

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), Theodore Brown (UCL), Raul Astudillo (MBZUAI), Peter Frazier, Alexander Terenin, and Ziv Scully (Cornell)

INFORMS Annual Meeting 2025 Job Market Showcase

Optimization Under Uncertainty

ML model training:

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

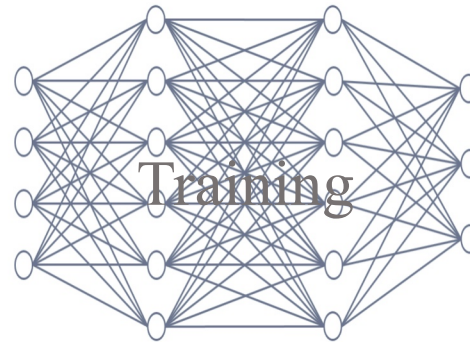


Accuracy

Optimization Under Uncertainty

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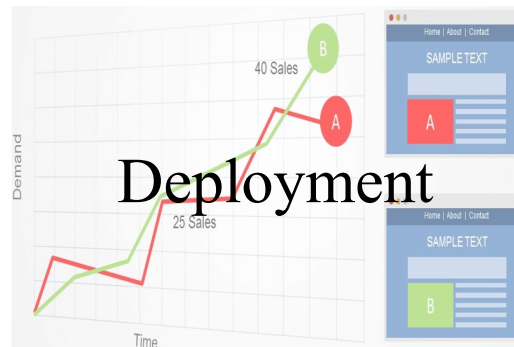
Training hyperparameters
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Accuracy

Adaptive experimentation:

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



Revenue

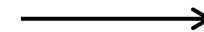
Optimization Under Uncertainty

Black-box optimization:

Input x



non-analytical &
no gradient info



Performance metric $f(x)$

ML model training:

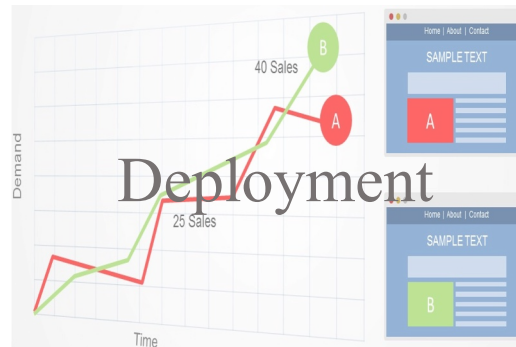
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Accuracy

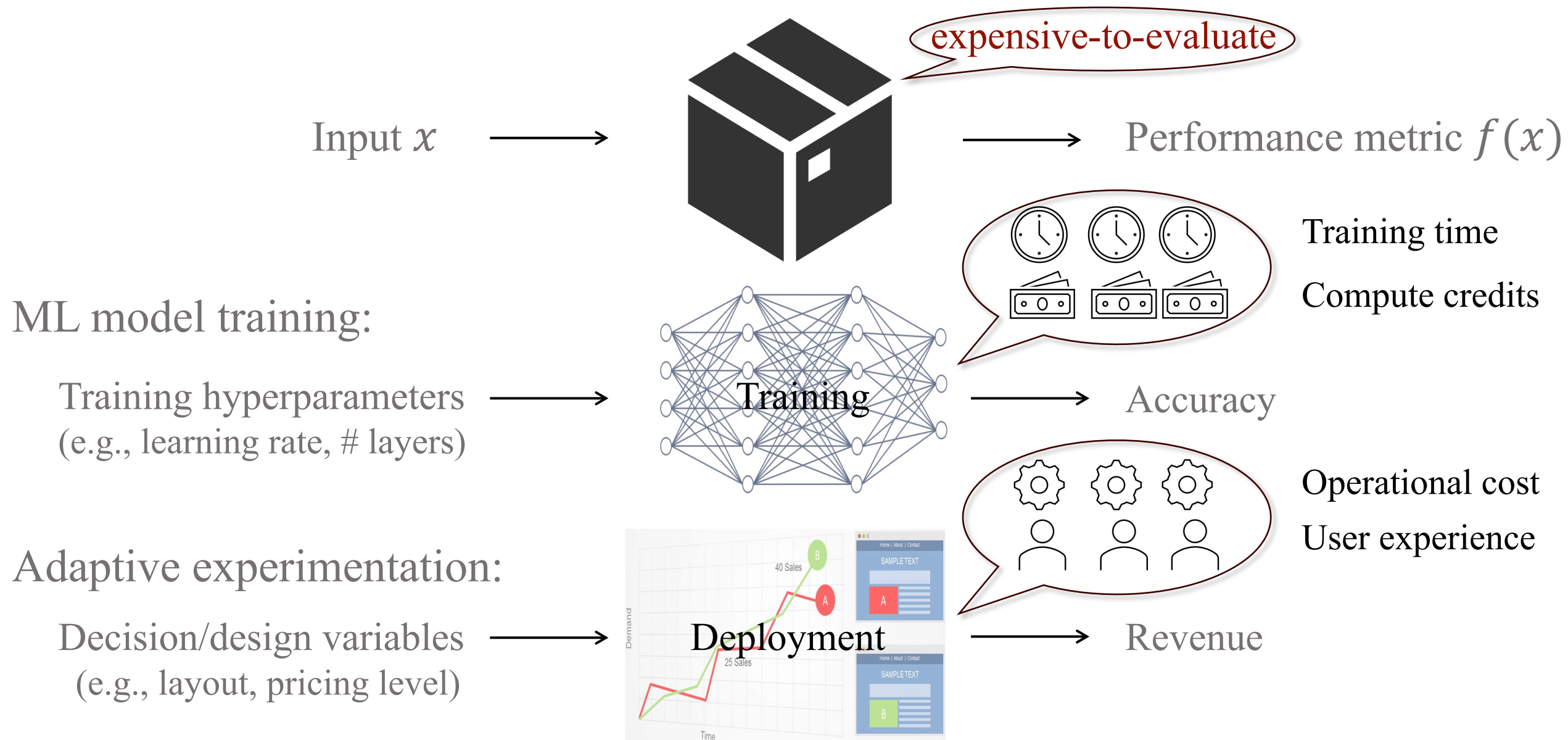
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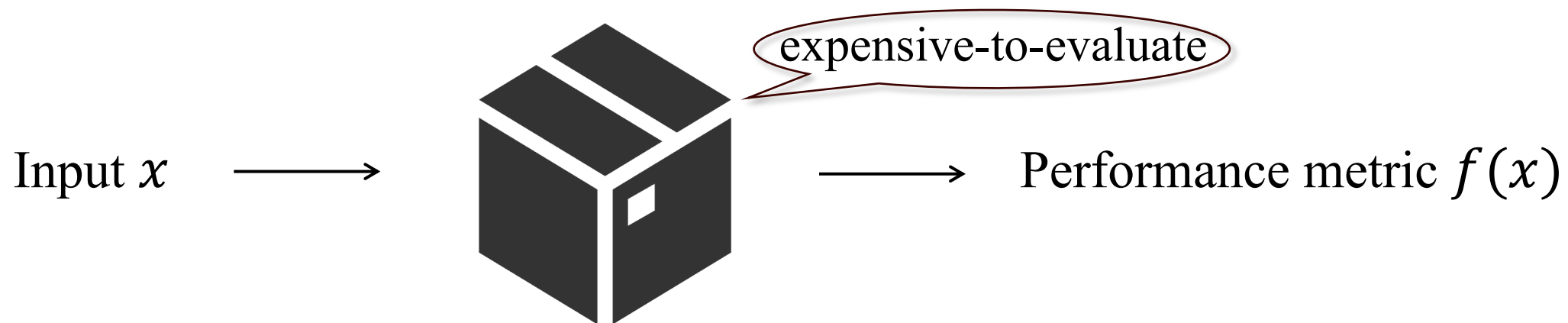


