

# Cost-Aware Bayesian Optimization with Adaptive Stopping via Gittins Indices

Qian Xie 谢倩 (Cornell ORIE)

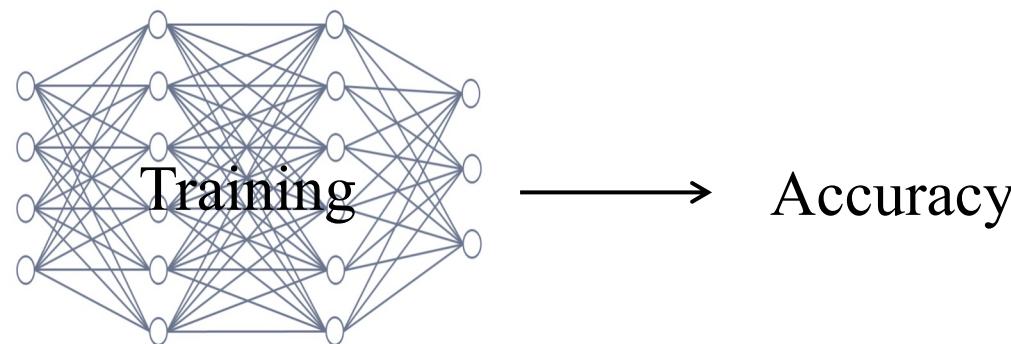
Joint work with Linda Cai (UC Berkeley), Theodore Brown (UCL), Raul Astudillo (MBZUAI), Peter Frazier, Alexander Terenin, and Ziv Scully (Cornell)

INFORMS Annual Meeting 2025 Job Market Showcase

# Optimization Under Uncertainty

ML model training:

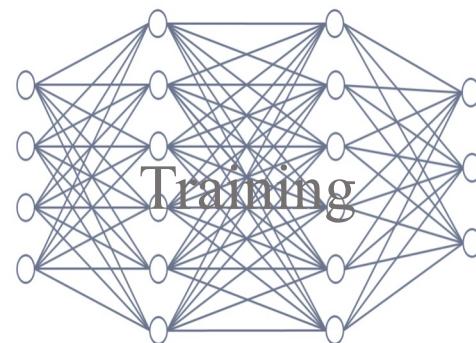
Training hyperparameters  
(e.g., learning rate, # layers)  $\longrightarrow$



# Optimization Under Uncertainty

ML model training:

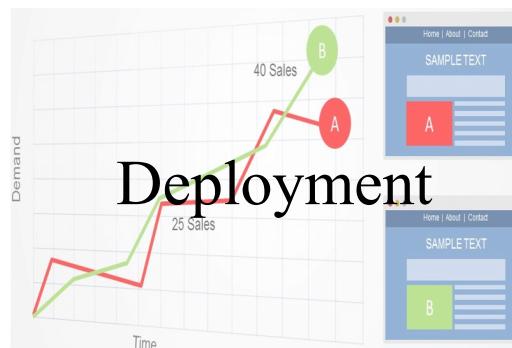
Training hyperparameters  
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Accuracy

Adaptive experimentation:

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

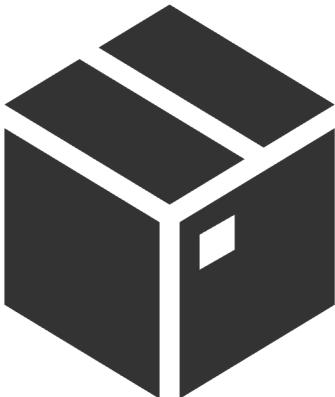


Revenue

# Optimization Under Uncertainty

Black-box optimization:

Input  $x$   $\longrightarrow$

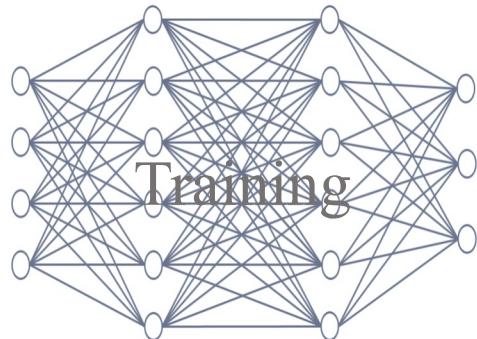


non-analytical &  
no gradient info

Performance metric  $f(x)$

ML model training:

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



Accuracy

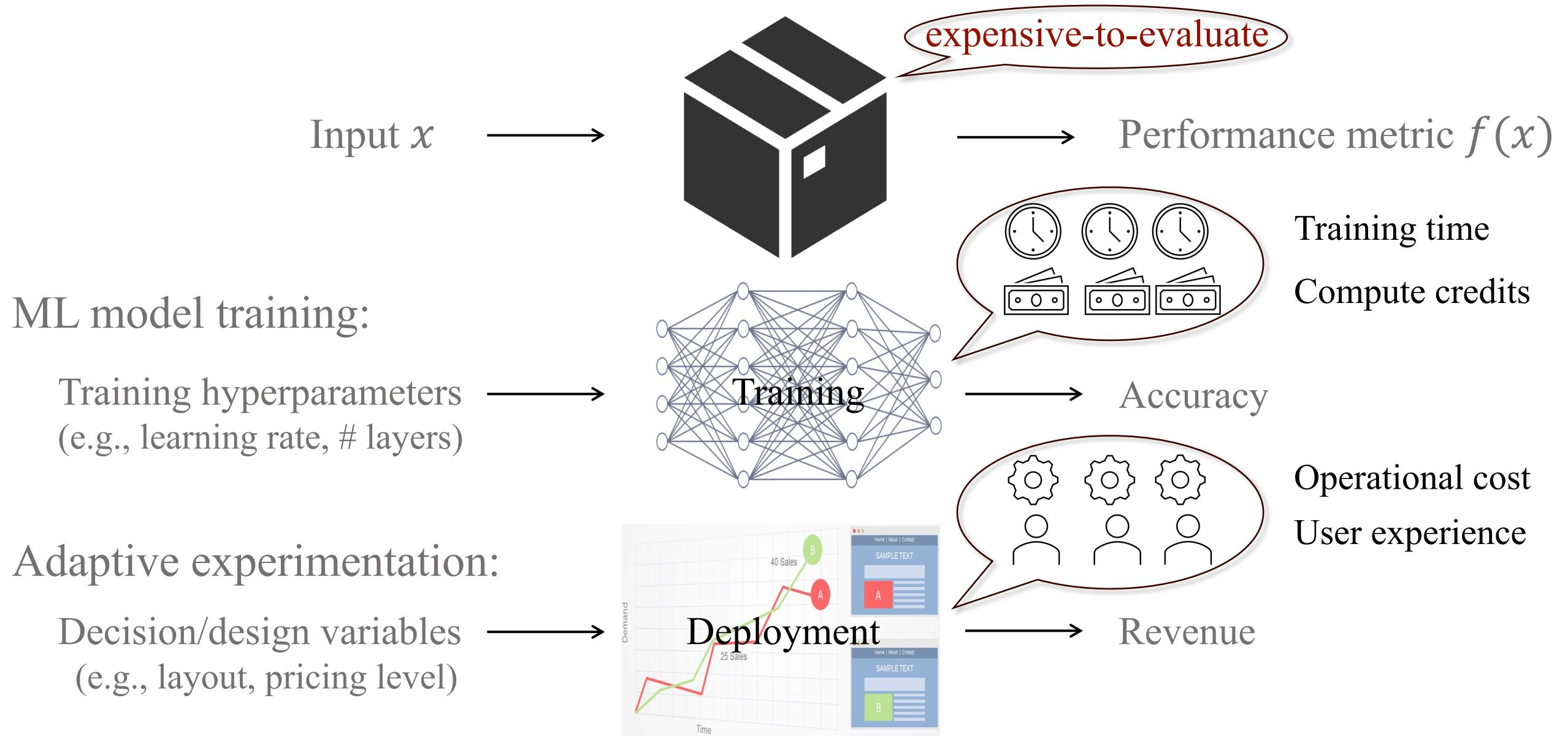
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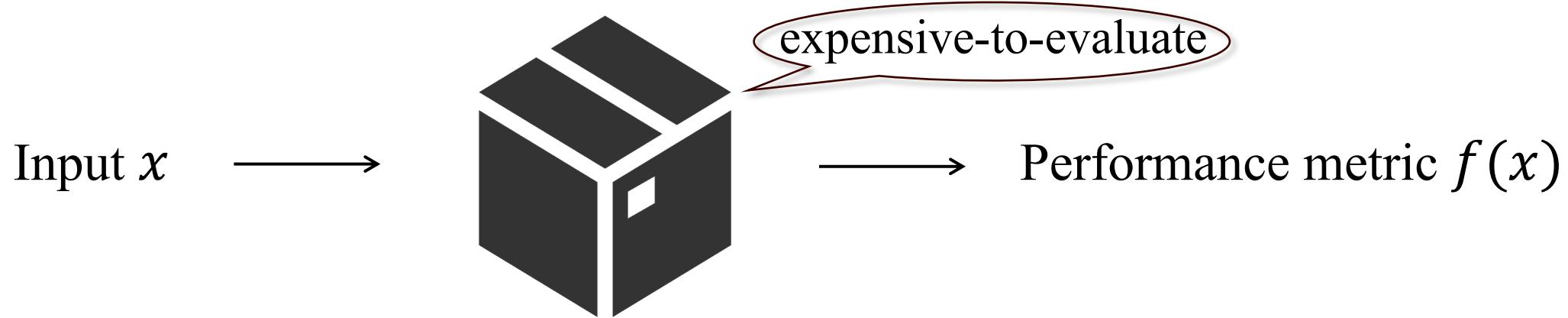


