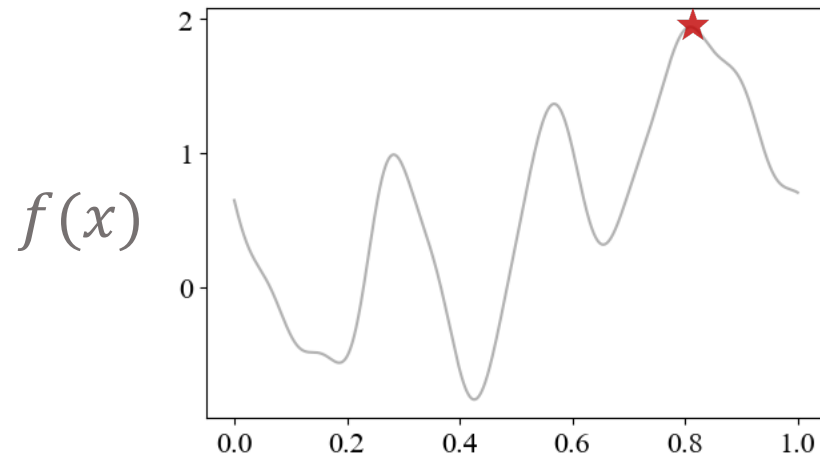
1. Naturally handles practical considerations
- 2. Performs competitively on benchmarks**
3. Comes with theoretical guarantees

Gittins Index vs Baselines on AutoML Benchmark



Bound on achievable performance

Bayesian Optimization



Continuous

Correlated

Fixed-budget / Flexible-stopping

Expected (cost-adjusted) regret

Is Gittins index good?

theoretically

Pandora's Box

[Weitzman'79]



Discrete

Independent

Flexible-stopping

Expected cost-adjusted regret

Gittins index is optimal

Our Contribution: Gittins Index Principle

- Improvement-based (e.g., LogEIPC)
- Entropy-based
- Confidence bounds
- 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)

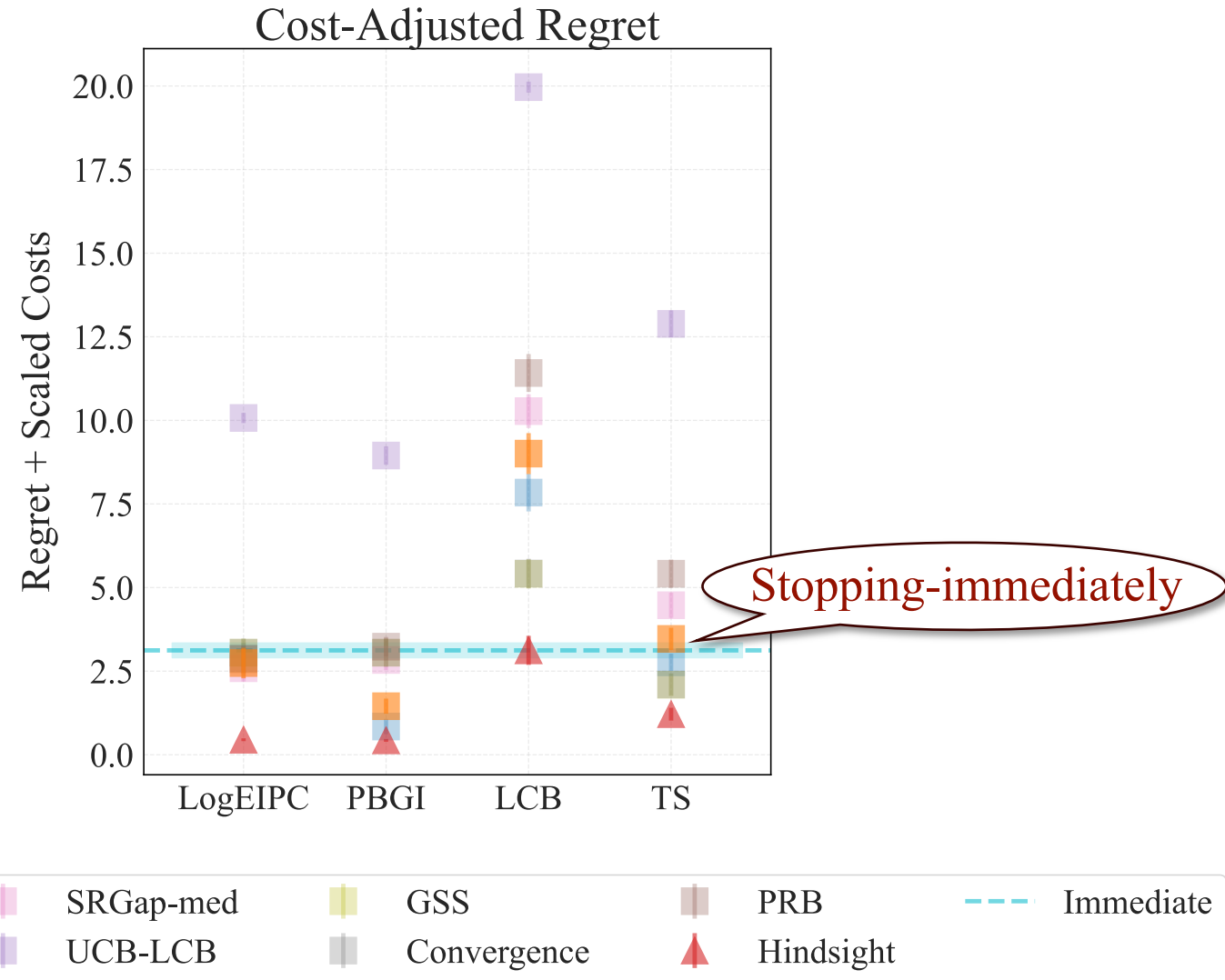
$$\mathbb{E}[R(\text{ours}; \text{PBGI})] \leq R[\text{stopping immediately}]$$