Revenue

Black-Box Optimization



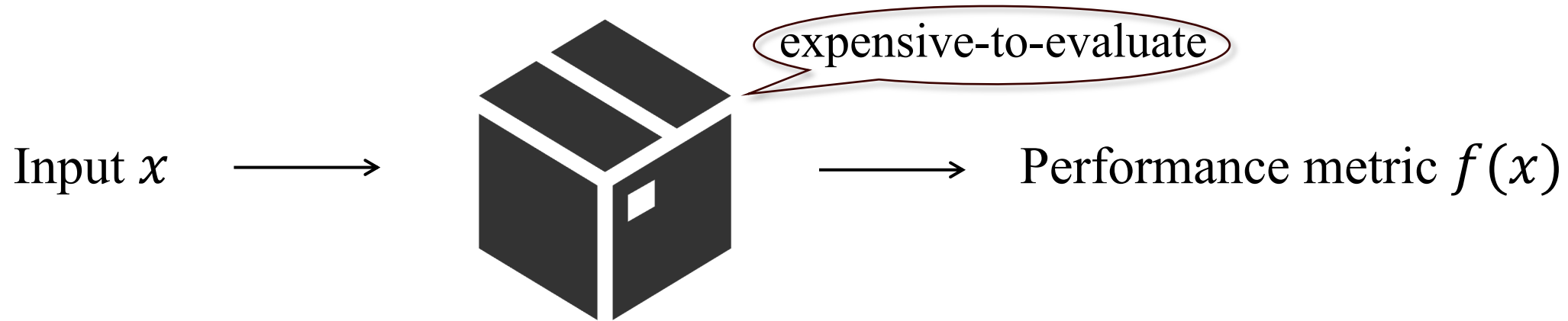
Black-Box Optimization



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



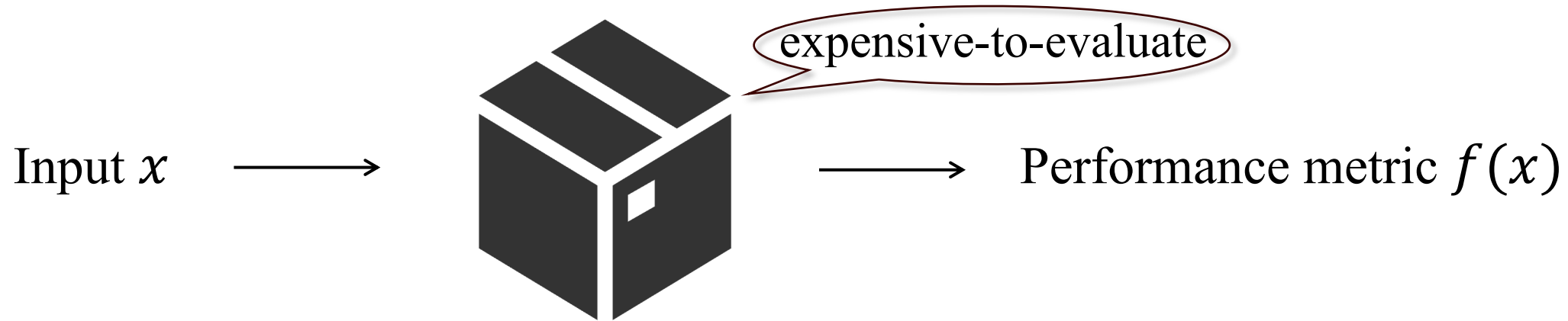
adaptively

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

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Fewer #evaluations

Data-Driven Black-Box Optimization



adaptively

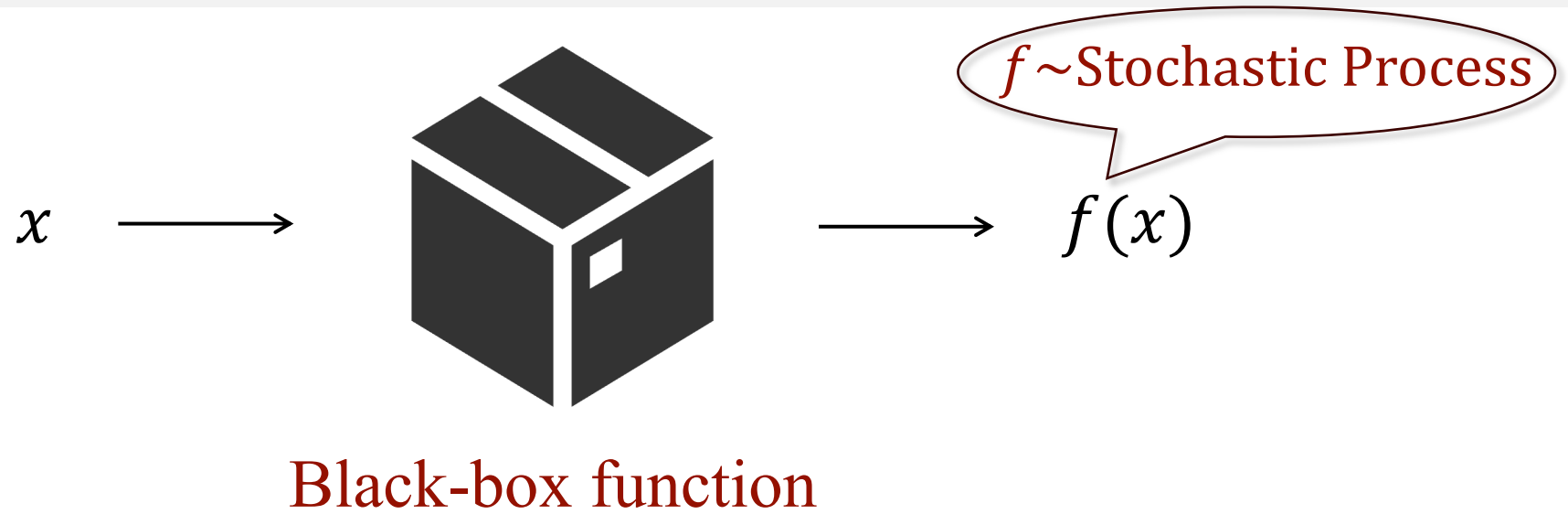
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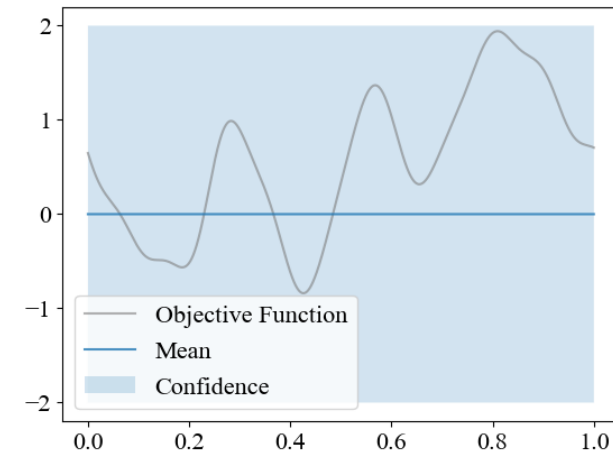
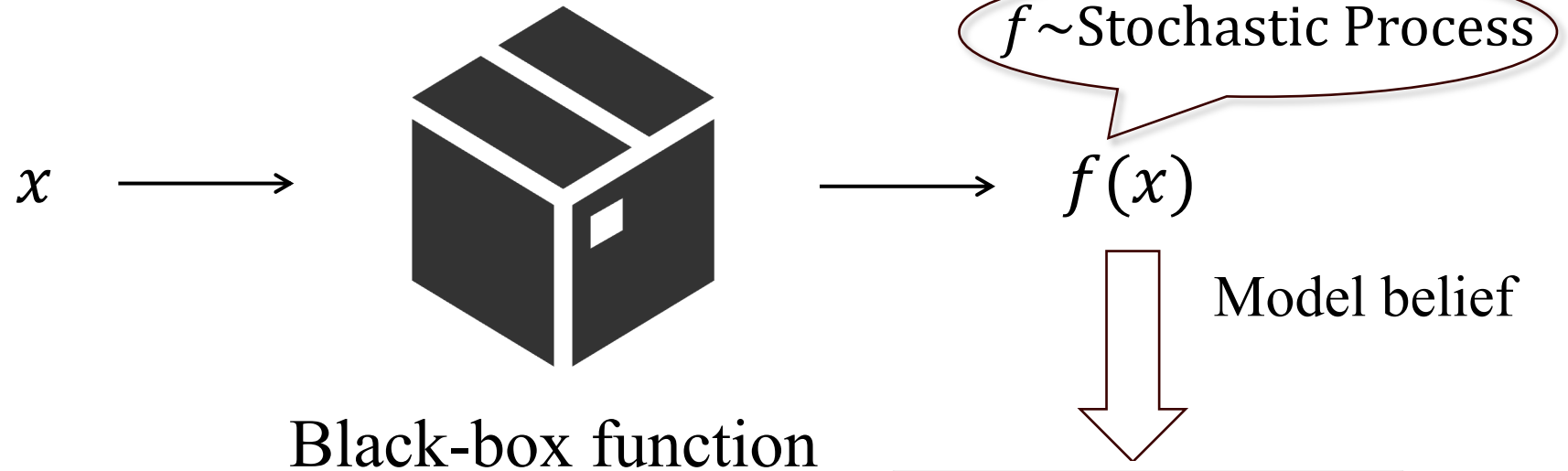
Efficient framework: Bayesian optimization

Bayesian Optimization



Bayesian Optimization

Time 0



Probabilistic model
(e.g., Gaussian process)

Bayesian Optimization

Time t

x_1, \dots, x_t



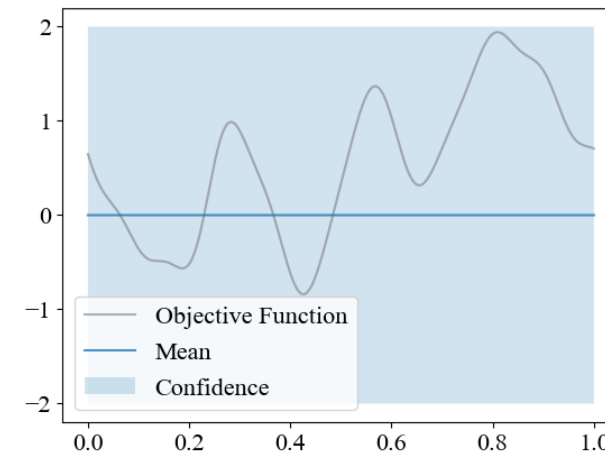
Black-box function



$f \sim \text{Stochastic Process}$

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

Model belief



Probabilistic model
(e.g., Gaussian process)

Bayesian Optimization

Time t

x_1, \dots, x_t



Black-box function

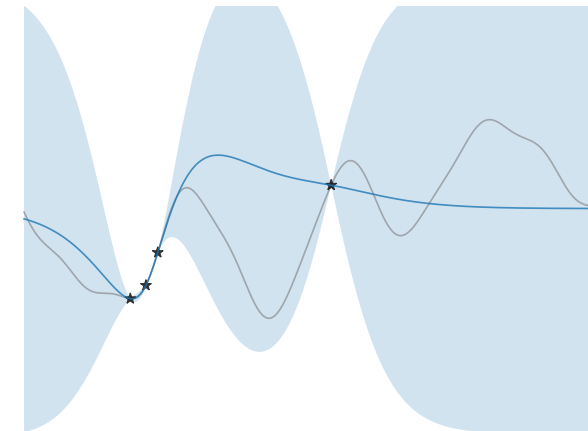


$f \sim \text{Stochastic Process}$

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



Update belief
(Bayes' rule)

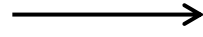


Probabilistic model
(e.g., Gaussian process)

Bayesian Optimization

Time t

x_1, \dots, x_t

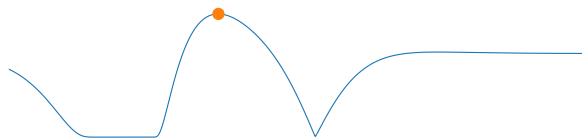


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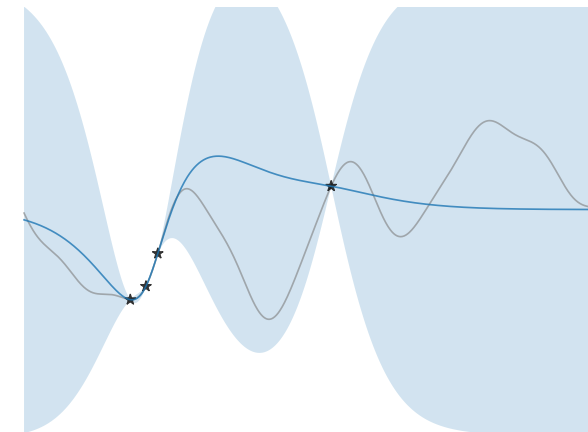
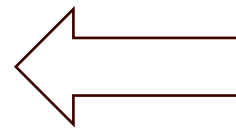
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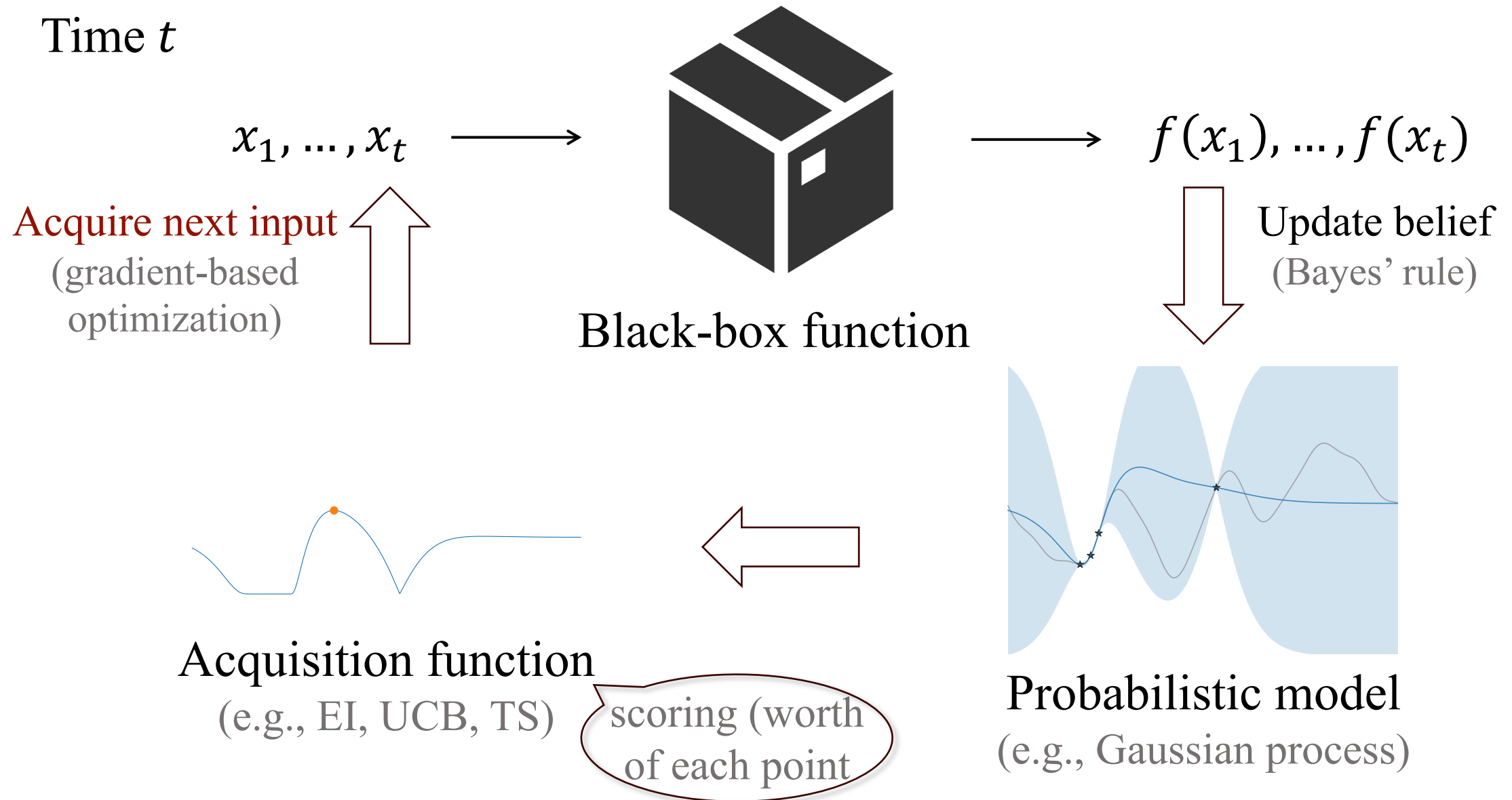
Acquisition function
(e.g., EI, UCB, TS)

scoring (worth
of each point)