Revenue

# Black-Box Optimization



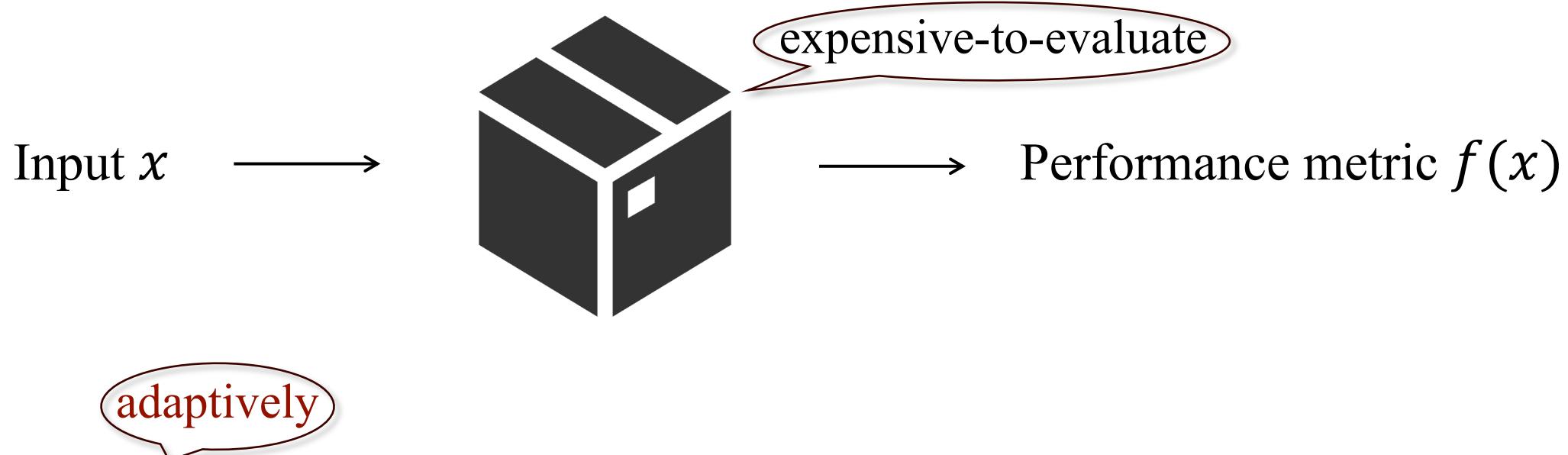
# Black-Box Optimization



**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

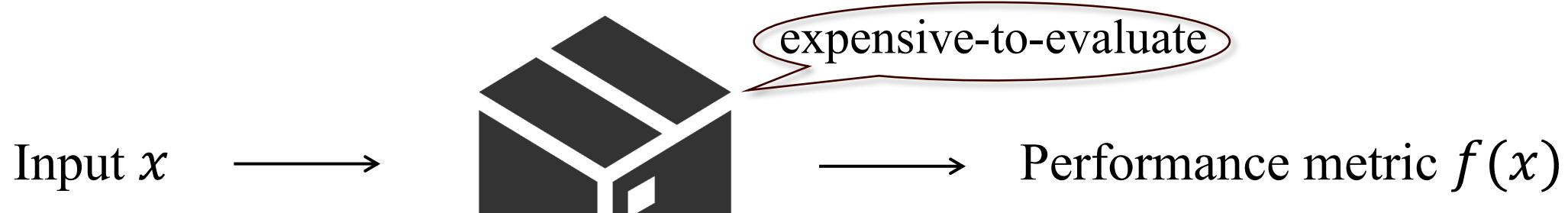


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Fewer #evaluations

# Data-Driven Black-Box Optimization



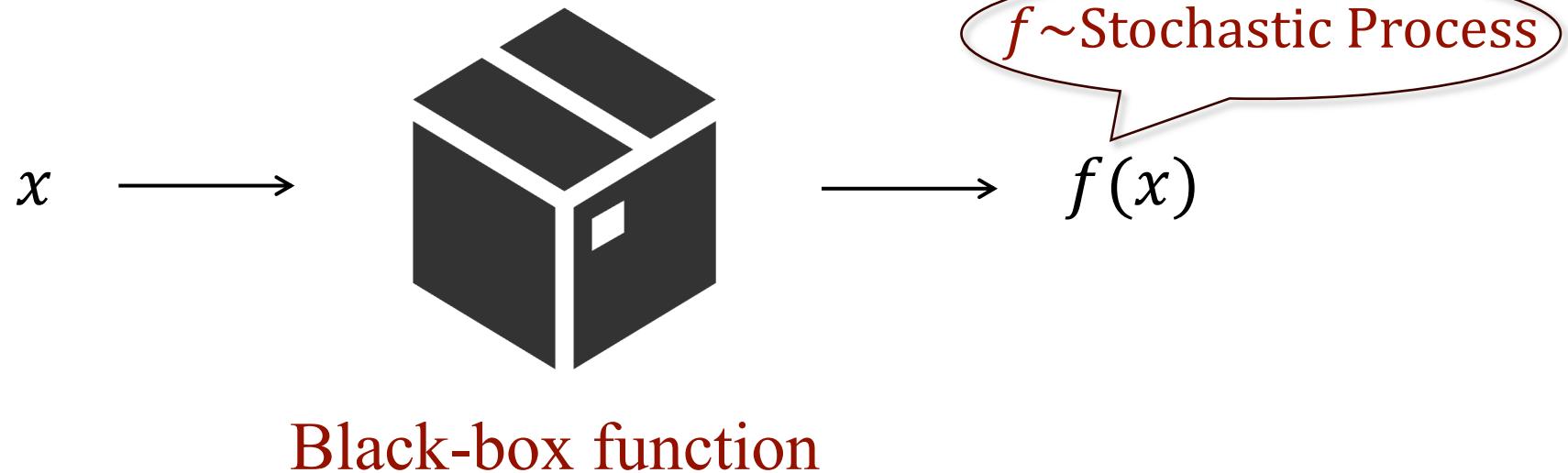
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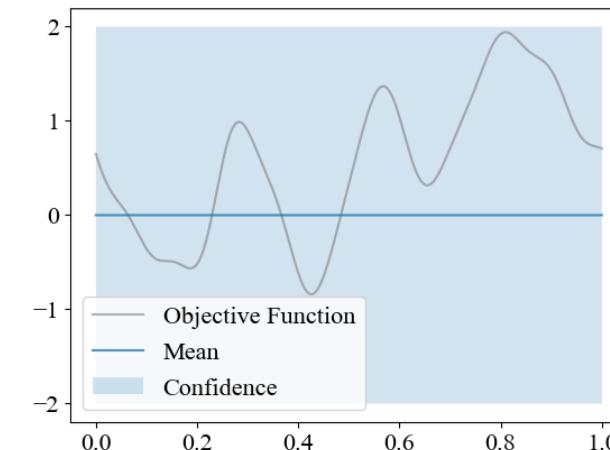
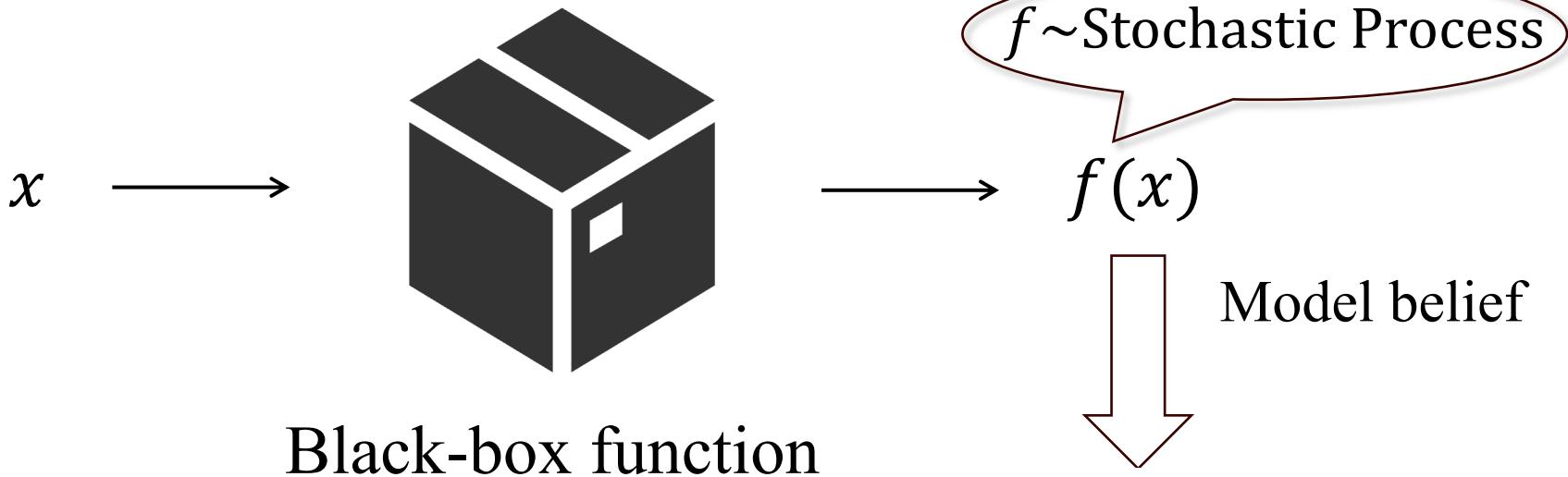
Efficient framework: Bayesian optimization

# Bayesian Optimization



# Bayesian Optimization

Time 0



Probabilistic model  
(e.g., Gaussian process)

# Bayesian Optimization

Time  $t$

$x_1, \dots, x_t$

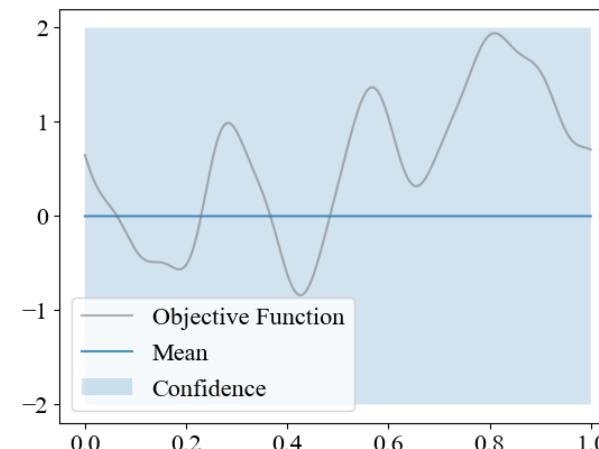


Black-box function

$f \sim \text{Stochastic Process}$

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

Model belief

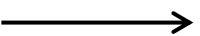


Probabilistic model  
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# Bayesian Optimization

Time  $t$

$x_1, \dots, x_t$

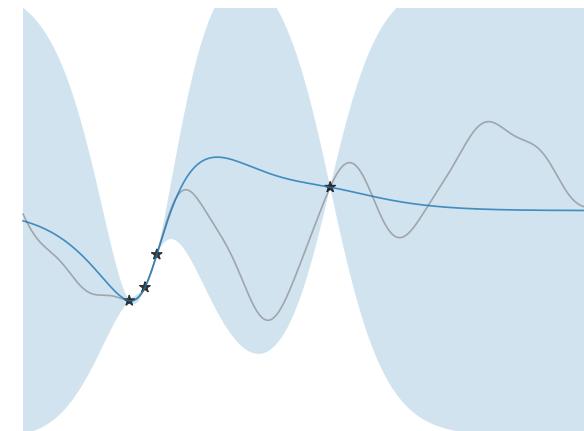


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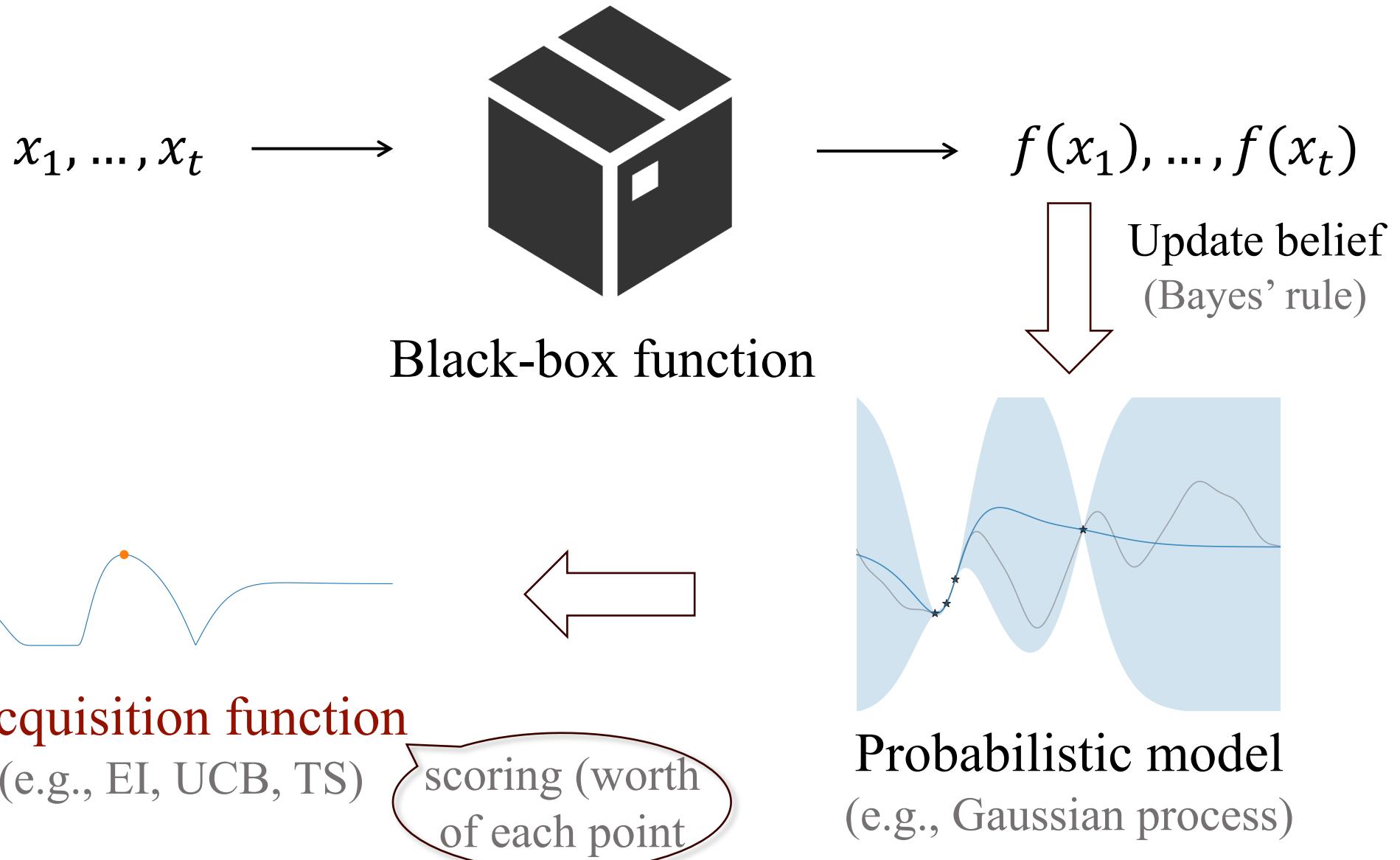
Update belief  
(Bayes' rule)