or LogEIPC

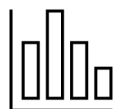
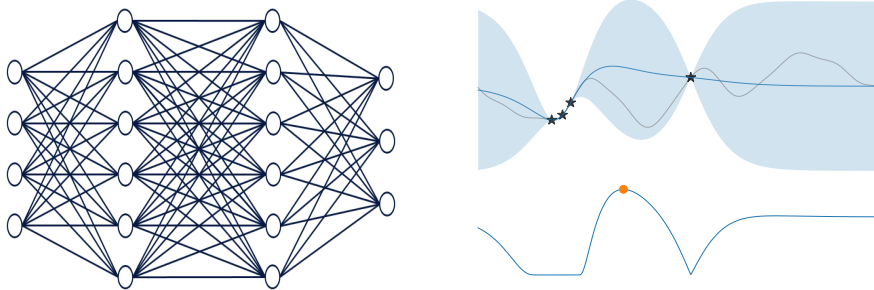
cost-adjusted regret

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

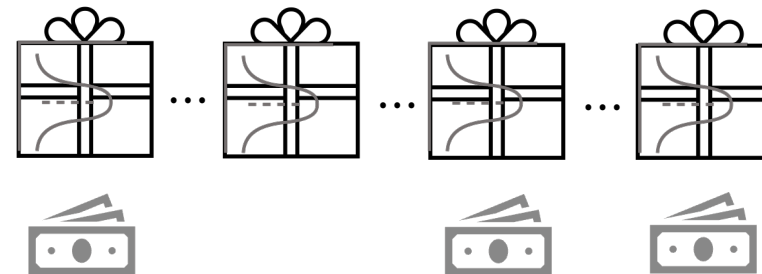


Varying evaluation costs



Adaptive stopping time

Key idea



Link to Pandora's Box problem
& Gittins index theory

Impact