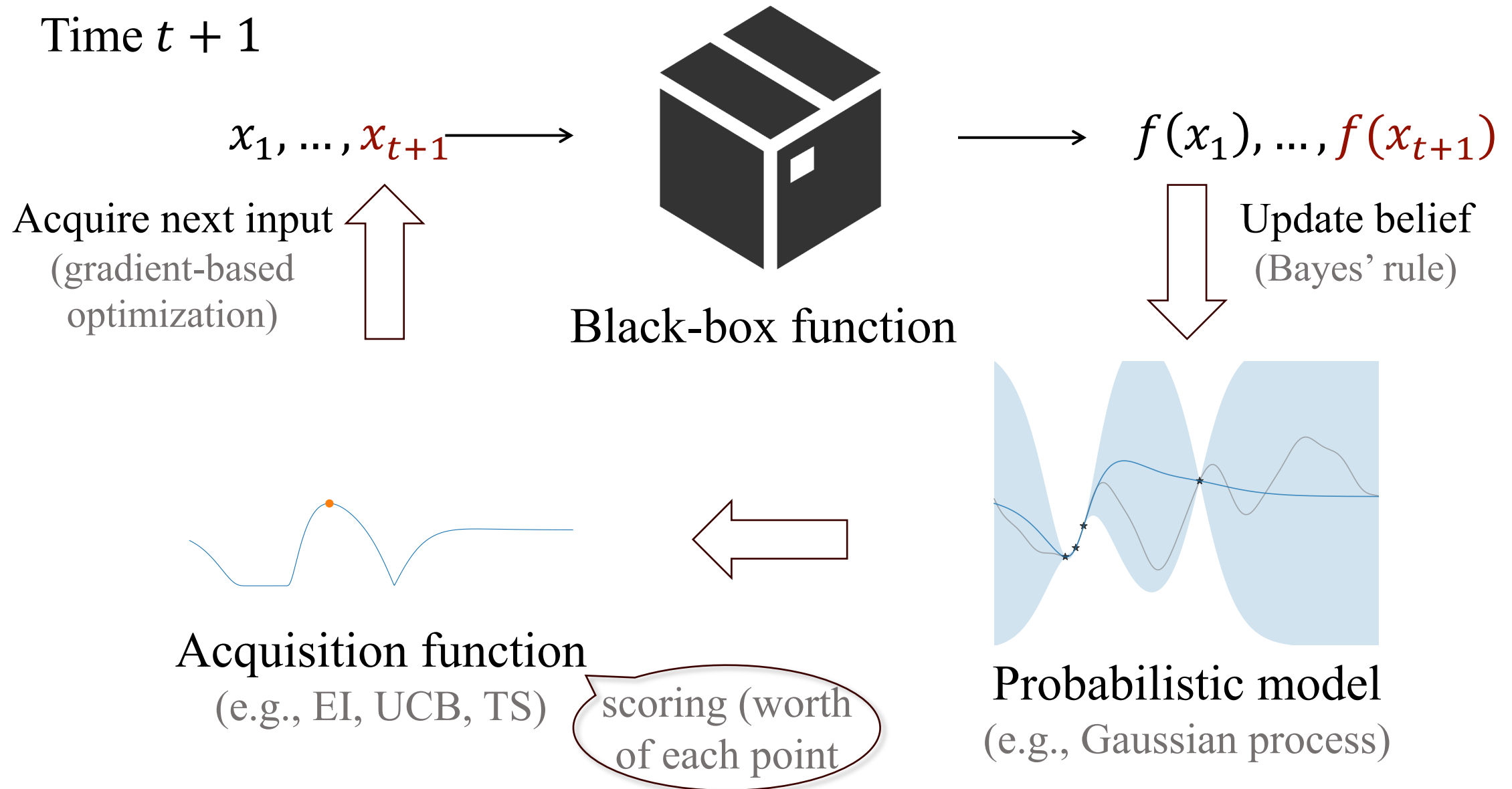


Probabilistic model
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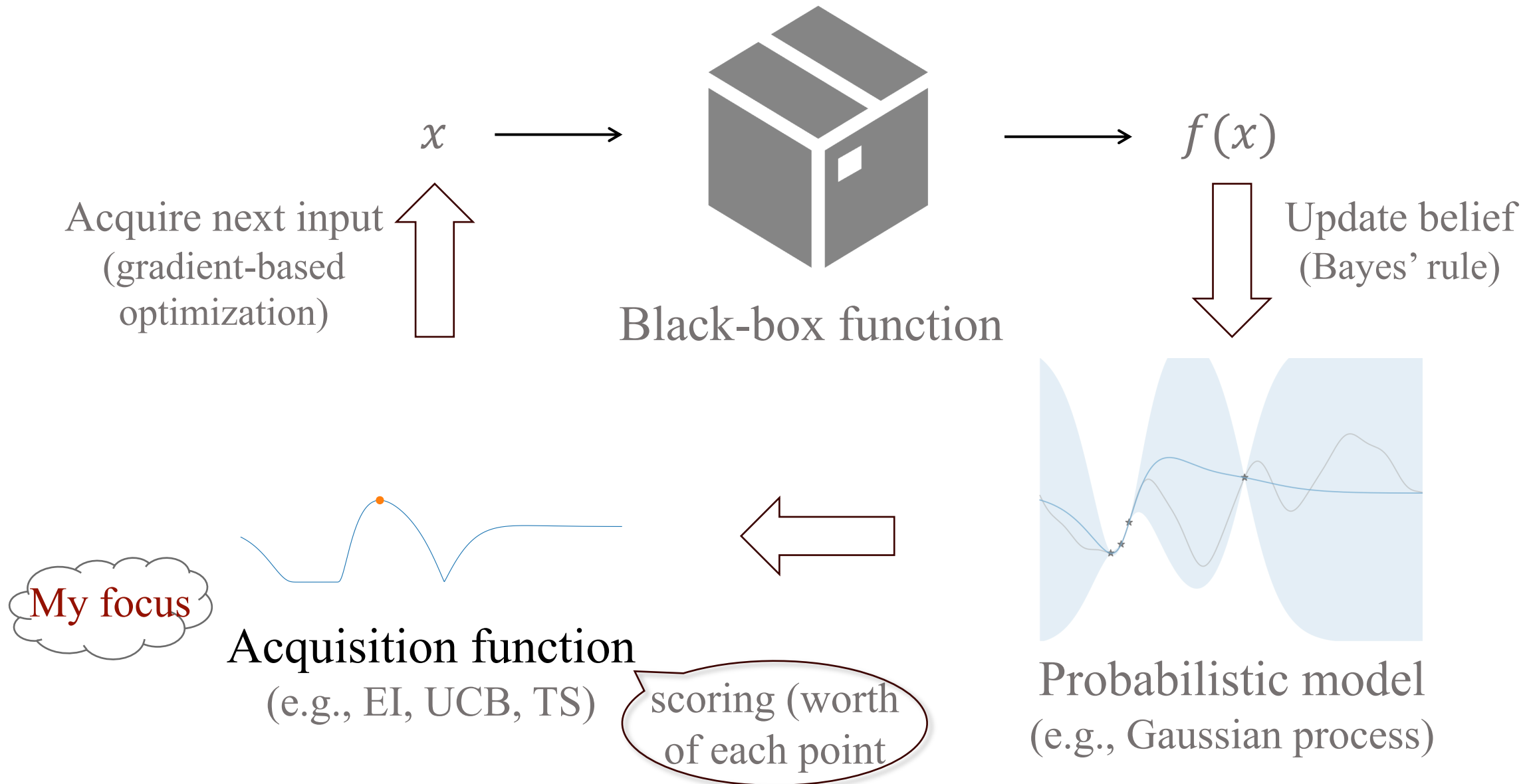
Bayesian Optimization



Bayesian Optimization



Bayesian Optimization



Existing Design Principles

- Improvement-based (e.g., EI)
- Entropy-based
- Confidence bounds (UCB/LCB)
- Thompson sampling (TS)

New Design Principle: Gittins Index

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? Why another principle?

Our Contribution: Gittins Index Principle

- Improvement-based (e.g., EI)
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 Why another principle?

1. Naturally incorporates side info and practical flexibility
2. Performs competitively on benchmarks
3. Comes with theoretical guarantees

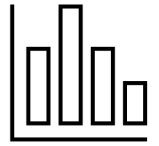
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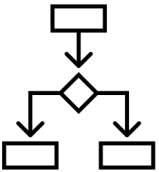
Under-explored Side Info and Flexibility



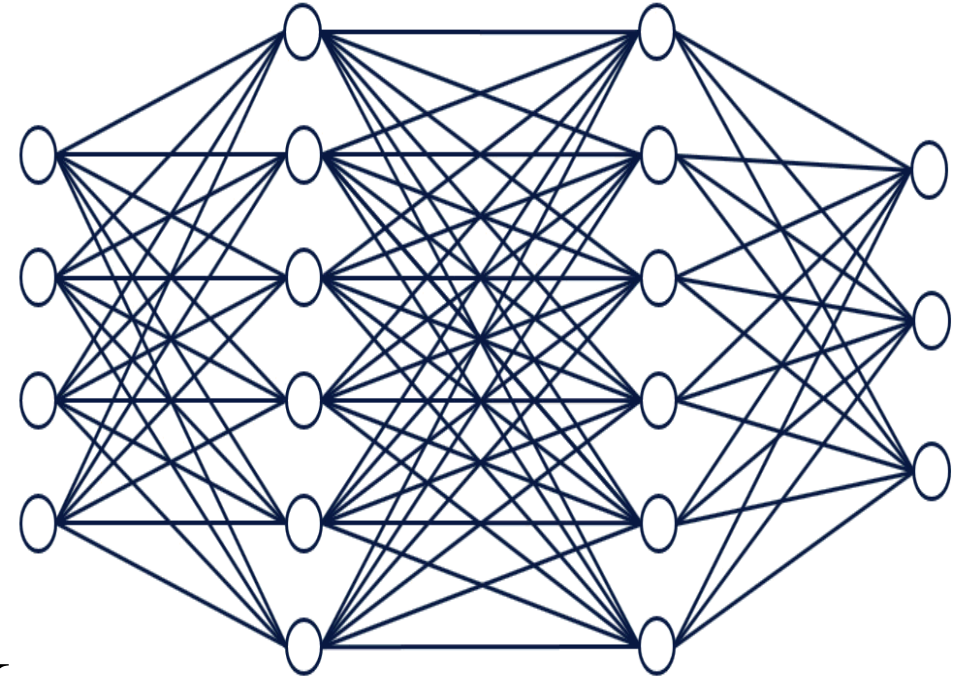
Varying evaluation costs



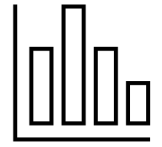
Smart stopping time



Observable multi-stage feedback



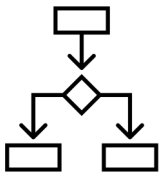
How does existing principle incorporate them?



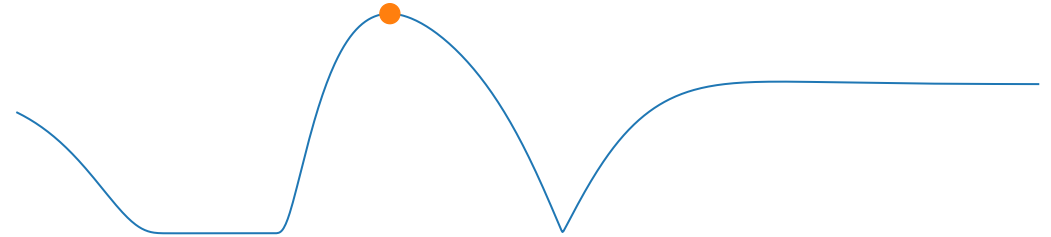
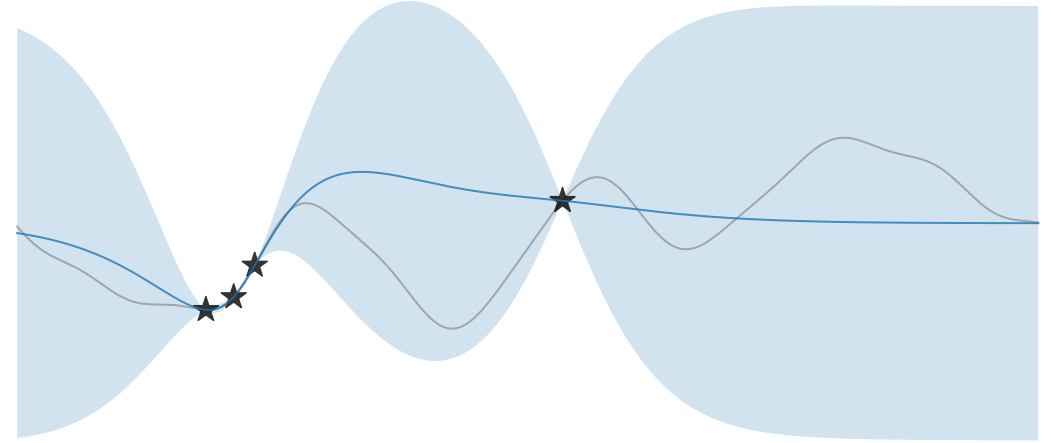
Varying evaluation costs



Smart stopping time

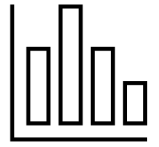


Observable multi-stage feedback



Expected improvement $EI(x)$

How does existing principle incorporate them?