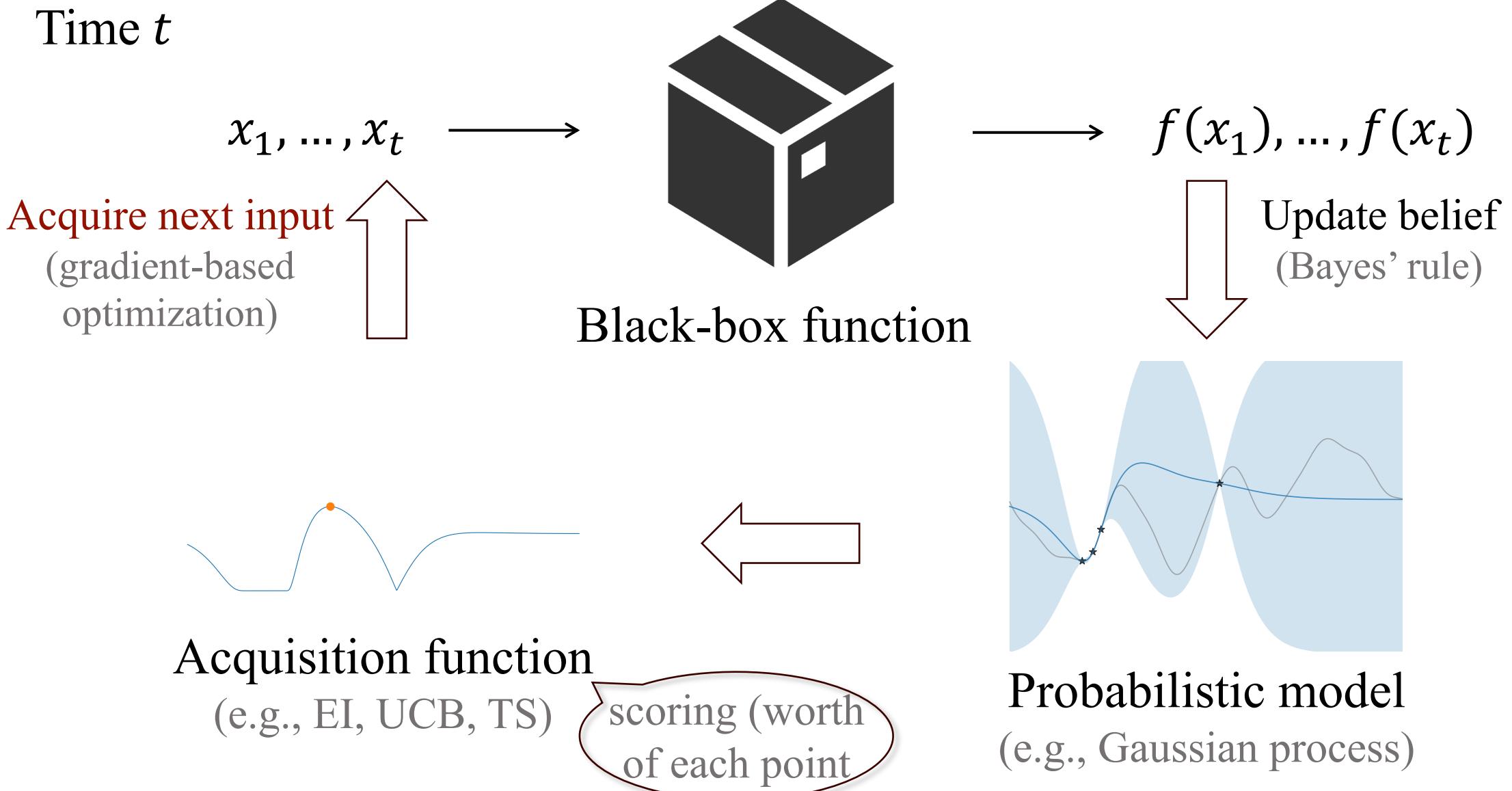
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# Bayesian Optimization

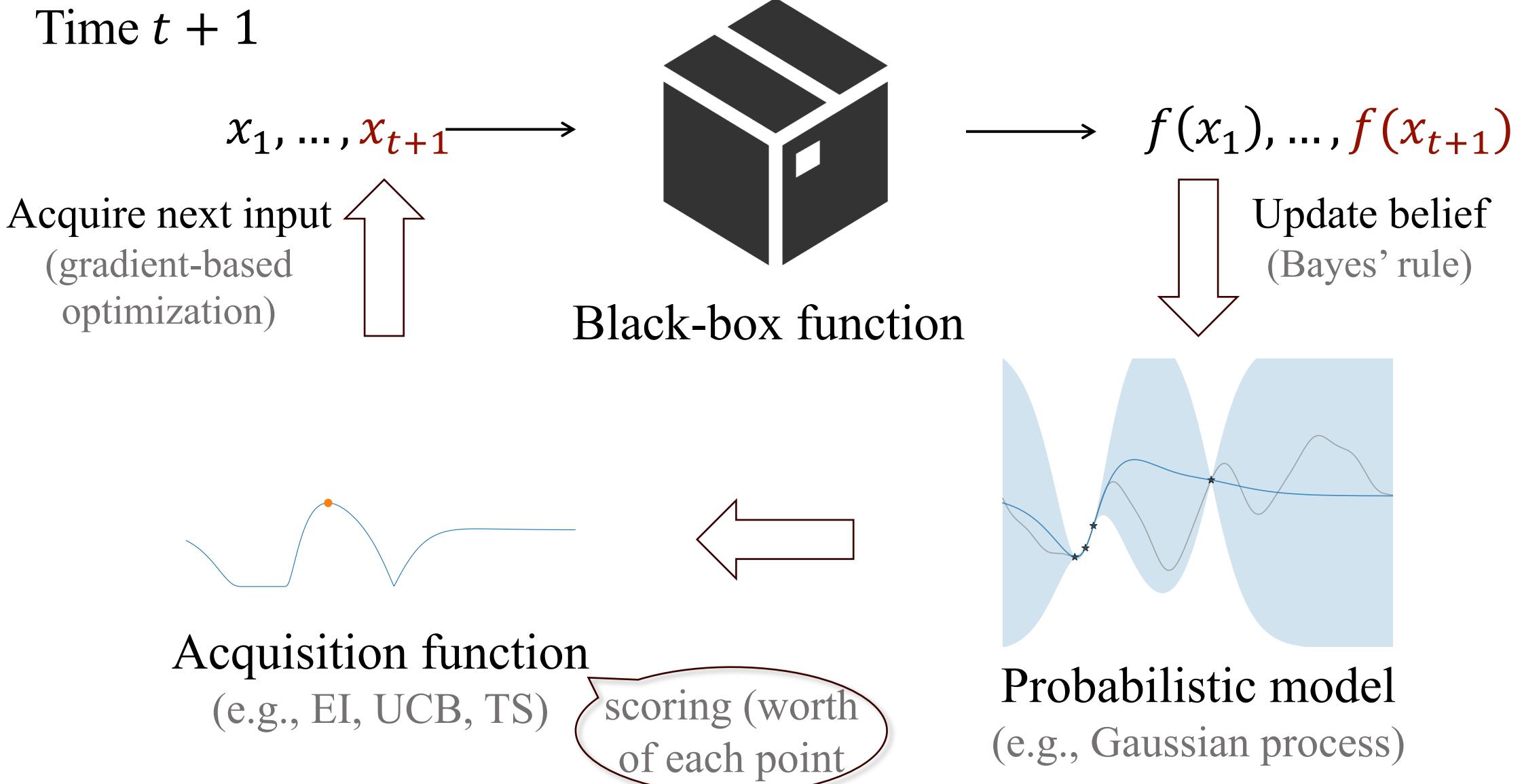
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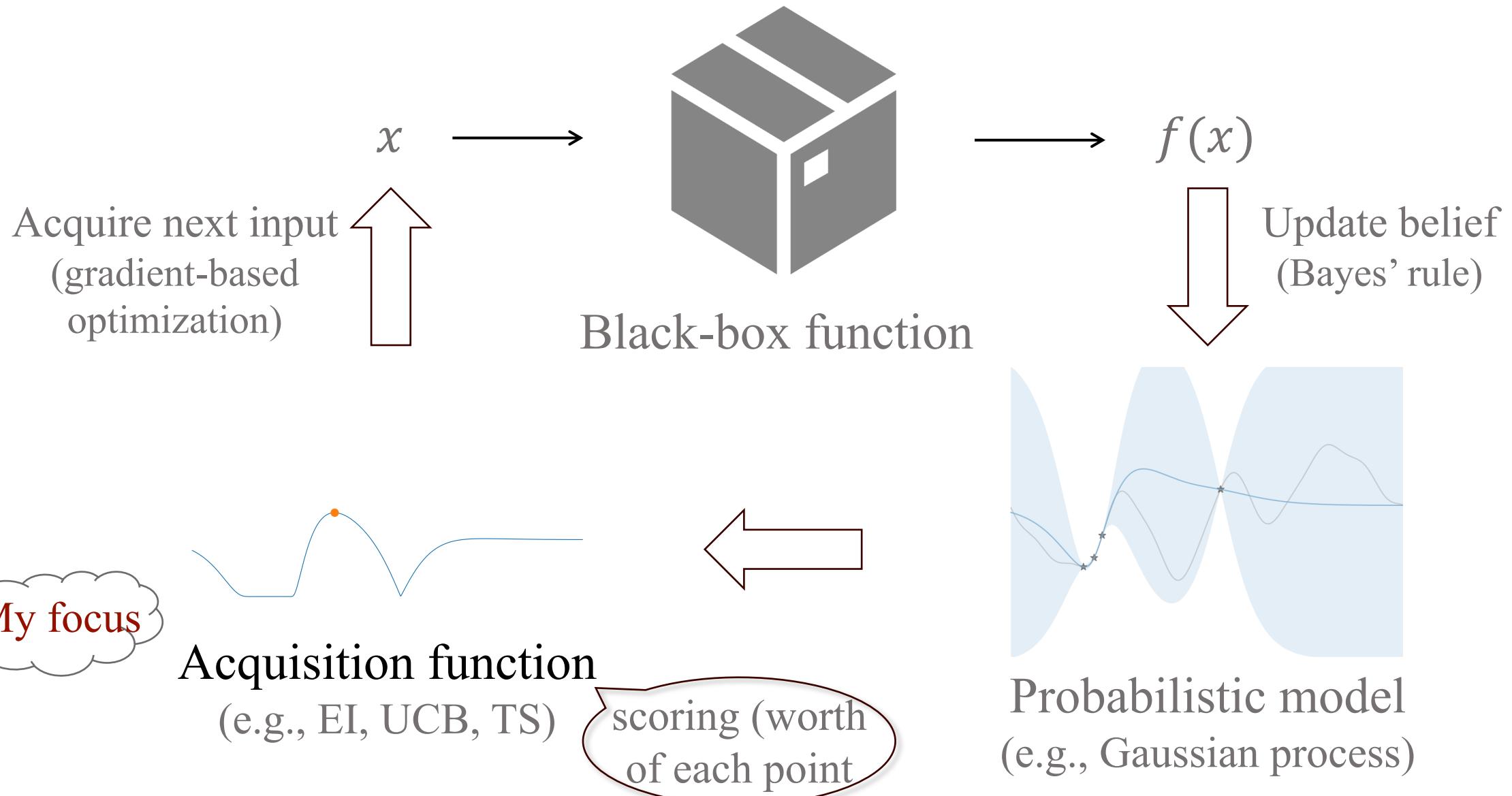
# Bayesian Optimization



# 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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- **Gittins Index**

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? Why another principle?

# Our Contribution: Gittins Index Principle

- Improvement-based (e.g., EI)
- Entropy-based
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- Gittins Index



Why another principle?

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

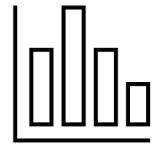
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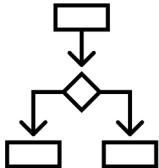
# Under-explored Side Info and Flexibility



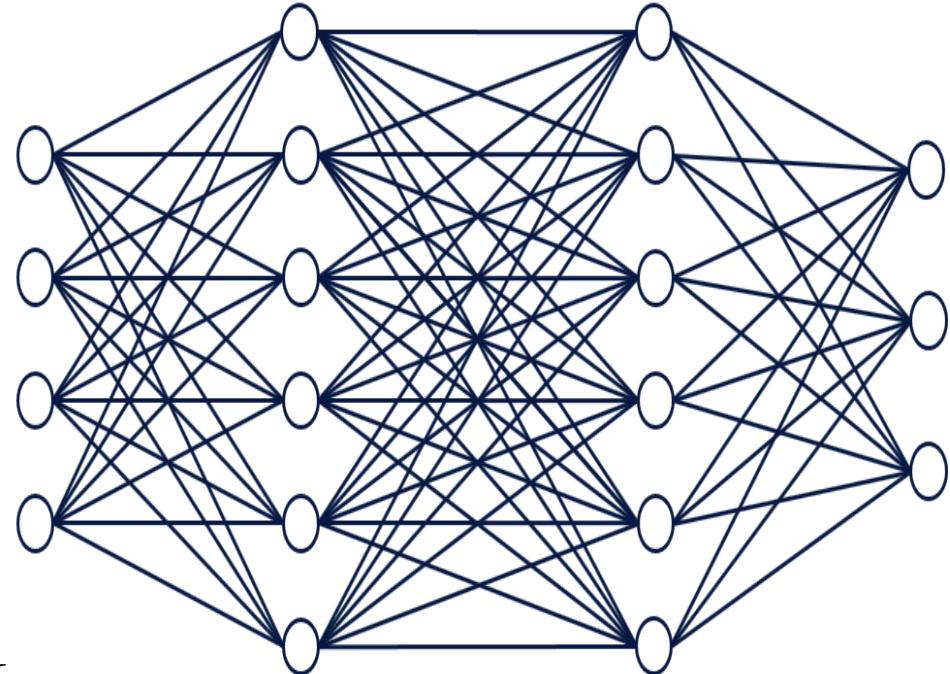
Varying evaluation costs



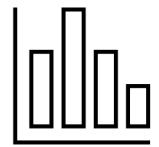
Smart stopping time



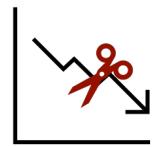
Observable multi-stage feedback



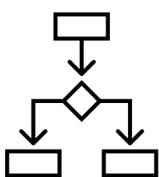
# How does existing principle incorporate them?