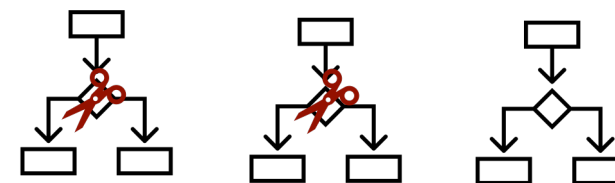


Competitive empirical performance &
interests from practitioners



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

Ongoing work

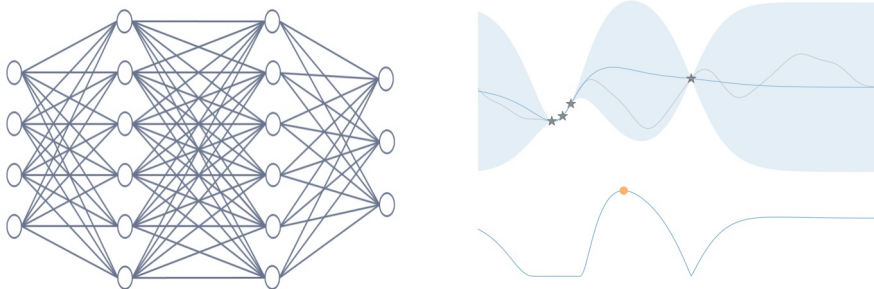


Sharper theoretical guarantees & black-
box optimization w/ multi-stage feedback



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

Studied problem