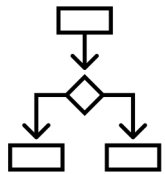
Varying evaluation costs

$$EI(x)/c(x)$$

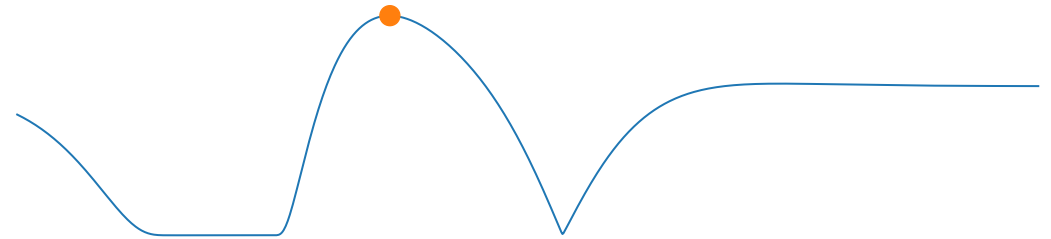
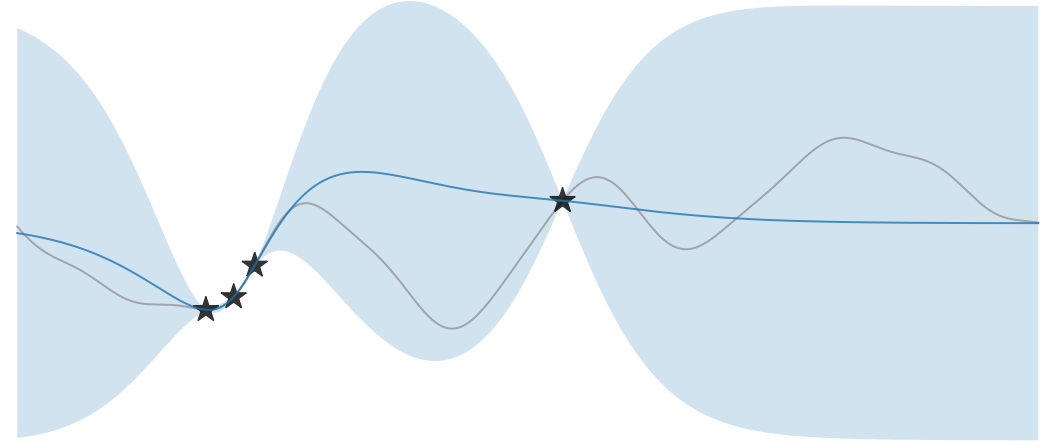
Why divide?



Smart stopping time

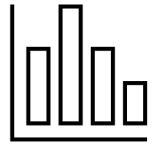


Observable multi-stage feedback



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Varying evaluation costs

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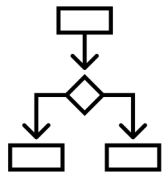
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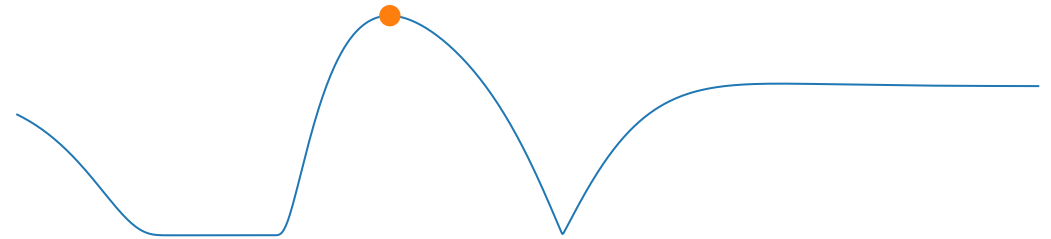
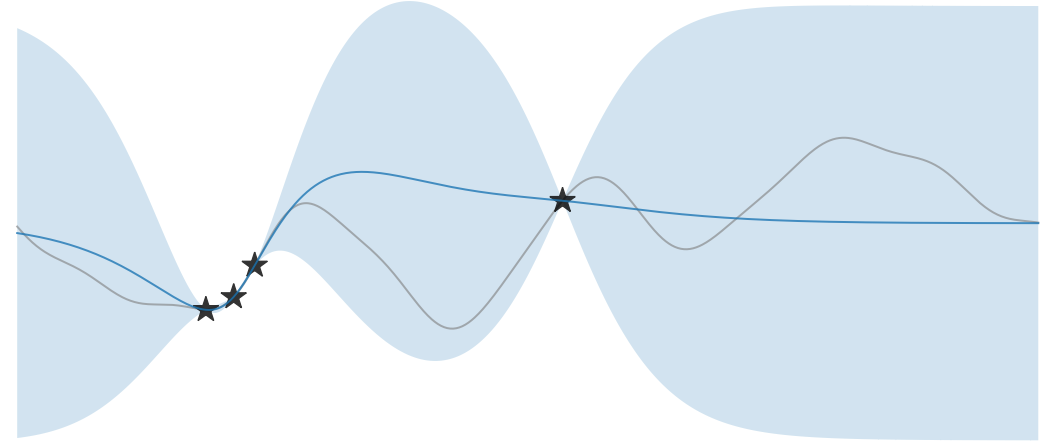
Smart stopping time

$$EI(x) \leq \theta$$

Which threshold?

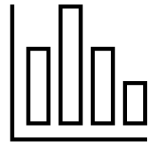


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Varying evaluation costs

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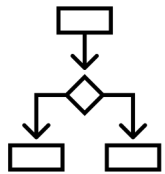
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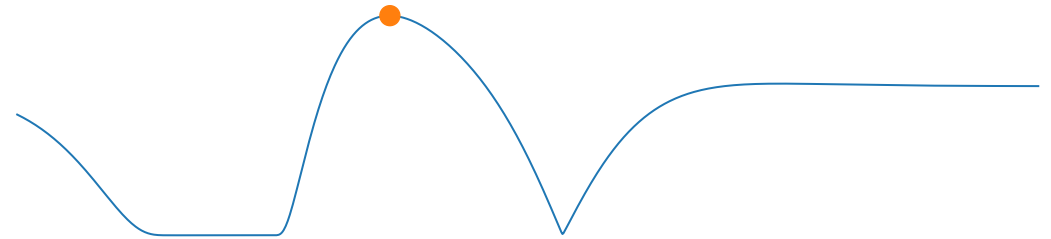
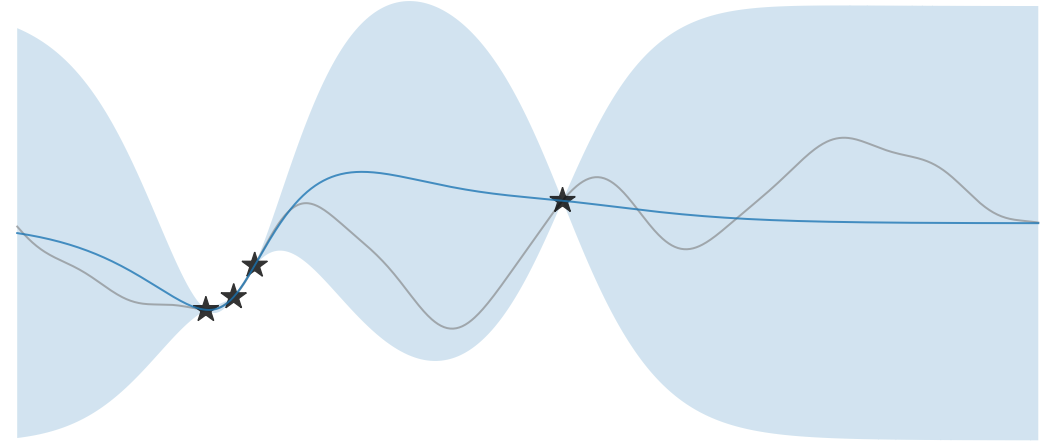
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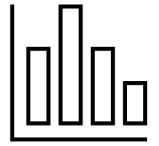
Observable multi-stage feedback

?



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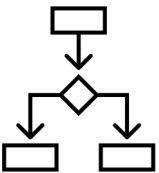
Under-explored Side Info and Flexibility



Varying evaluation costs



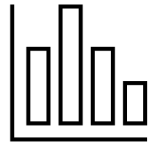
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Observable multi-stage feedback

New design principle:
Gittins index

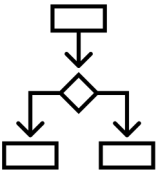
Why Gittins index?



Varying evaluation costs



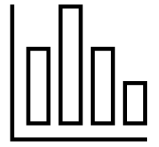
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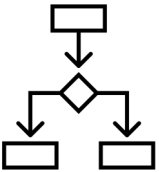
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Varying evaluation costs



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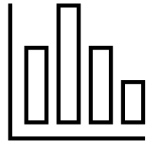


Observable multi-stage feedback

New design principle:
Gittins index

Optimal in related sequential
decision problems

Why Gittins index?



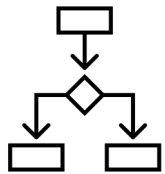
Varying evaluation costs

Features in Pandora's box



Smart stopping time

Features in Pandora's box

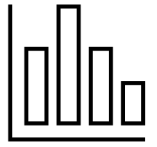


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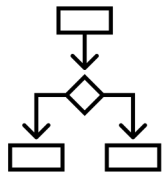
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Smart stopping time

Features in Pandora's box



Observable multi-stage feedback

Features in **Markovian bandits**

New design principle:
Gittins index

Optimal in related sequential
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What is Pandora's Box?



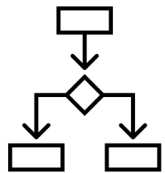
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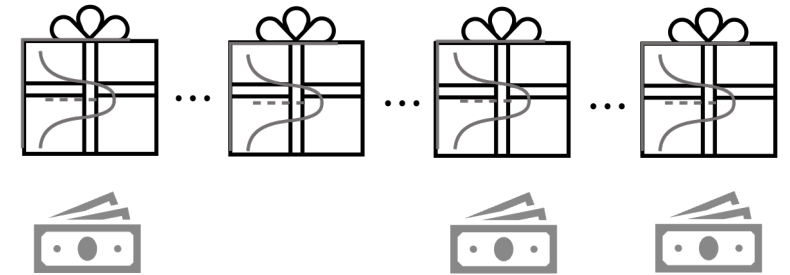


Observable multi-stage feedback

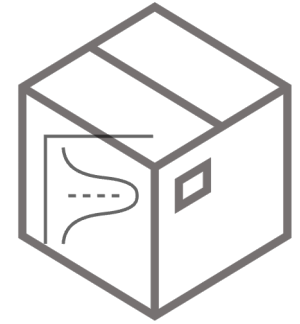
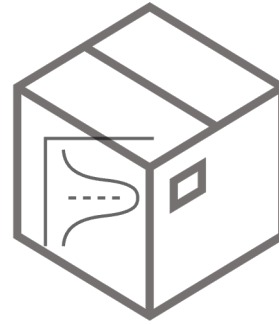
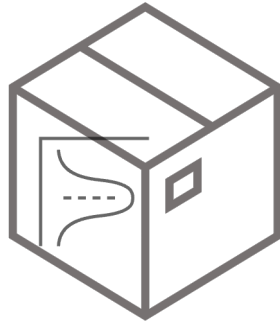
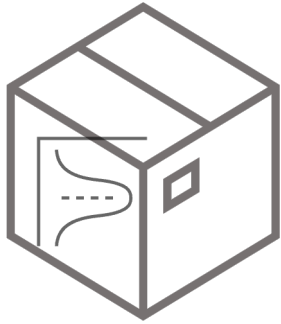
Features in Markovian bandits

New design principle:
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Pandora's Box



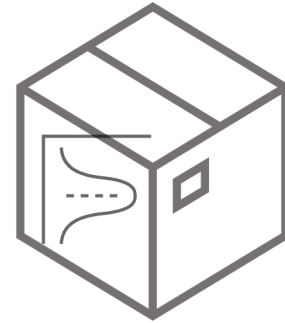
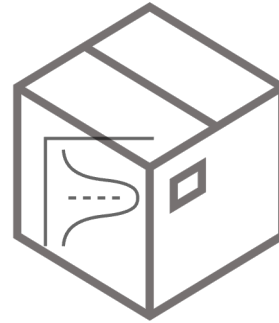
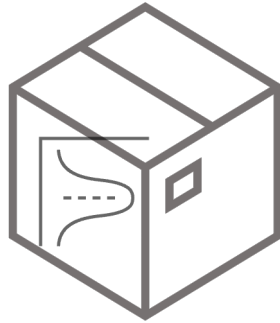
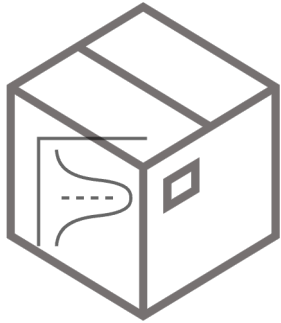
High-level goal: Choose box x_1, \dots, x_T to open to maximize the expected utility

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

Flexible stopping time

Pandora's Box

$t = 0$

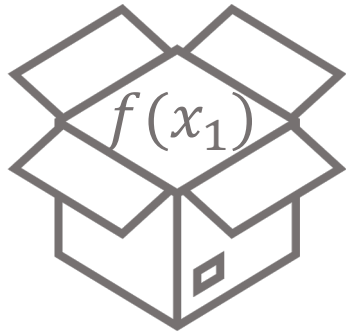


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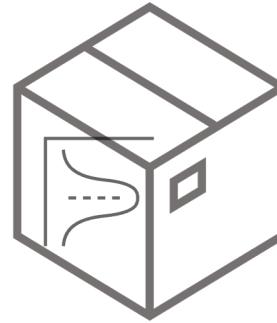
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Pandora's Box