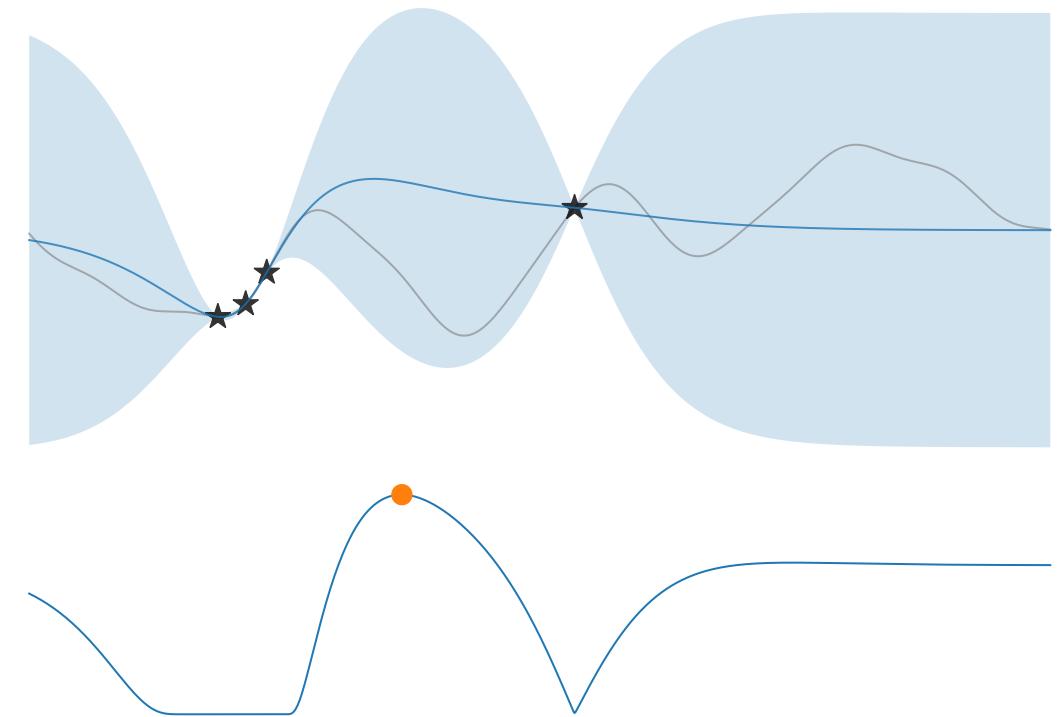
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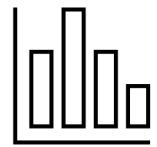


Observable multi-stage feedback



Expected improvement  $EI(x)$

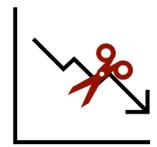
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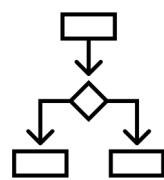
Varying evaluation costs

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

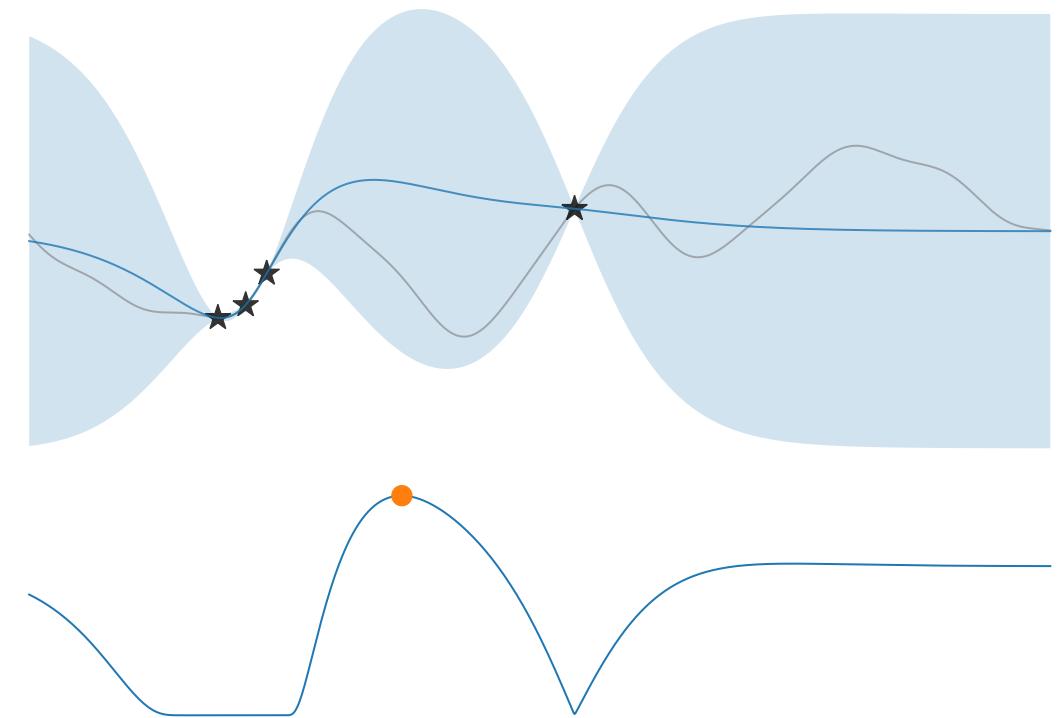
Why divide?



Smart stopping time



Observable multi-stage feedback



Expected improvement  $EI(x)$

# How does existing principle incorporate them?



Varying evaluation costs

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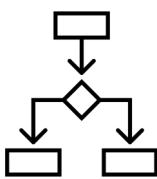
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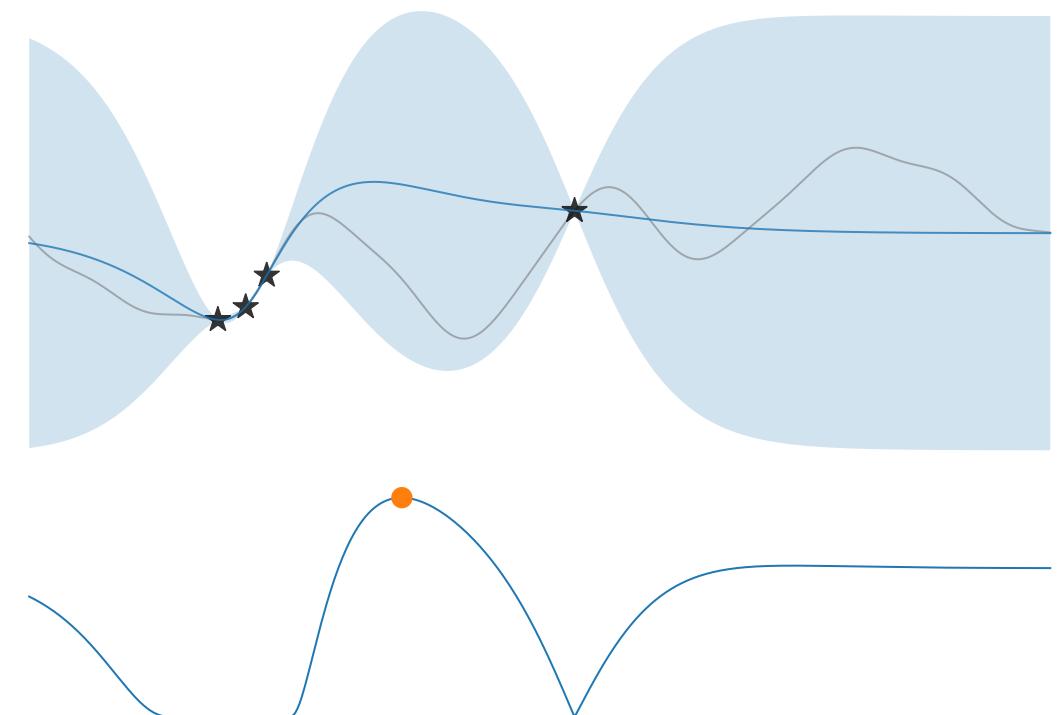
Smart stopping time

$$\text{EI}(x) \leq \theta$$

Which threshold?



Observable multi-stage feedback



Expected improvement  $\text{EI}(x)$

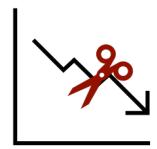
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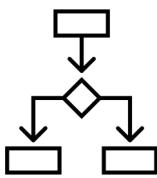
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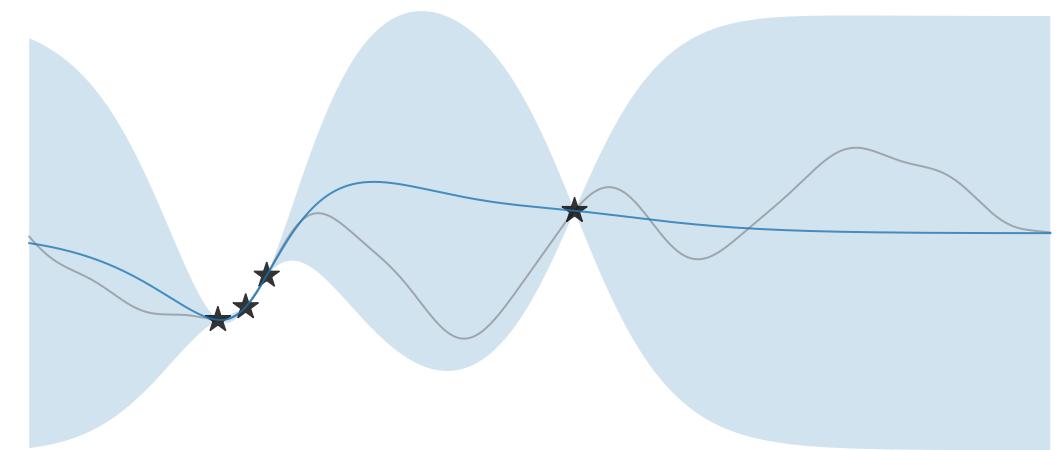
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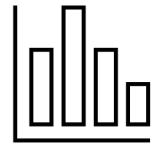
Observable multi-stage feedback

?



Expected improvement  $EI(x)$

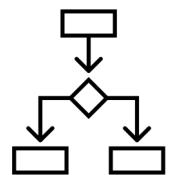
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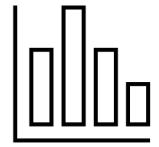
Smart stopping time



Observable multi-stage feedback

New design principle:  
**Gittins index**

# Why Gittins index?

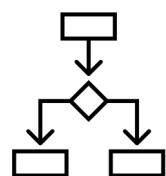


Varying evaluation costs

New design principle:  
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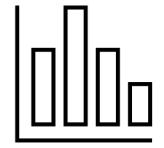


Smart stopping time

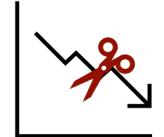


Observable multi-stage feedback

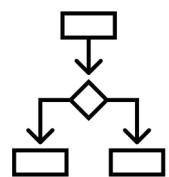
# Why Gittins index?



Varying evaluation costs



Smart stopping time



Observable multi-stage feedback

New design principle:  
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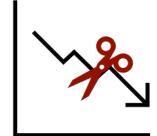
**Optimal** in related sequential  
decision problems

# Why Gittins index?



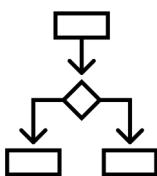
Varying evaluation costs

Features in **Pandora's box**



Smart stopping time

Features in **Pandora's box**



Observable multi-stage feedback

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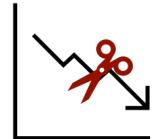
# Why Gittins index?



Varying evaluation costs

Features in Pandora's box

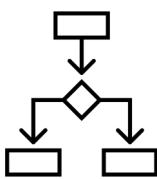
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Observable multi-stage feedback

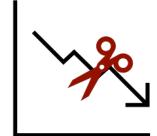
Features in **Markovian bandits**

# What is Pandora's Box?



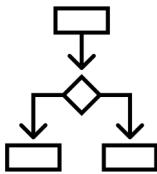
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Smart stopping time

Features in **Pandora's box**



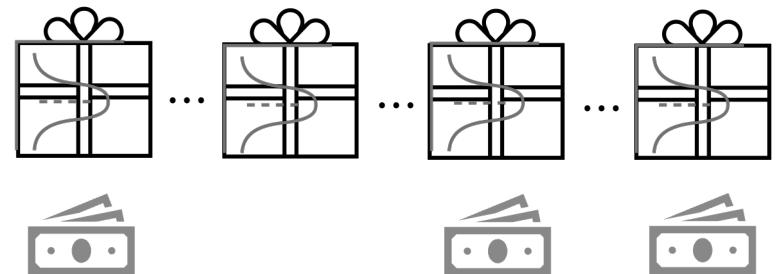
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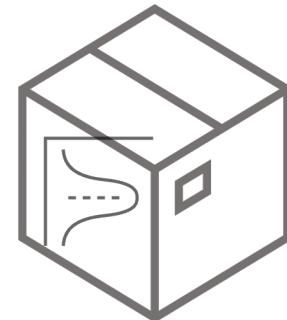
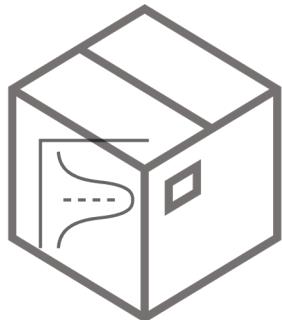
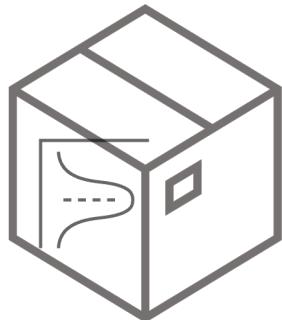
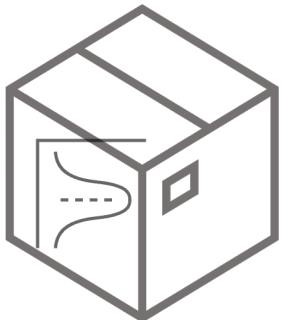