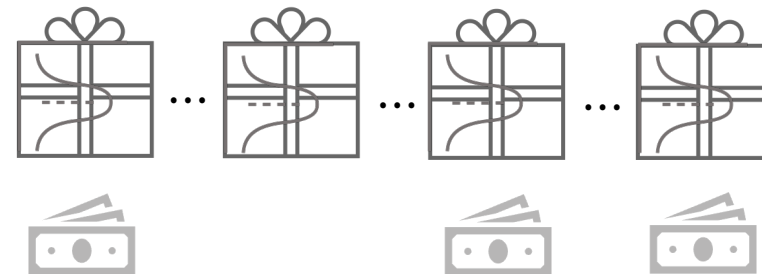


Varying evaluation costs



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Ongoing work



ChatGPT



deepseek



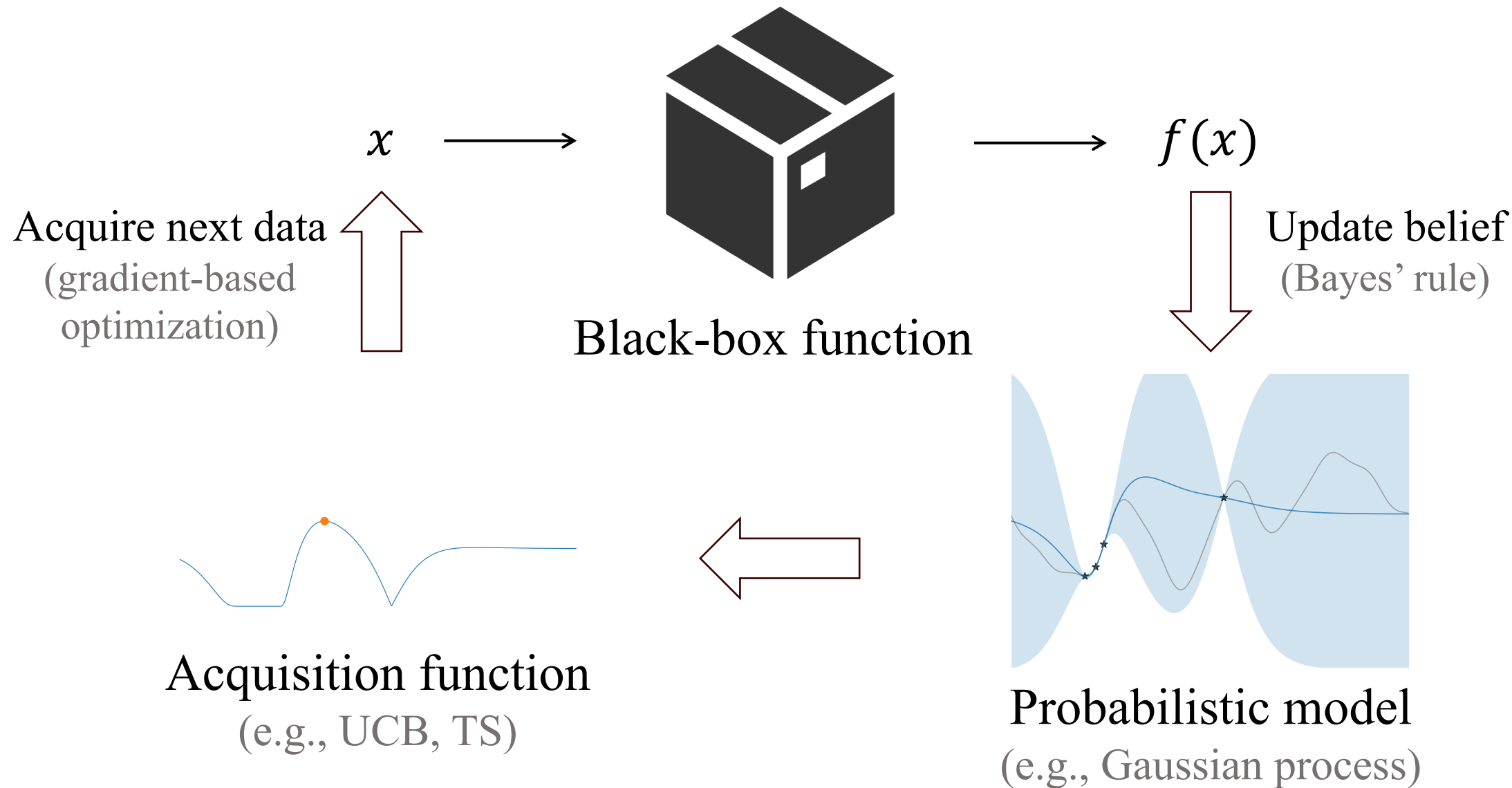
Claude

LLM-driven black-box optimization

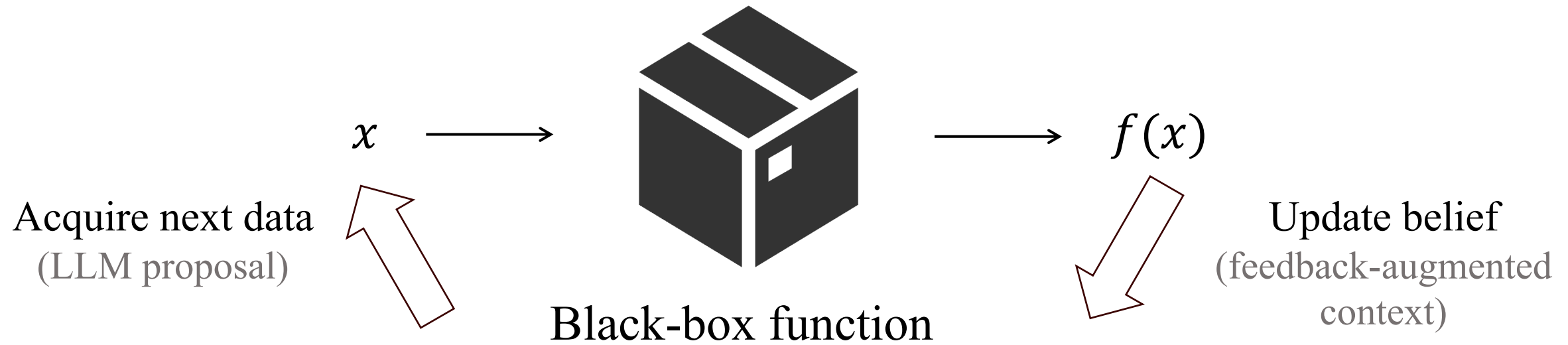


"Cost-aware Stopping for Bayesian
Optimization." Under review.