$t = 1$



$c(x_1)$

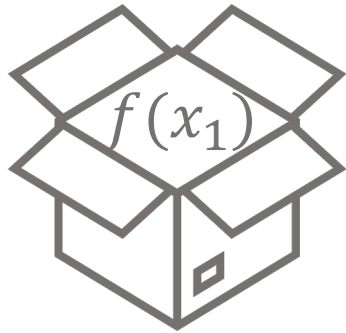


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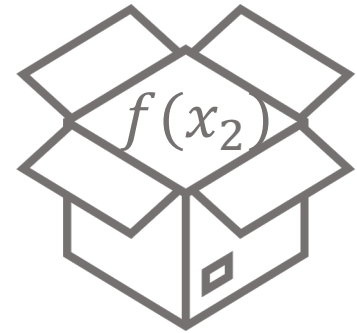
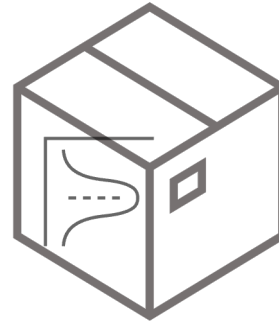
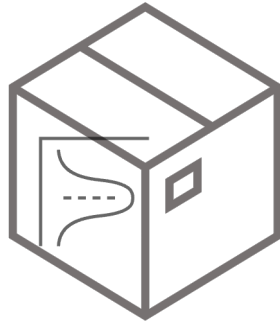
$$\mathbb{E} \max_{t=1,2,\dots,T} f(x_t) - \mathbb{E} \sum_{t=1}^T c(x_t)$$

Pandora's Box

$t = 2$



$c(x_1)$



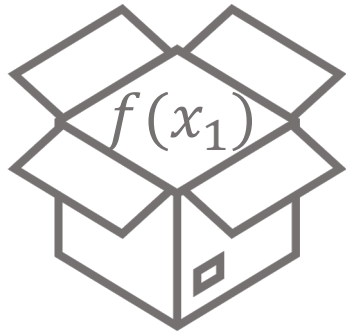
$c(x_2)$

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

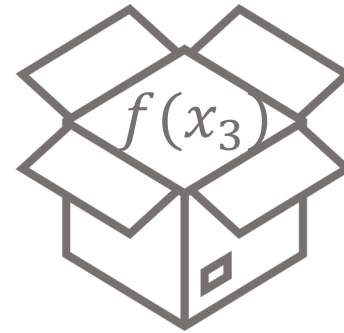
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Pandora's Box

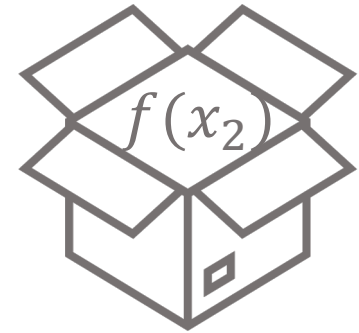
$t = 3$



$c(x_1)$



$c(x_3)$



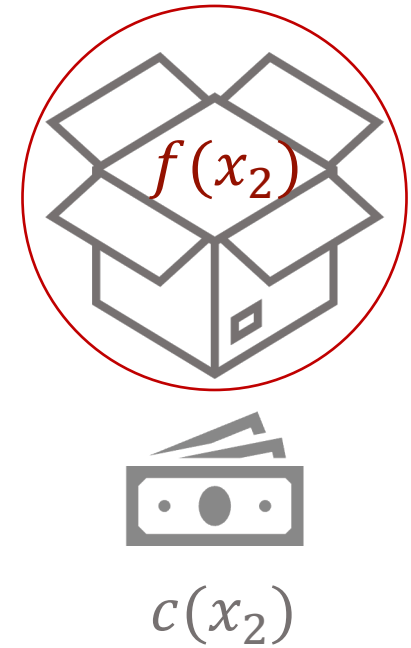
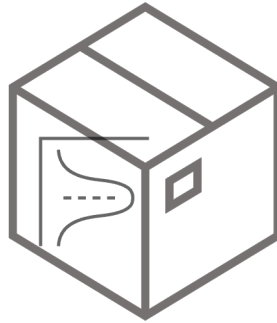
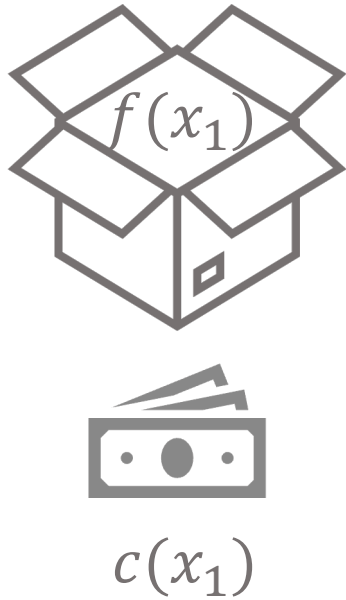
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High-level goal: Choose box x_1, \dots, x_T to open to maximize the expected utility

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

Pandora's Box

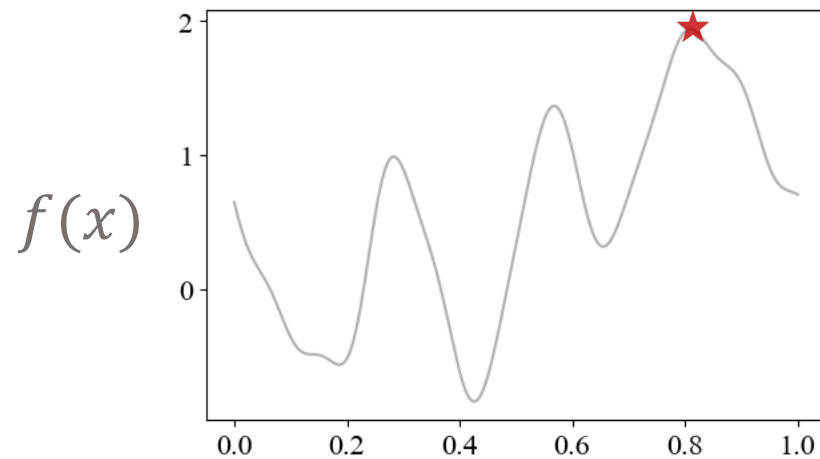
$t = T$, stop



High-level goal: Choose box x_1, \dots, x_T to open 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

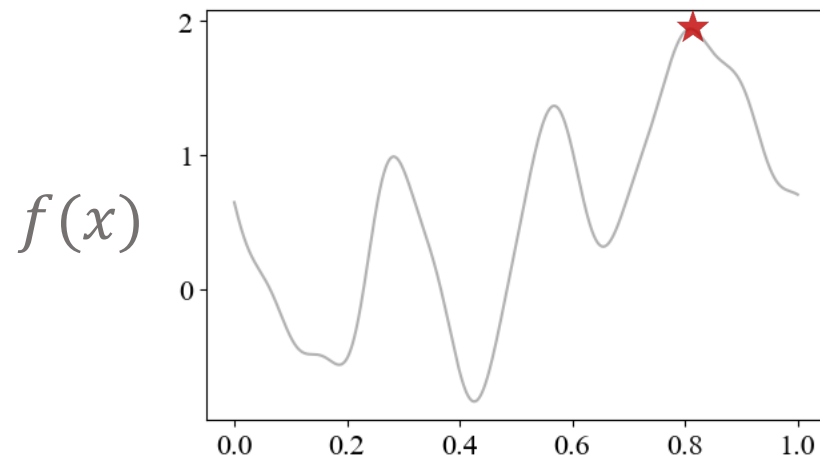
Flexible-stopping

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

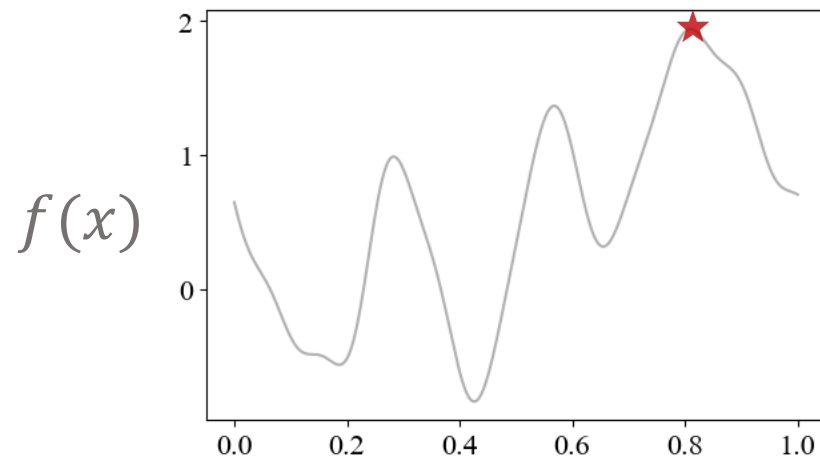
Flexible-stopping

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

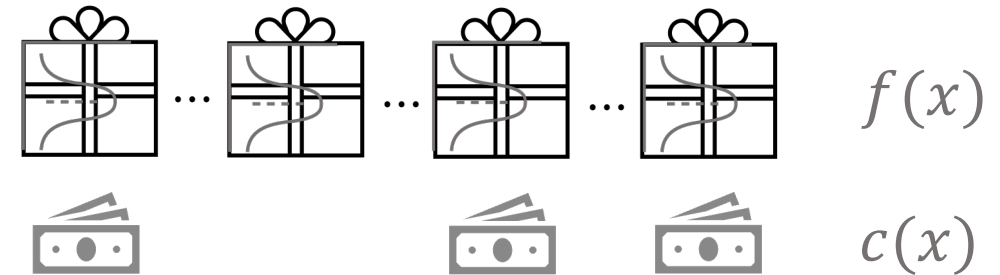
Fixed-iteration

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

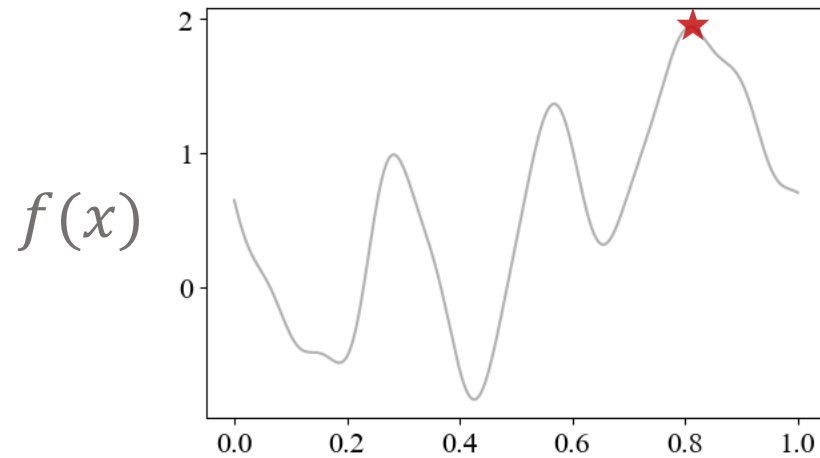
Flexible-stopping

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

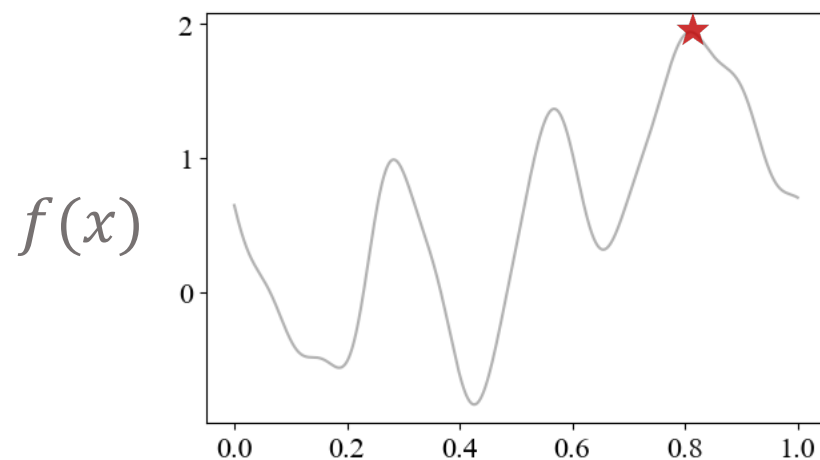
Flexible-stopping

Expected cost-adjusted regret

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

cumulative cost

Bayesian Optimization



Continuous

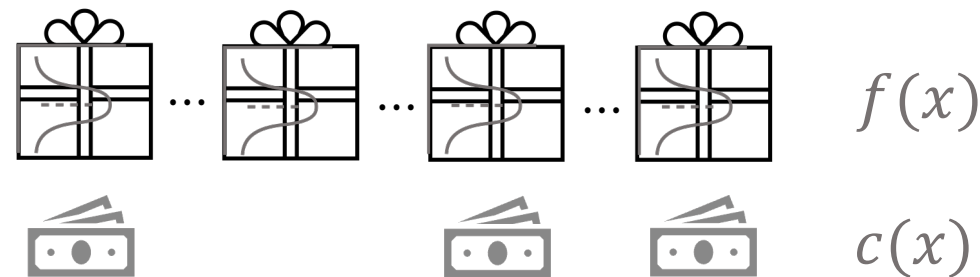
Correlated

Fixed-budget / Flexible-stopping

Expected (cost-adjusted) regret

Pandora's Box

[Weitzman'79]