New design principle:  
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Optimal in related sequential  
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# Pandora's Box



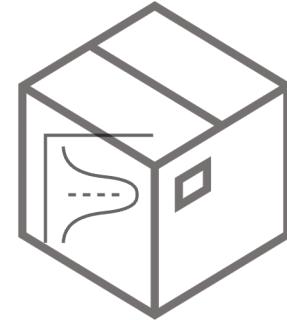
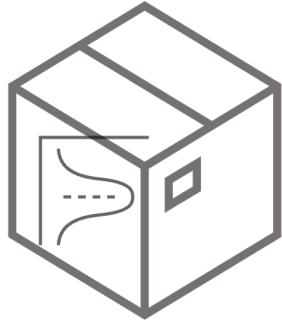
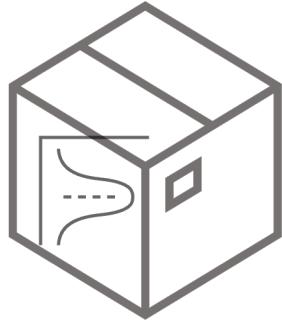
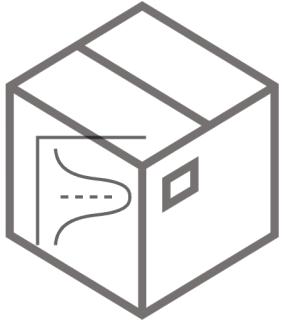
**High-level goal:** Choose box  $x_1, \dots, x_T$  to open to maximize the expected utility

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

Flexible stopping time

# Pandora's Box

$t = 0$

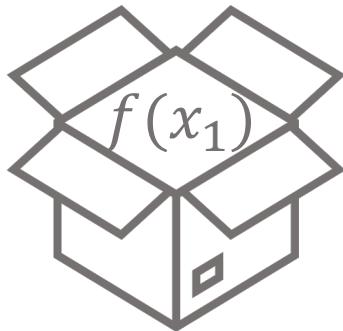


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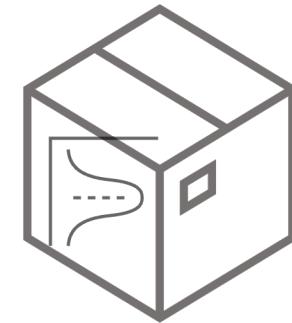
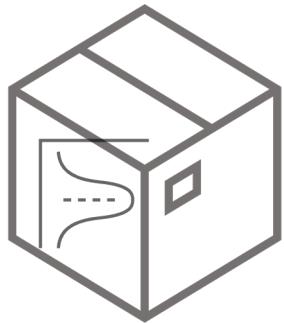
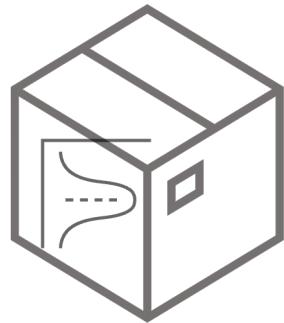
$$\mathbb{E} \max_{t=1,2,\dots,T} f(x_t) - \mathbb{E} \sum_{t=1}^T c(x_t)$$

# Pandora's Box

$t = 1$



$c(x_1)$

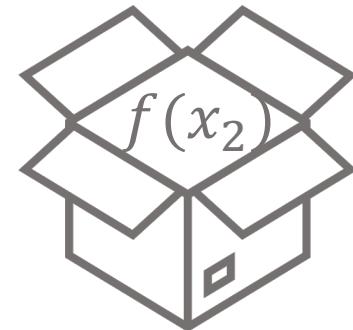
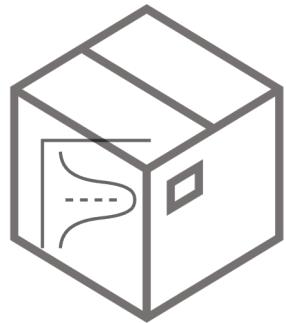
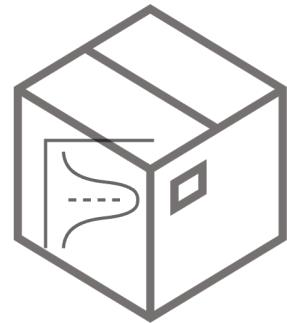
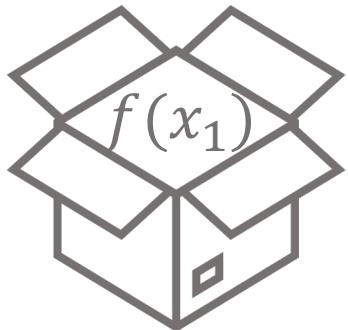


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# Pandora's Box

$t = 2$

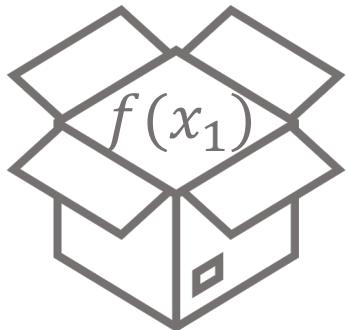


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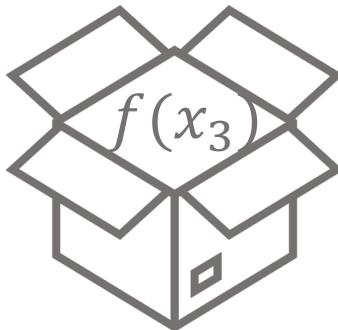
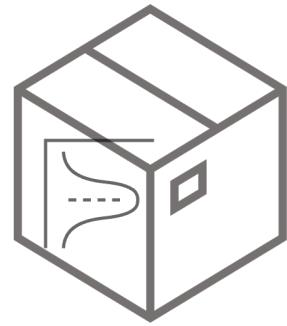
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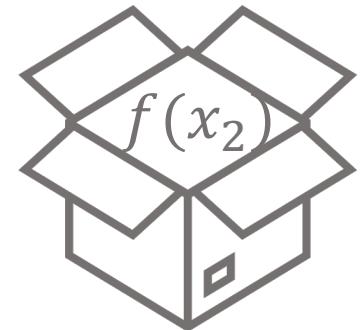
$t = 3$



$c(x_1)$



$c(x_3)$



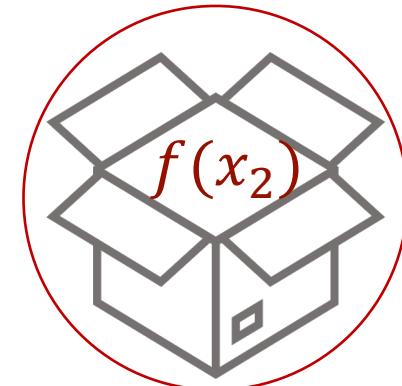
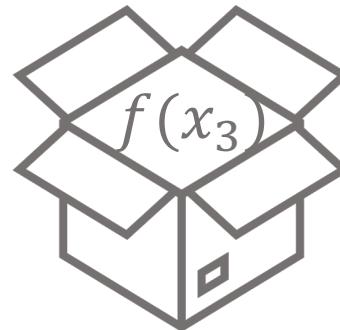
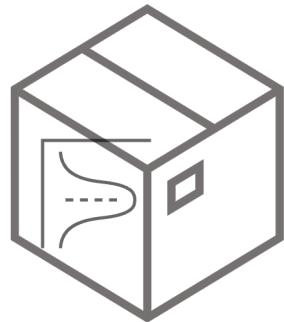
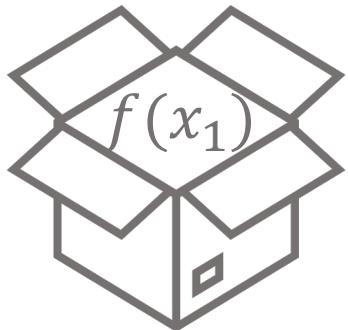
$c(x_2)$

**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

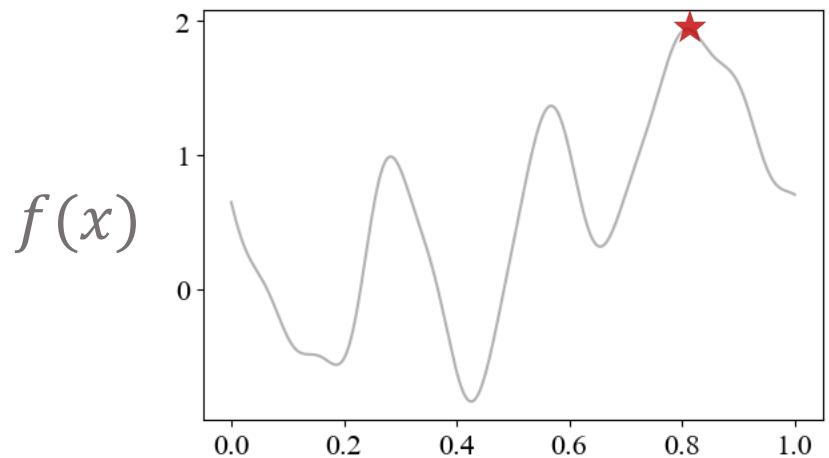
$t = T$ , stop



**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

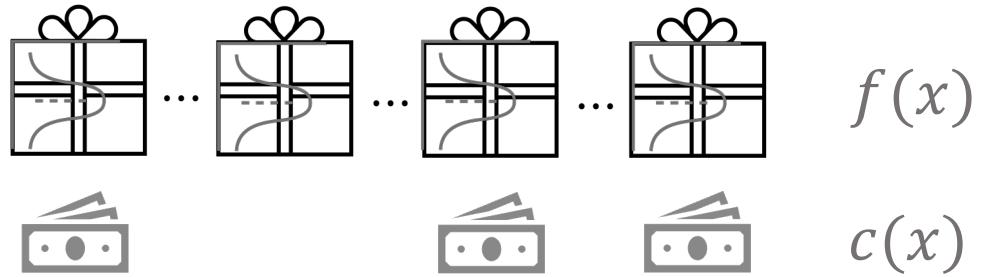
Fixed-iteration

Expected best-observed value

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

# Pandora's Box

[Weitzman'79]



Discrete

Independent

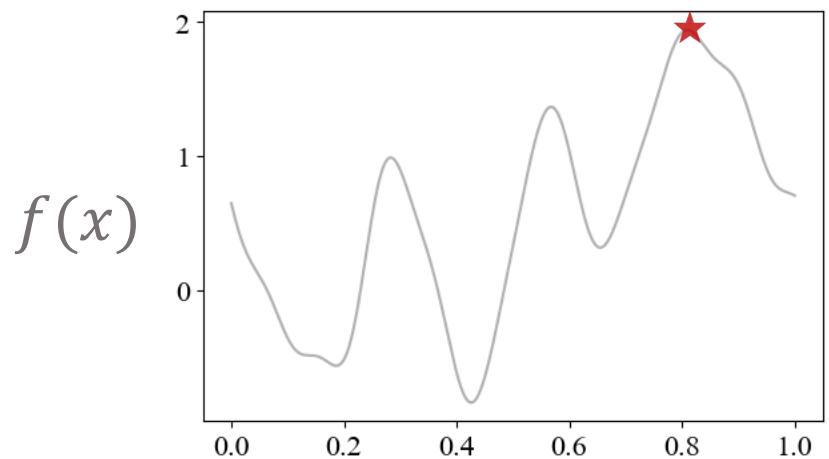
Flexible-stopping

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

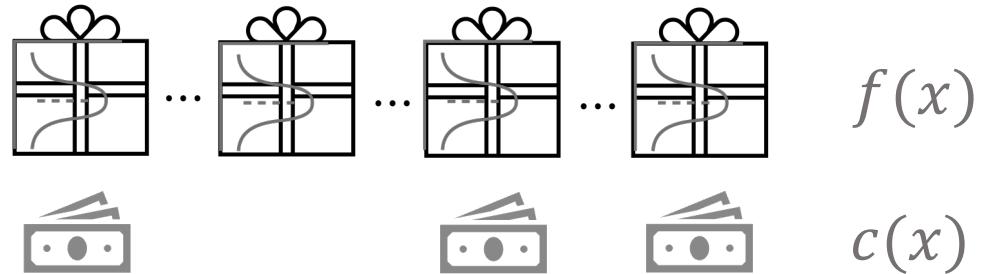
Fixed-iteration

Expected best-observed value

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

# Pandora's Box

[Weitzman'79]



Discrete

Independent

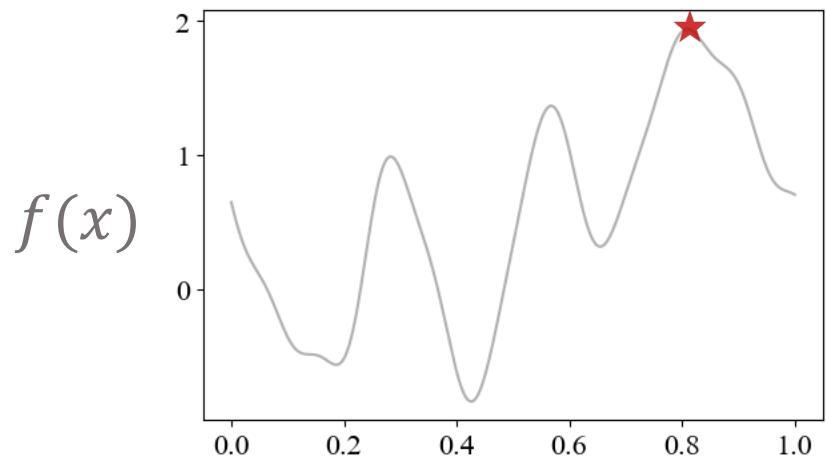
Flexible-stopping

Expected utility

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

A red oval highlights the term  $\sum_{t=1}^T c(x_t)$  in the equation, with an arrow pointing to it from the text "cumulative cost" in the adjacent column.