Recap: Bayesian Optimization



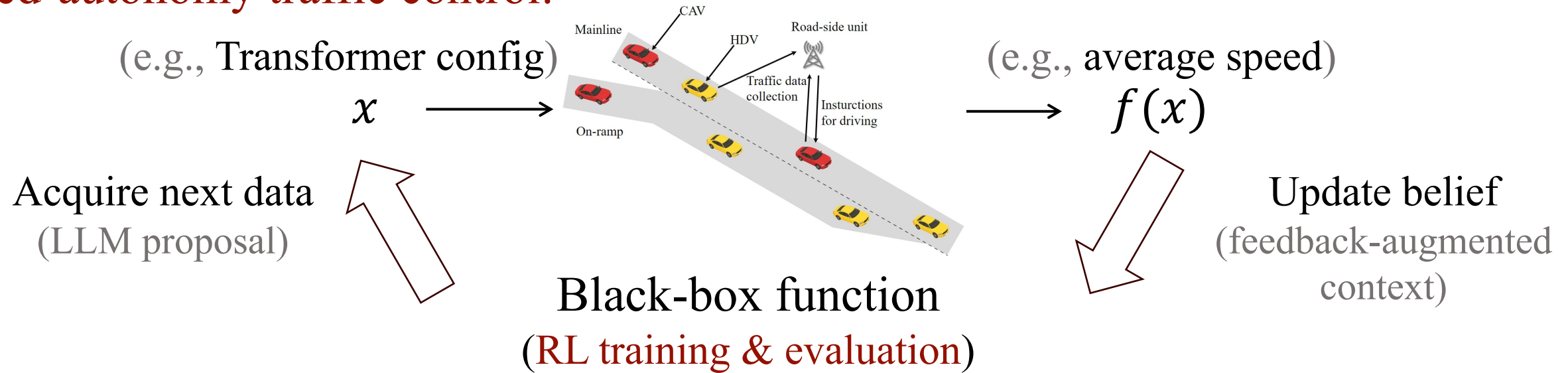
Ongoing: LLM-Driven Black-Box Optimization



Large language model

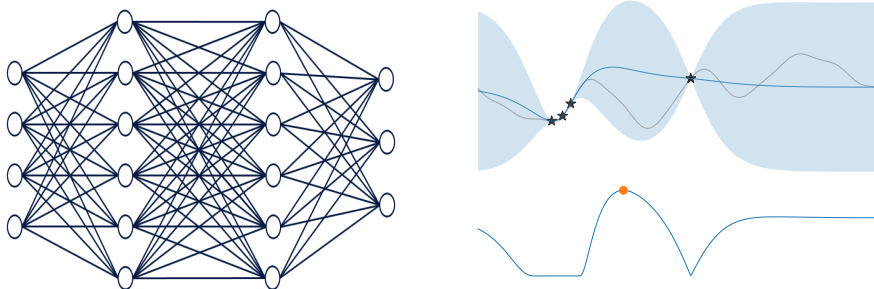
Ongoing: LLM-Driven Black-Box Optimization

Mixed-autonomy traffic control:



Large language model

Studied problem

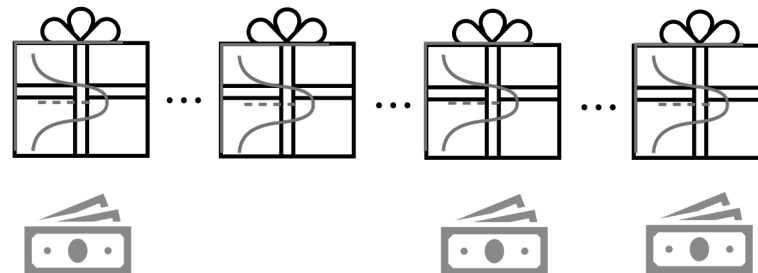


Varying evaluation costs



Adaptive stopping time

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Ongoing work



ChatGPT



Gemini



deepseek



Claude

LLM-driven black-box optimization



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