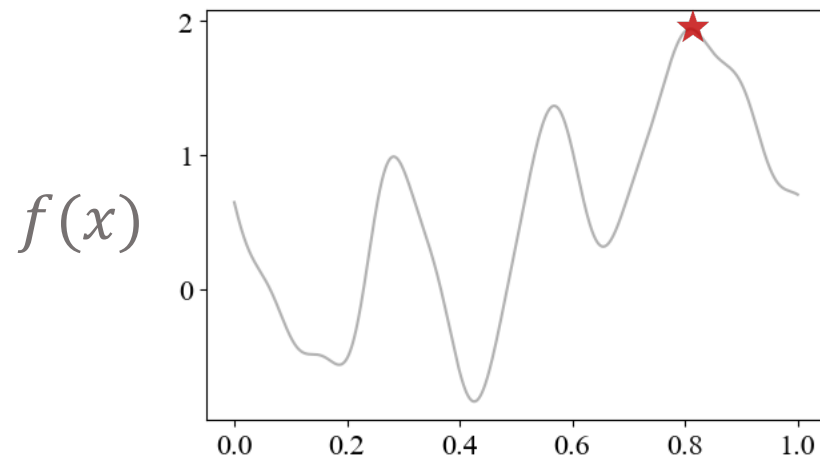
Discrete

Independent

Flexible-stopping

Expected cost-adjusted regret

Bayesian Optimization



Continuous

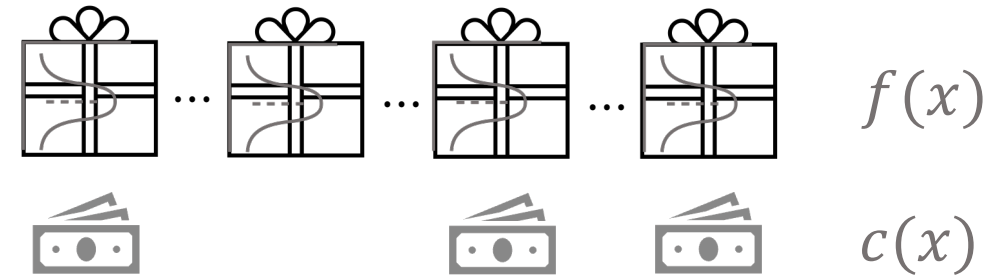
Correlated

Fixed-budget / Flexible-stopping

Expected (cost-adjusted) regret

Pandora's Box

[Weitzman'79]



Discrete

Independent

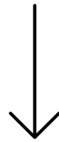
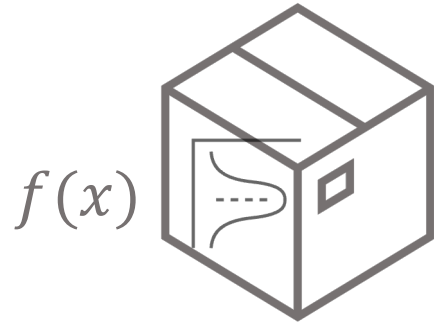
Flexible-stopping

Expected cost-adjusted regret

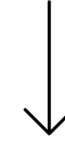
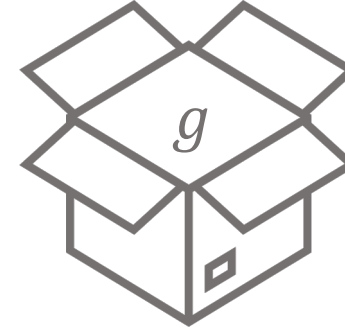
Optimal policy: Gittins index

Optimal Policy: Gittins Index

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



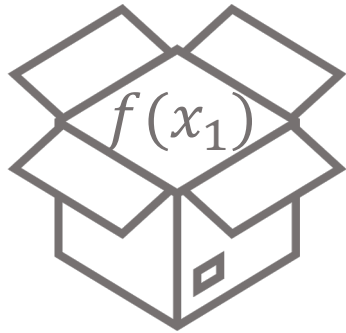
$GI_f(x; c(x))$



g

Optimal Policy: Gittins Index

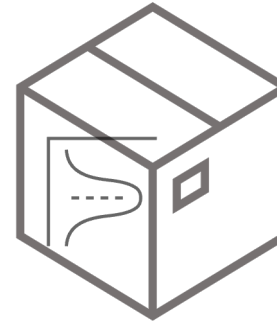
Step 2: **Open** the box with highest index if it is closed



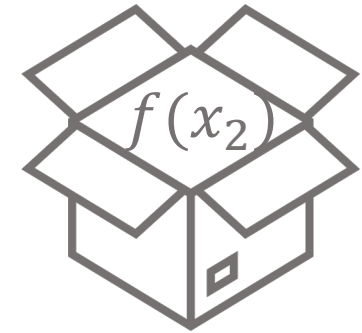
↓
 $f(x_1)$



↓
 $GI_f(x; c(x))$



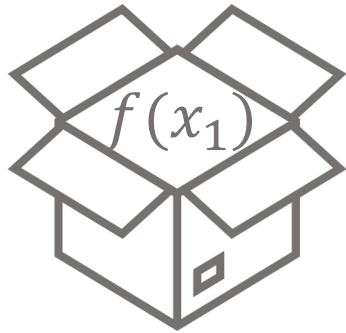
↓
 $GI_f(x'; c(x'))$



↓
 $f(x_2)$

Optimal Policy: Gittins Index

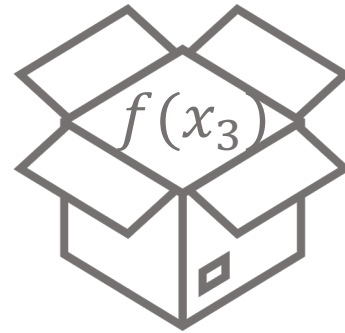
Step 2': **Select** the box with highest index if it is opened and **stop**



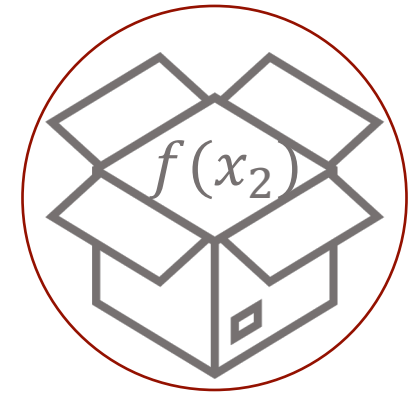
↓
 $f(x_1)$



↓
 $GI_f(x; c(x))$

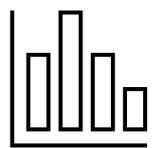


↓
 $f(x_3)$



↓
 $f(x_2)$

Optimal Policy: Gittins Index



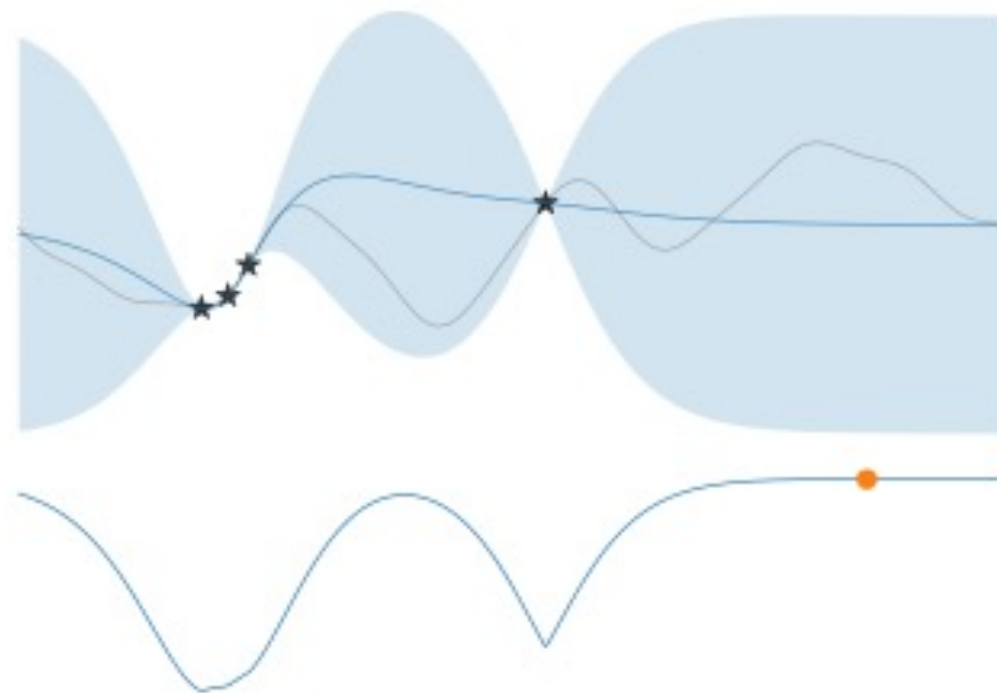
Varying evaluation costs

$$GI(x; c(x))$$



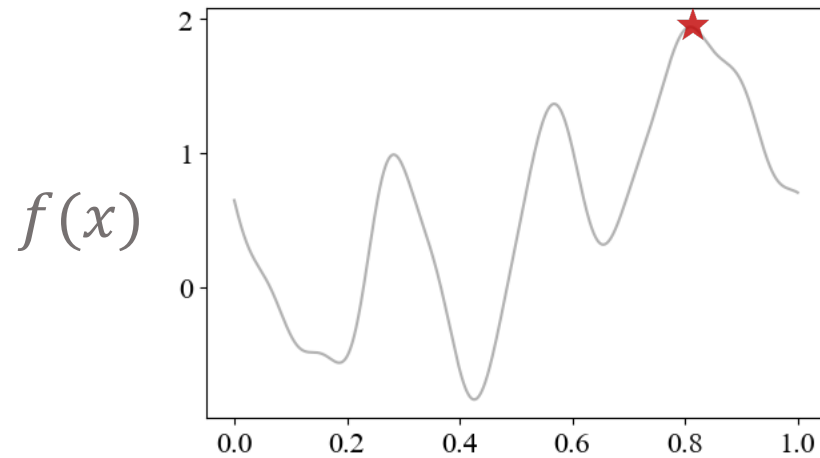
Smart stopping time

$$\max_x GI(x; c(x)) \leq \max_x f(x)$$



Gittins index $GI(x)$

Bayesian Optimization



Continuous

Correlated

Fixed-budget / Flexible-stopping

Expected (cost-adjusted) regret

Is Gittins index good?

Pandora's Box

[Weitzman'79]