# Bayesian Optimization



Continuous

Correlated

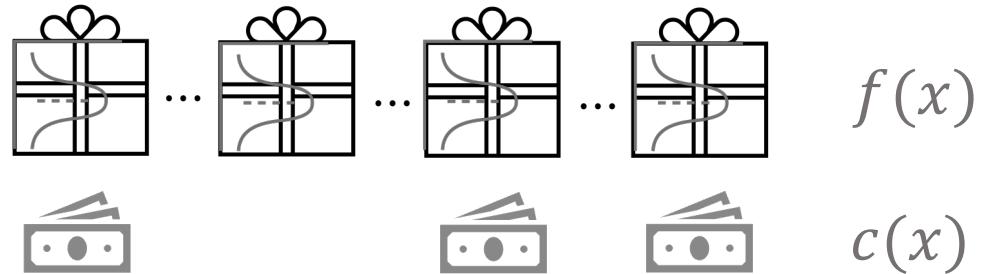
Fixed-iteration

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

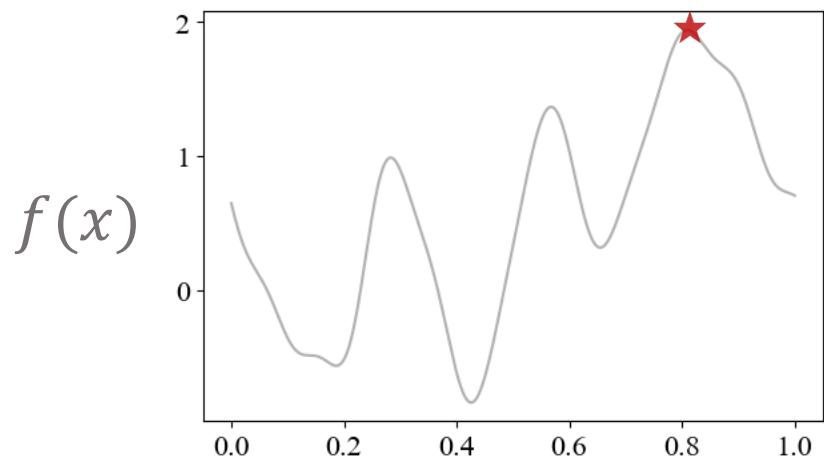
Flexible-stopping

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

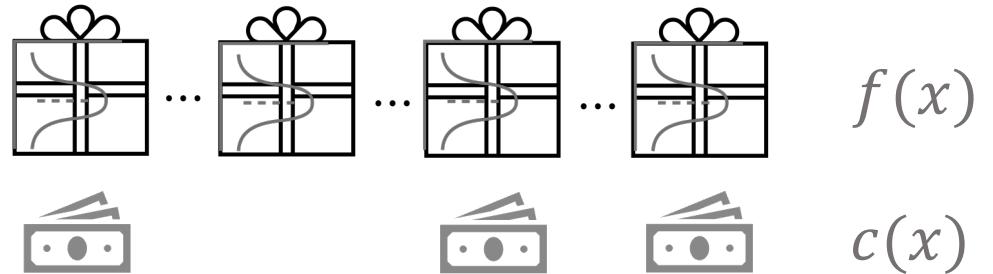
Fixed-iteration

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

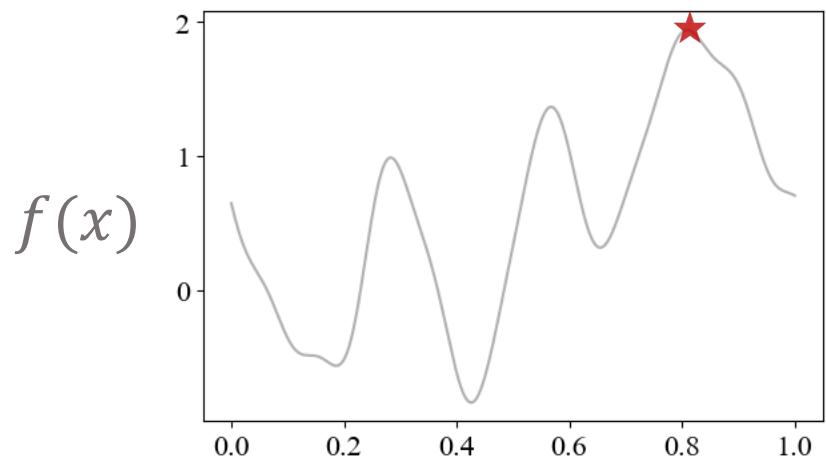
Flexible-stopping

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

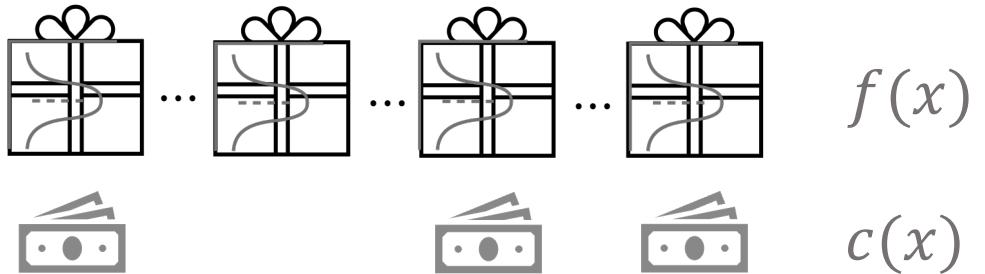
Correlated

Fixed-budget / Flexible-stopping

Expected (cost-adjusted) regret

# Pandora's Box

[Weitzman'79]



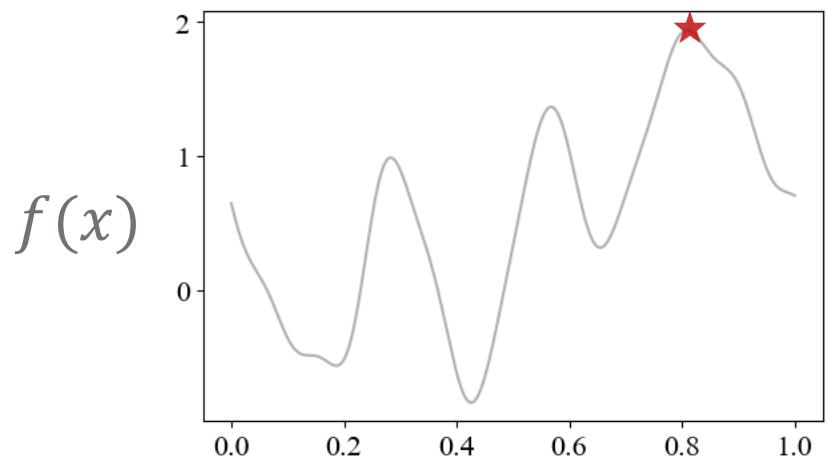
Discrete

Independent

Flexible-stopping

Expected cost-adjusted regret

# Bayesian Optimization



Continuous

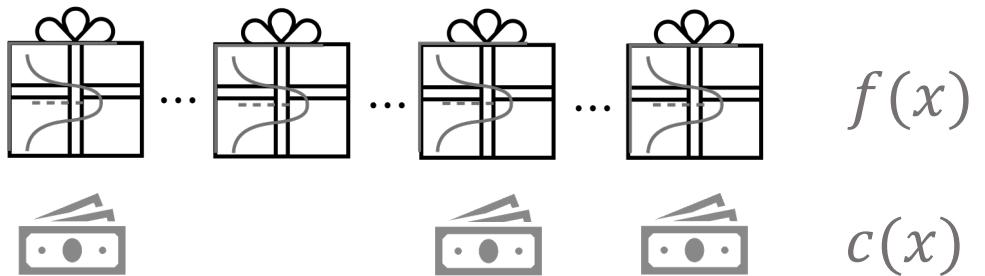
Correlated

Fixed-budget / Flexible-stopping

Expected (cost-adjusted) regret

# Pandora's Box

[Weitzman'79]



Discrete

Independent

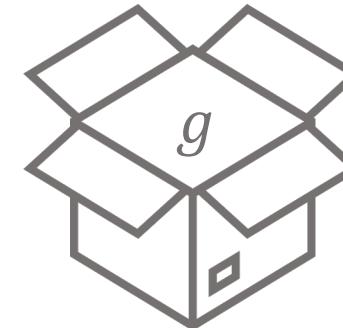
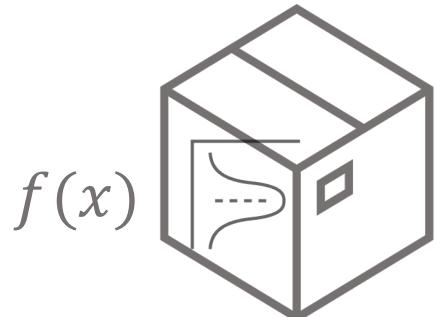
Flexible-stopping

Expected cost-adjusted regret

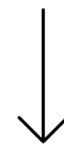
Optimal policy: Gittins index

# Optimal Policy: Gittins Index

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



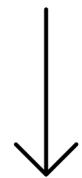
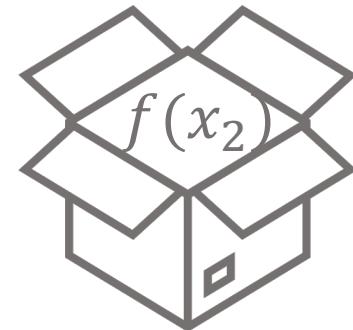
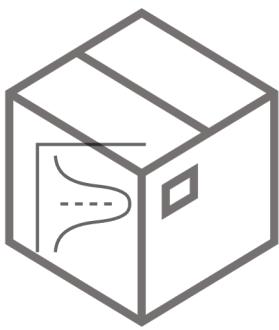
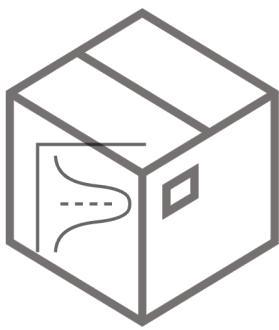
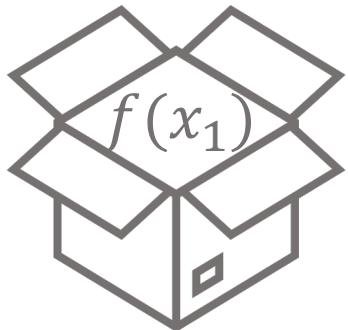
$$\text{GI}_f(x; c(x))$$



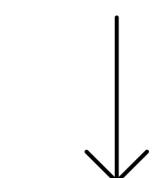
$$g$$

# Optimal Policy: Gittins Index

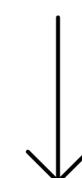
Step 2: Open the box with highest index if it is closed



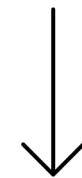
$$f(x_1)$$



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



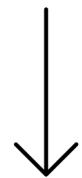
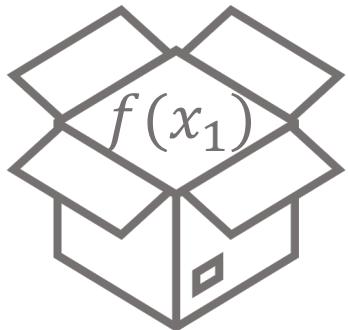
$$\text{GI}_f(x'; c(x'))$$



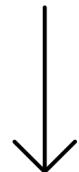
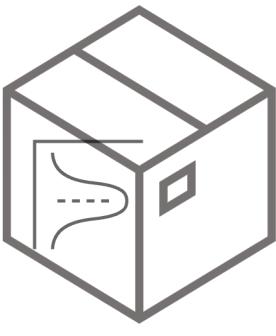
$$f(x_2)$$

# Optimal Policy: Gittins Index

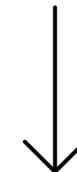
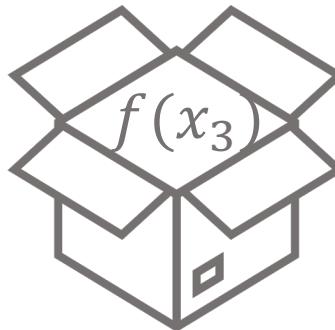
Step 2': **Select** the box with highest index if it is opened and **stop**



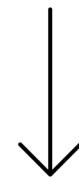
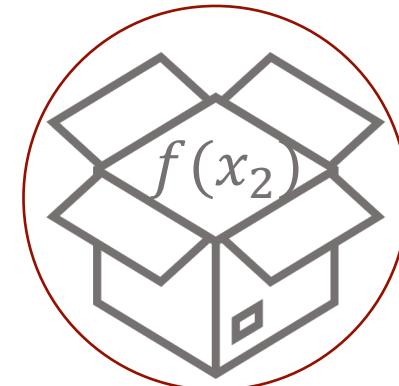
$$f(x_1)$$