Discrete

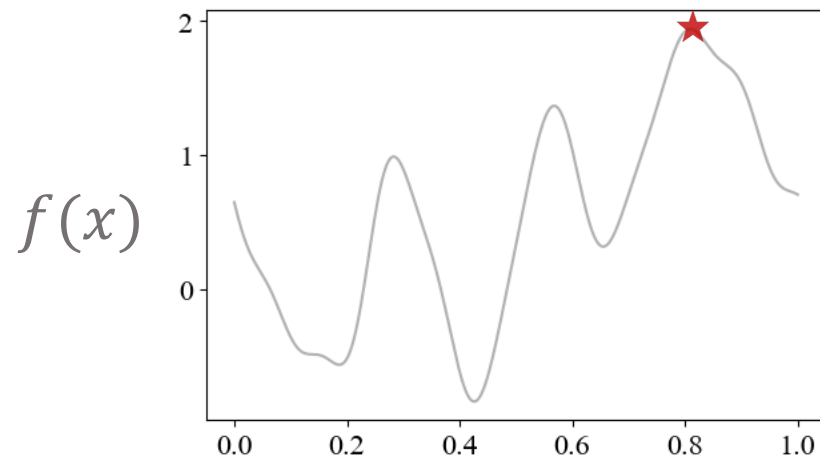
Independent

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

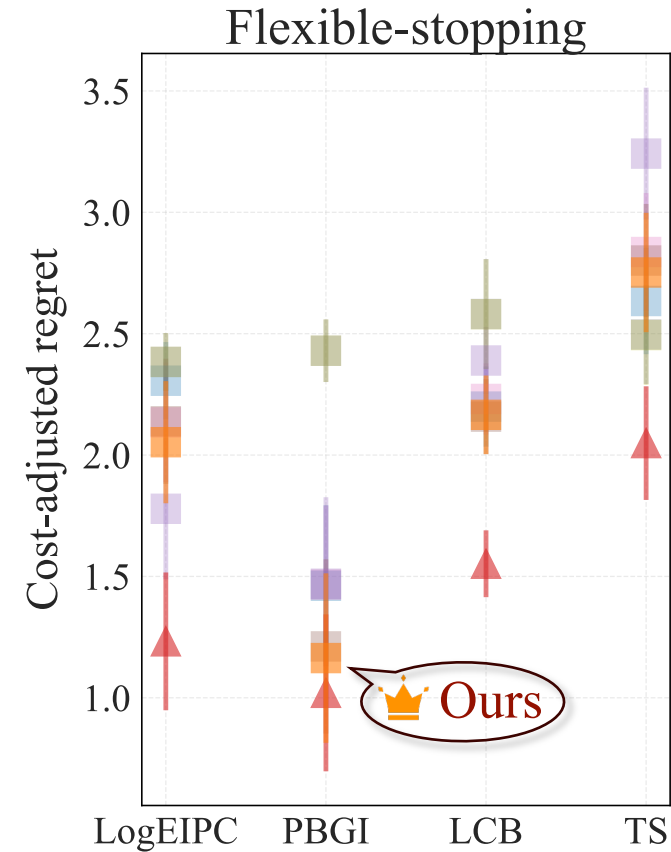
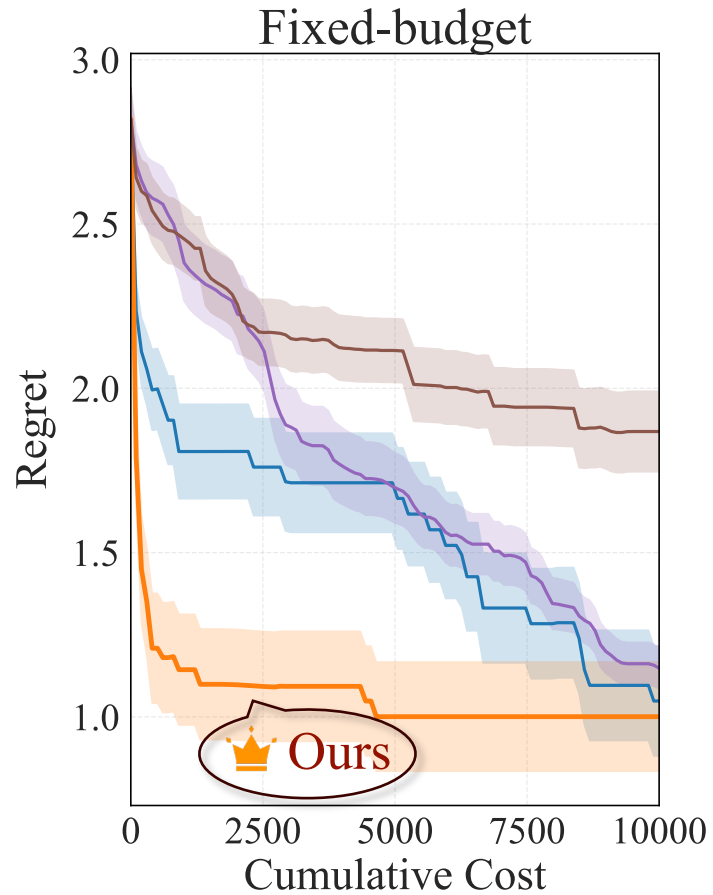
Our Contribution: Gittins Index Principle

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

 Why another principle?

1. Naturally incorporates side info and practical flexibility
- 2. Performs competitively on benchmarks**
3. Comes with theoretical guarantees

Gittins Index vs Baselines on AutoML Benchmark

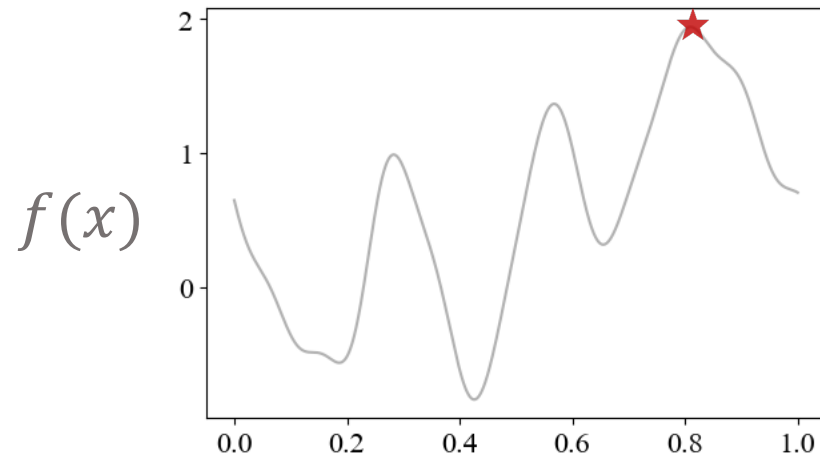


Lower the better



Bound on achievable performance

Bayesian Optimization



Continuous

Correlated

Fixed-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 incorporates side info and practical flexibility
2. Performs competitively on benchmarks
- 3. Comes with theoretical guarantees**

Theoretical Guarantee and Empirical Validation

Theorem (No worse than stopping-immediately)

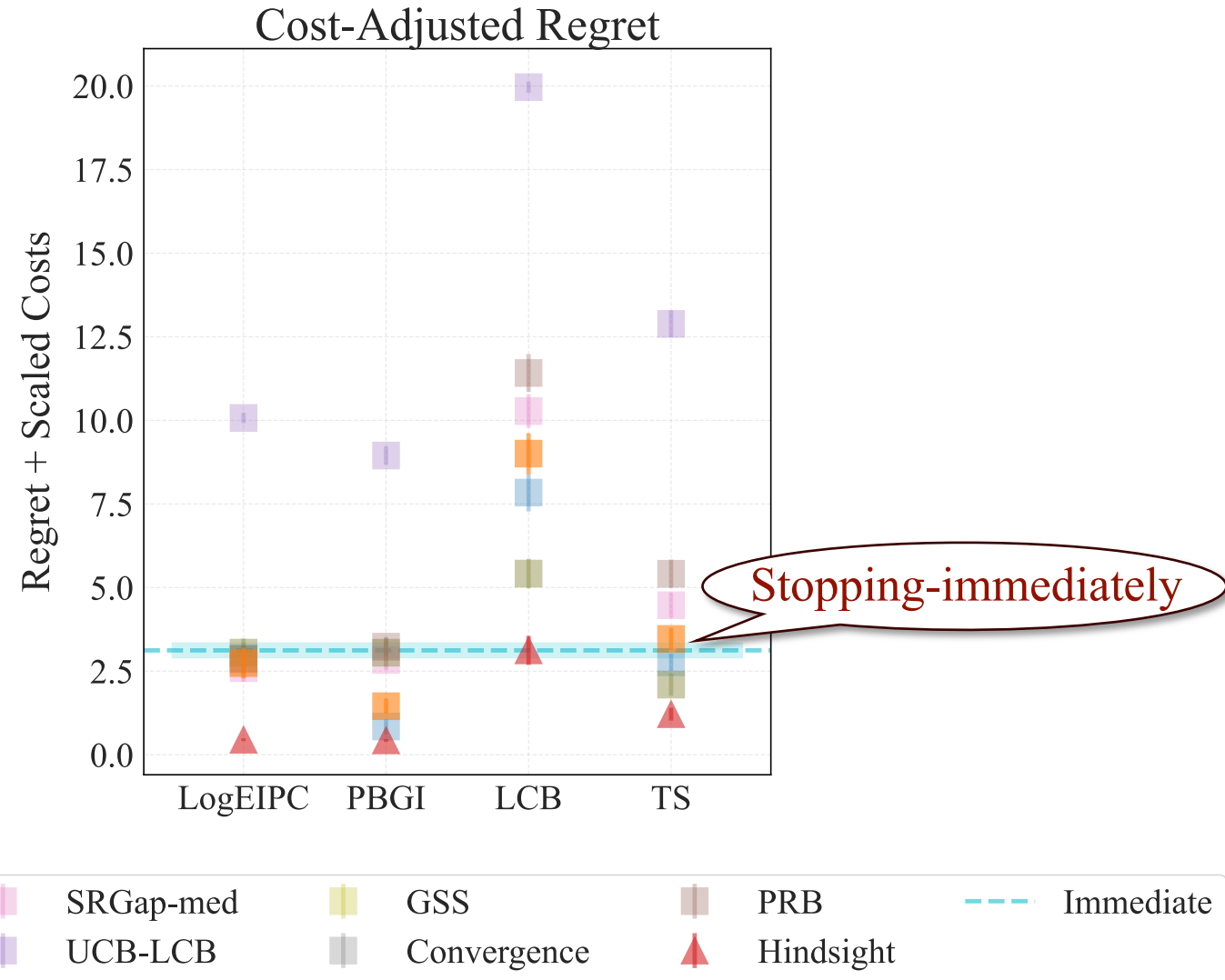
$$\mathbb{E}[R(\text{ours}; \text{PBGI})] \leq R[\text{stopping immediately}]$$

or LogEIPC

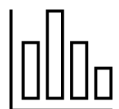
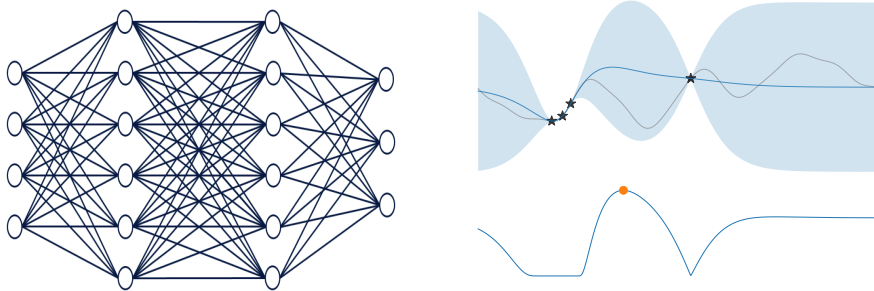
cost-adjusted regret

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

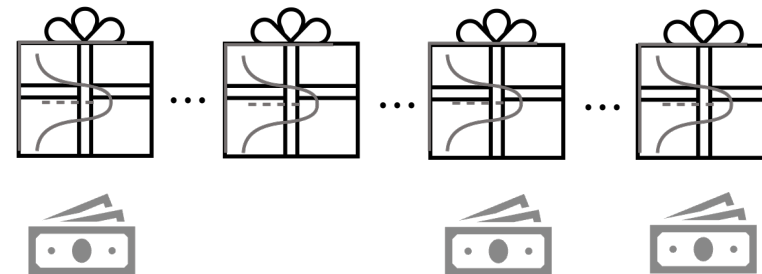


Varying evaluation costs



Adaptive stopping time

Key idea



Link to Pandora's Box problem
& Gittins index theory

Impact



BoTorch



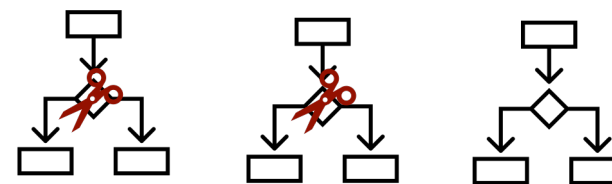
Ax

Competitive empirical performance &
interests from practitioners



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

Ongoing work

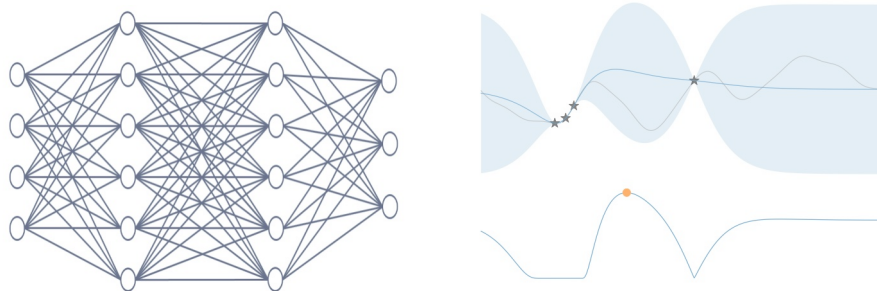


Sharper theoretical guarantees & black-
box optimization w/ multi-stage feedback



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

Studied problem

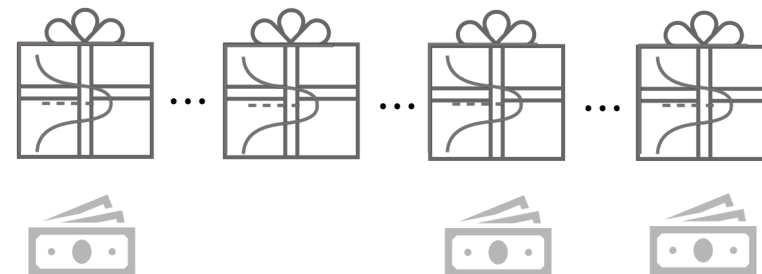


Varying evaluation costs



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Ongoing work



ChatGPT



Gemini



deepseek



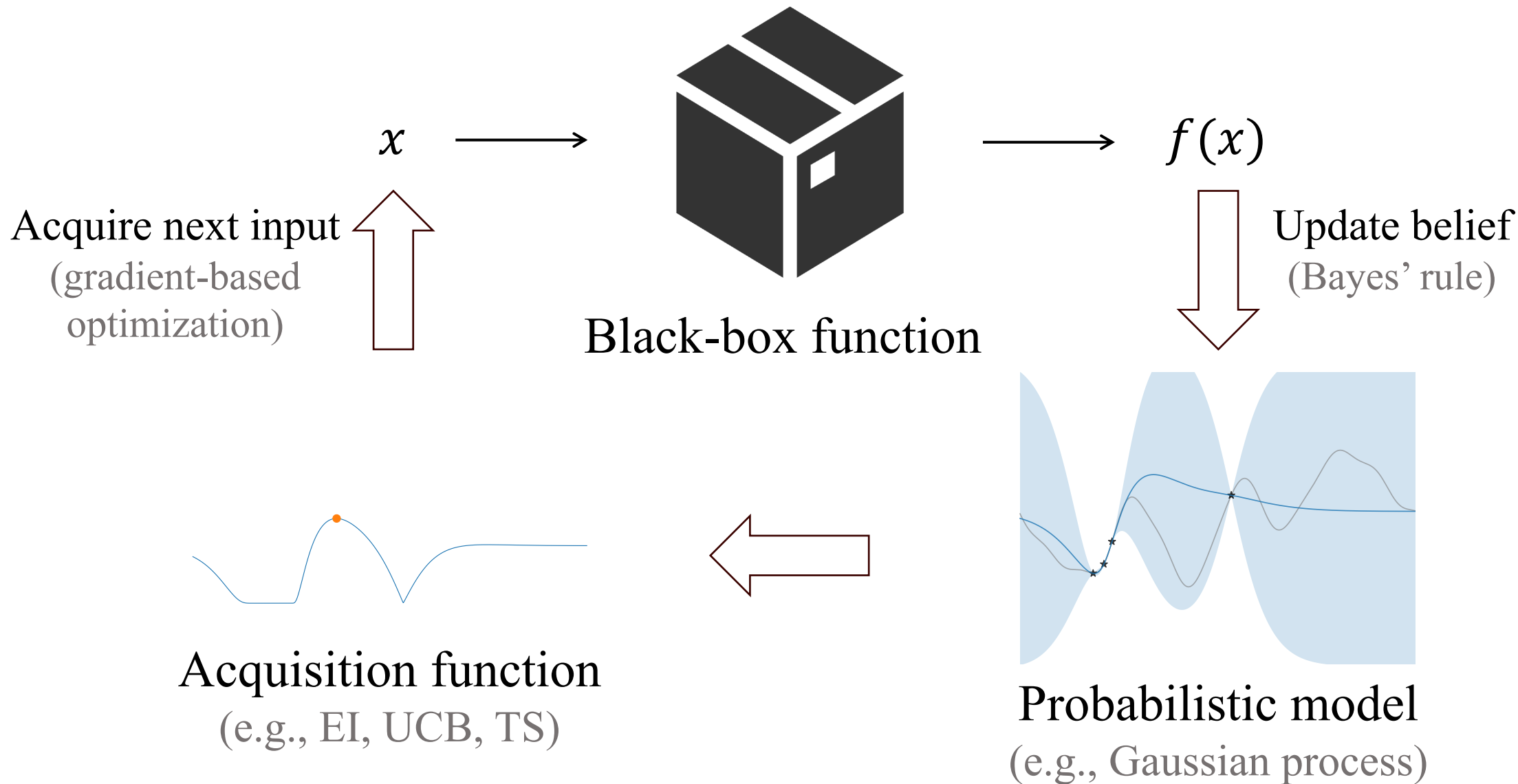
Claude

LLM-driven black-box optimization



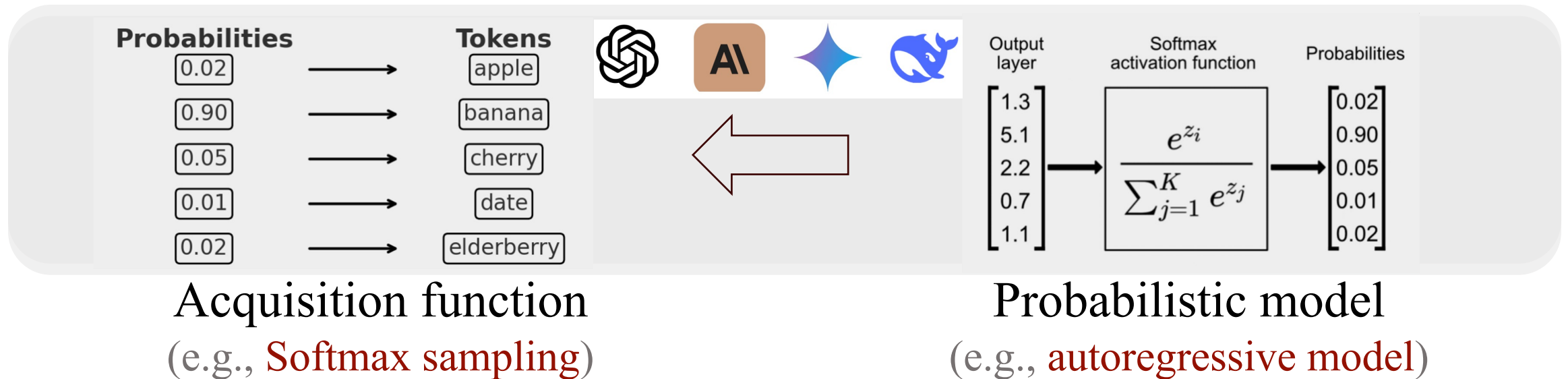
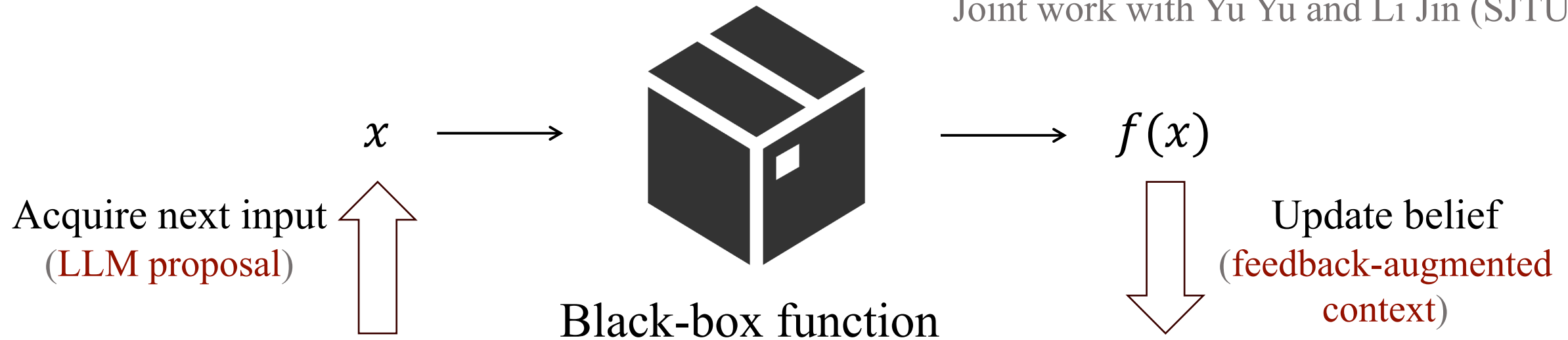
"Cost-aware Stopping for Bayesian
Optimization." Under review.

Recap: Bayesian Optimization



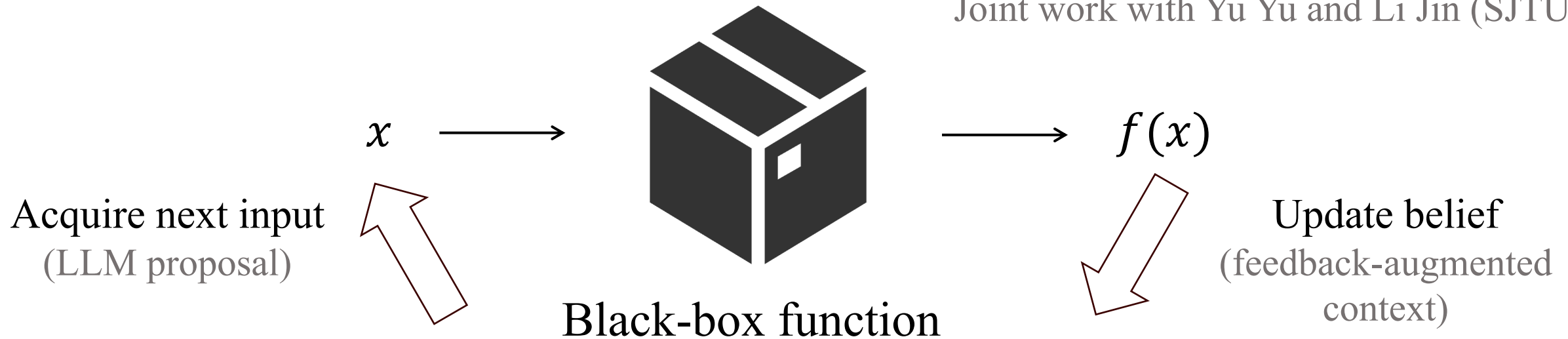
Ongoing: LLM-Driven Black-Box Optimization

Joint work with Yu Yu and Li Jin (SJTU)



Ongoing: LLM-Driven Black-Box Optimization

Joint work with Yu Yu and Li Jin (SJTU)



Large language model

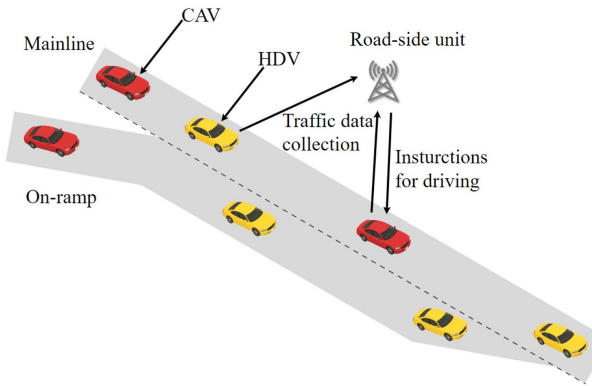
Ongoing: LLM-Driven Black-Box Optimization

Mixed-autonomy traffic control:

(e.g., Transformer config)

RL state representation

Acquire next input
(LLM proposal)



Joint work with Yu Yu and Li Jin (SJTU)

Average speed

Update belief
(feedback-augmented context)

Black-box function
(RL training & evaluation)



Large language model

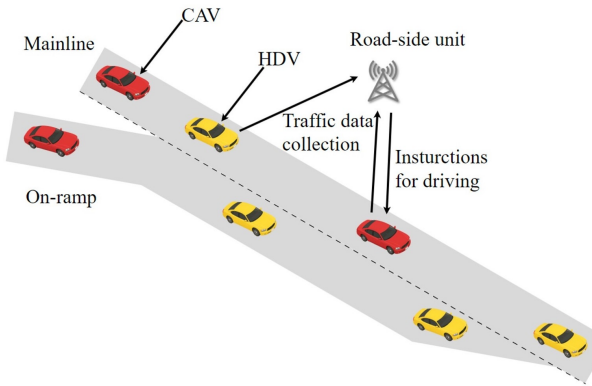
Ongoing: LLM-Driven Black-Box Optimization

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Black-box function
(RL training & evaluation)

Joint work with Yu Yu and Li Jin (SJTU)

Average speed

Update belief
(feedback-augmented context)

Can side info help?



Large language model

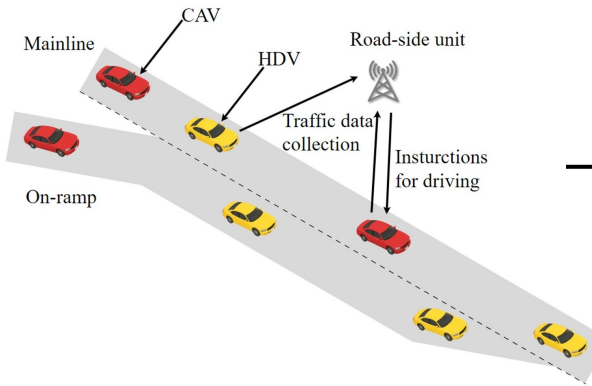
Our LLM-Driven Method: Incorporate Side Info

Mixed-autonomy traffic control:

(e.g., Transformer config)

RL state representation

Acquire next input
(LLM proposal)



Joint work with Yu Yu and Li Jin (SJTU)

Average speed

Black-box function
(RL training & evaluation)

Update belief
(feedback-augmented context)

performance metric +
representation quality



Large language model

Find our papers on arXiv!



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



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