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

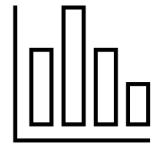


$$f(x_3)$$

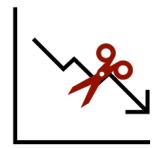


$$f(x_2)$$

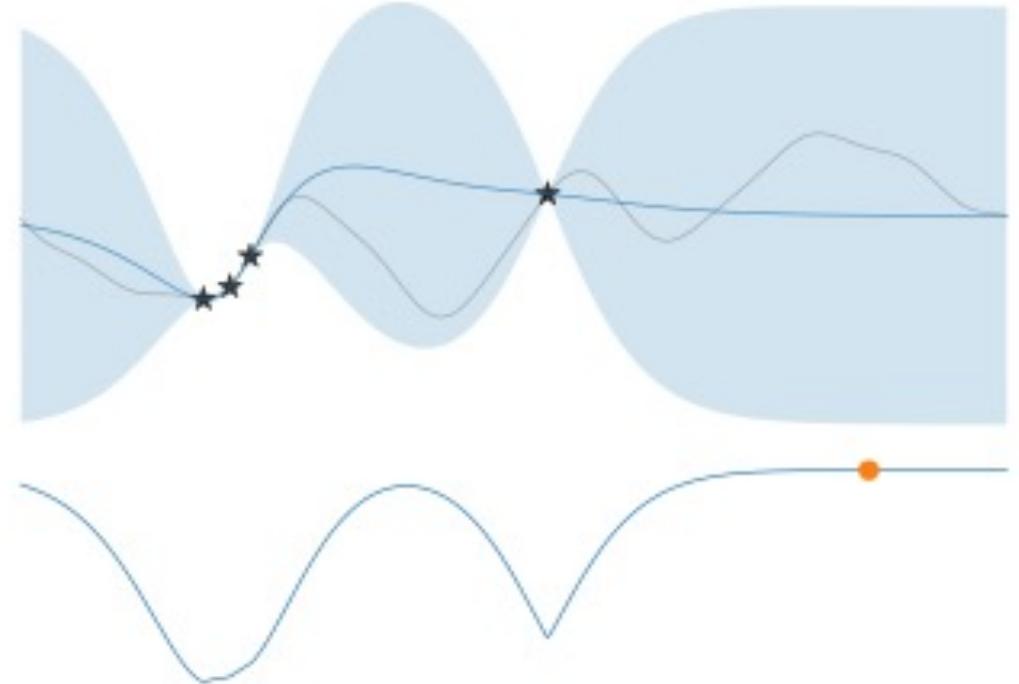
# Optimal Policy: Gittins Index



Varying evaluation costs  
 $GI(x; c(x))$

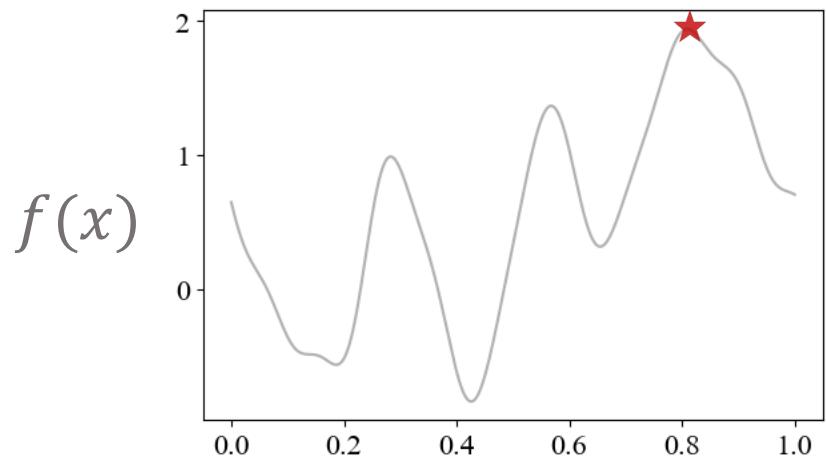


Smart stopping time  
 $\max_x GI(x; c(x)) \leq \max_x f(x)$



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

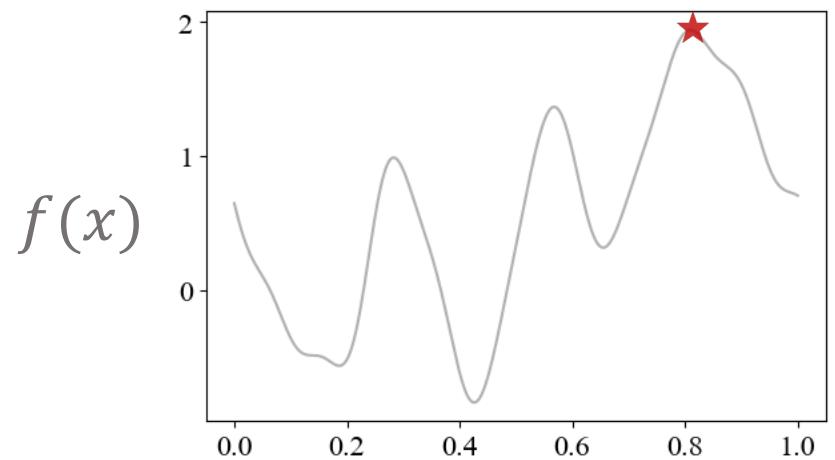
Independent

Flexible-stopping

Expected cost-adjusted regret

Gittins index is optimal

# Bayesian Optimization



Continuous

Correlated

Fixed-budget / Flexible-stopping

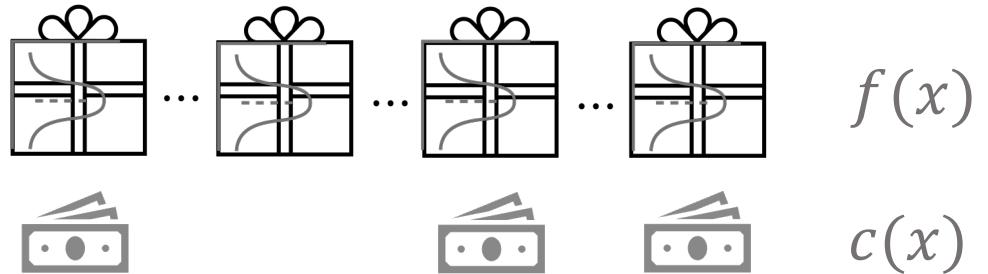
Expected (cost-adjusted) regret

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

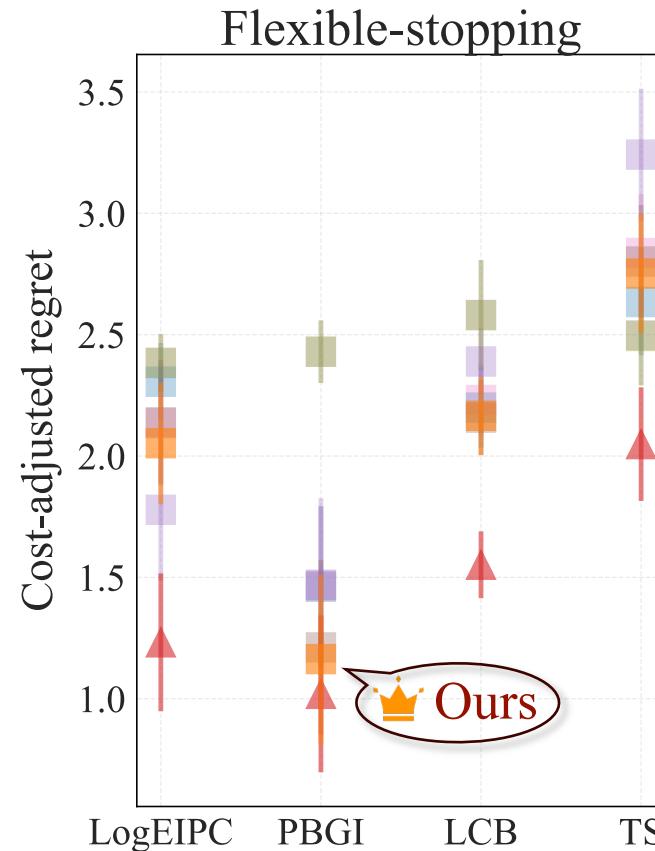
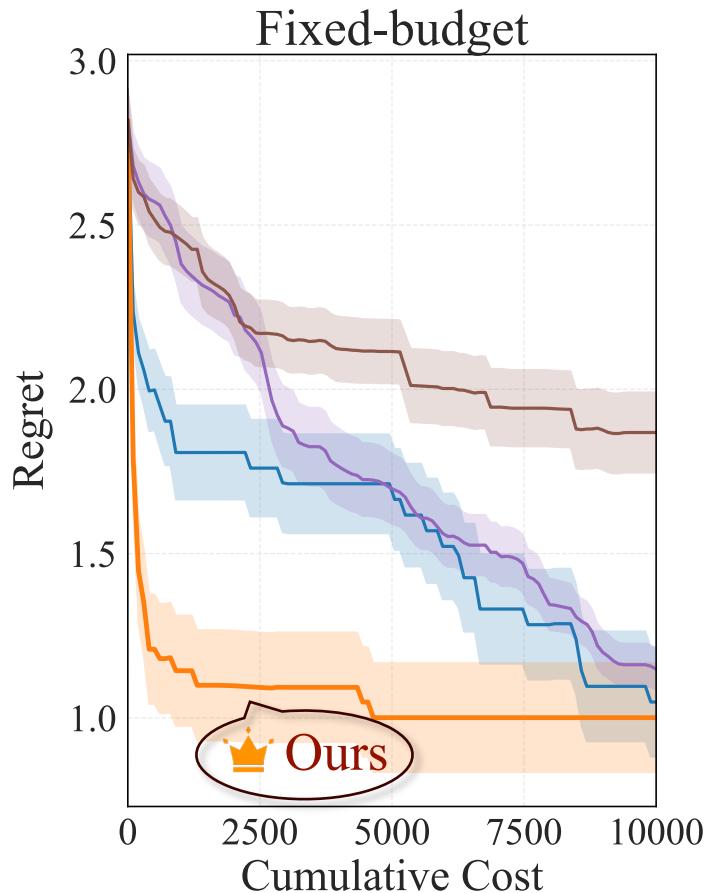
- Improvement-based (e.g., LogEIPC)
- Entropy-based
- Confidence bounds (UCB/LCB)
- Thompson sampling (TS)
- Gittins Index (PBGI)



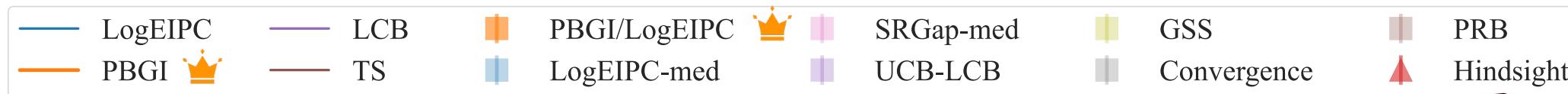
Why another principle?

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

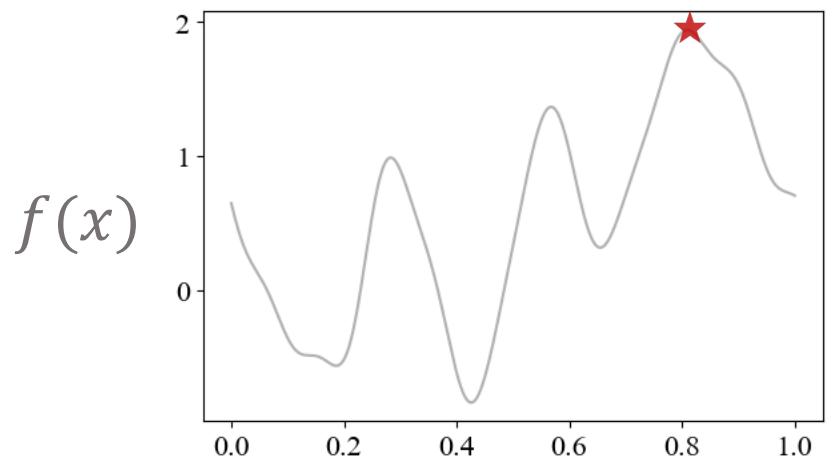


Lower the better



Bound on achievable performance

# Bayesian Optimization



Continuous

Correlated

Fixed-budget / Flexible-stopping

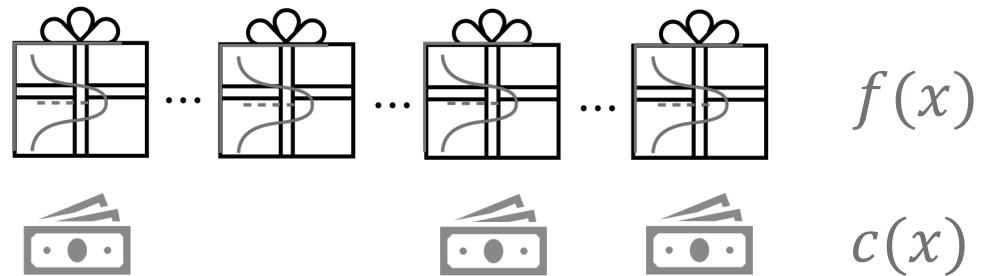
Expected (cost-adjusted) regret

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)

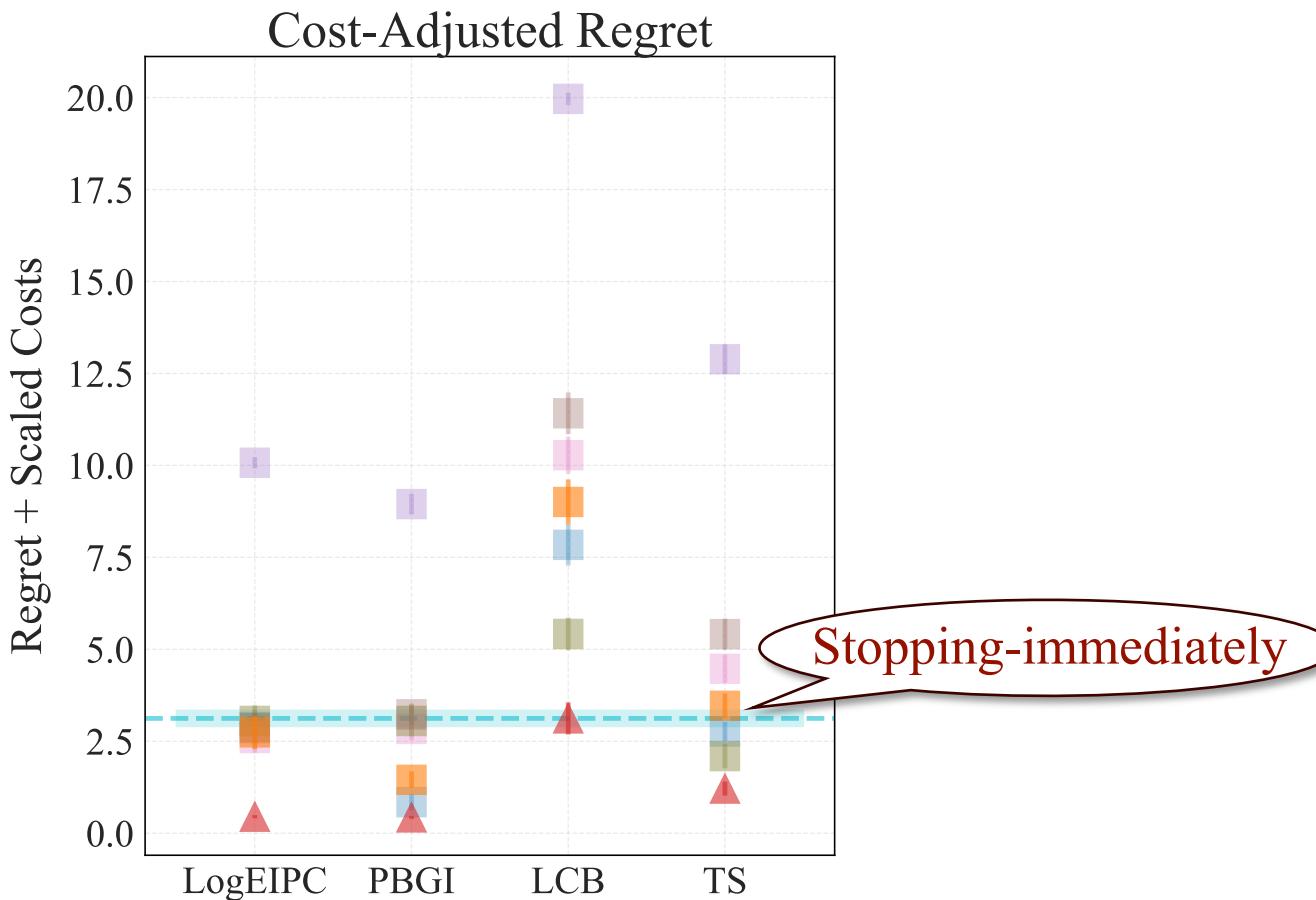
$$\mathbb{E}[R(\text{ours}; \text{PBGI})] \leq R[\text{stopping immediately}]$$

or LogEIPC

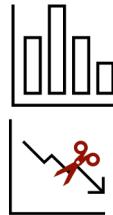
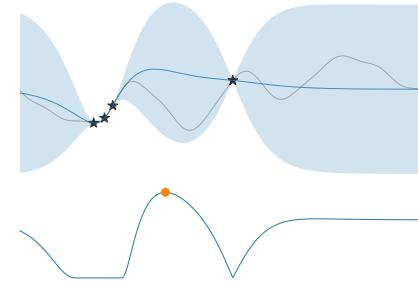
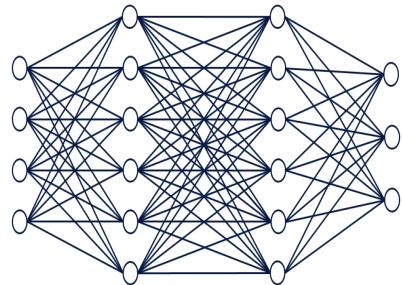
cost-adjusted regret

## 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

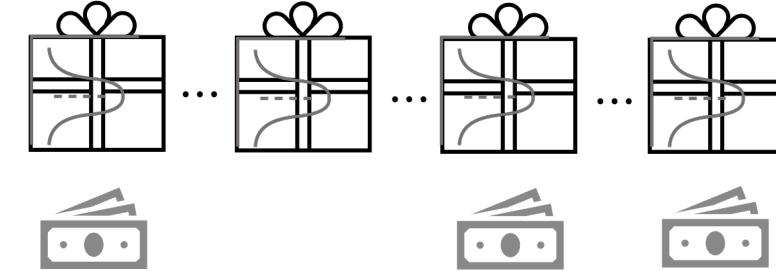


Varying evaluation costs



Adaptive stopping time

## Key idea



Link to Pandora's Box problem  
& Gittins index theory

## Impact

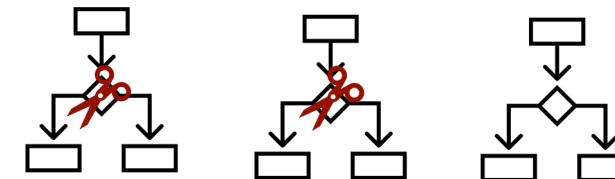


Competitive empirical performance &  
interests from practitioners



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

## Ongoing work

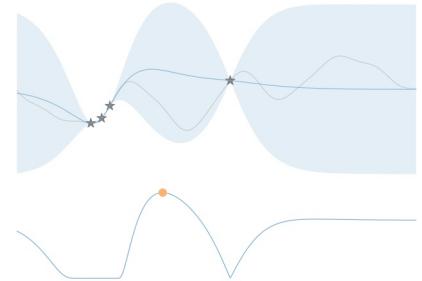
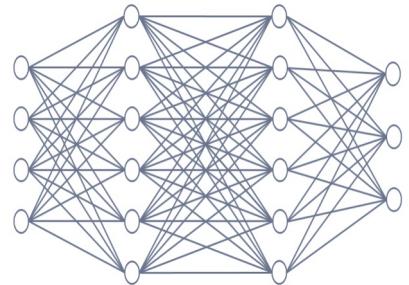


Sharper theoretical guarantees & black-  
box optimization w/ multi-stage feedback



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

# Studied problem

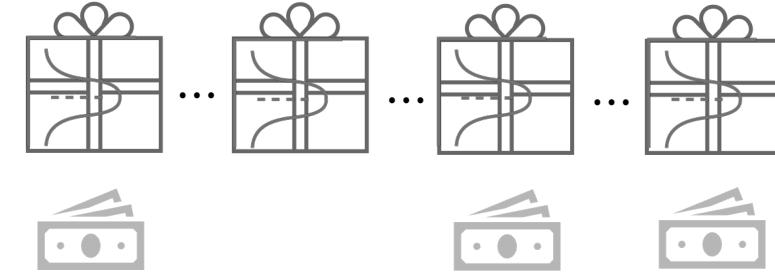


Varying evaluation costs



Adaptive stopping time

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## Impact



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"Cost-aware Bayesian Optimization via the  
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## Ongoing work



ChatGPT



deepseek

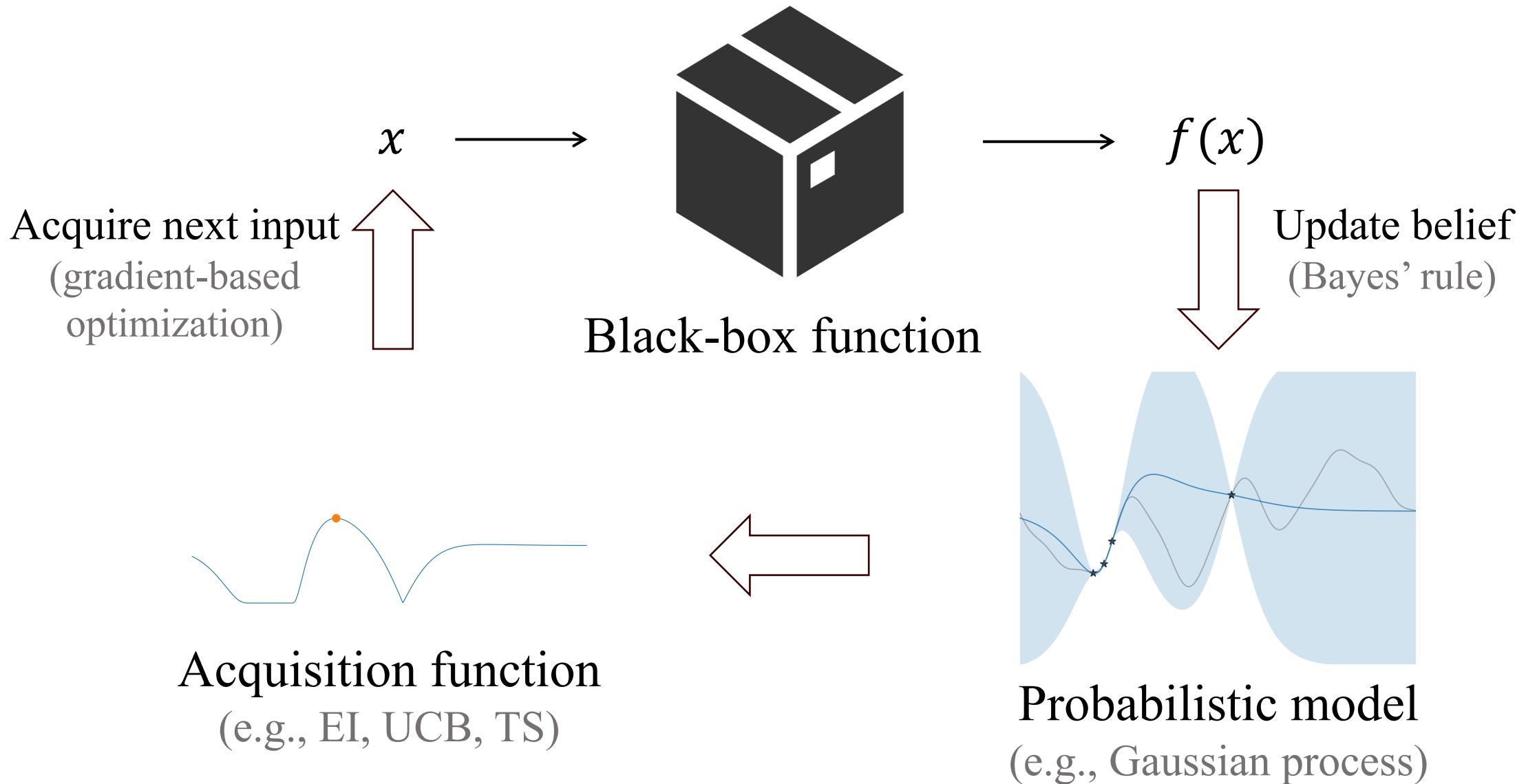


## LLM-driven black-box optimization



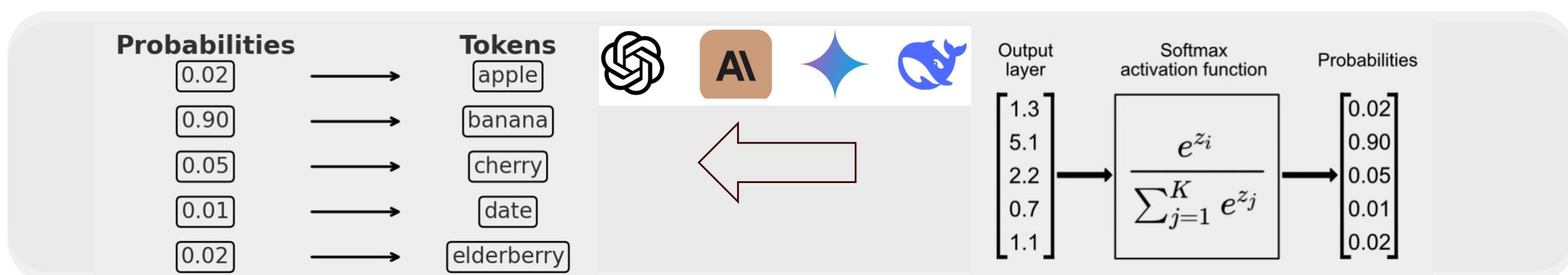
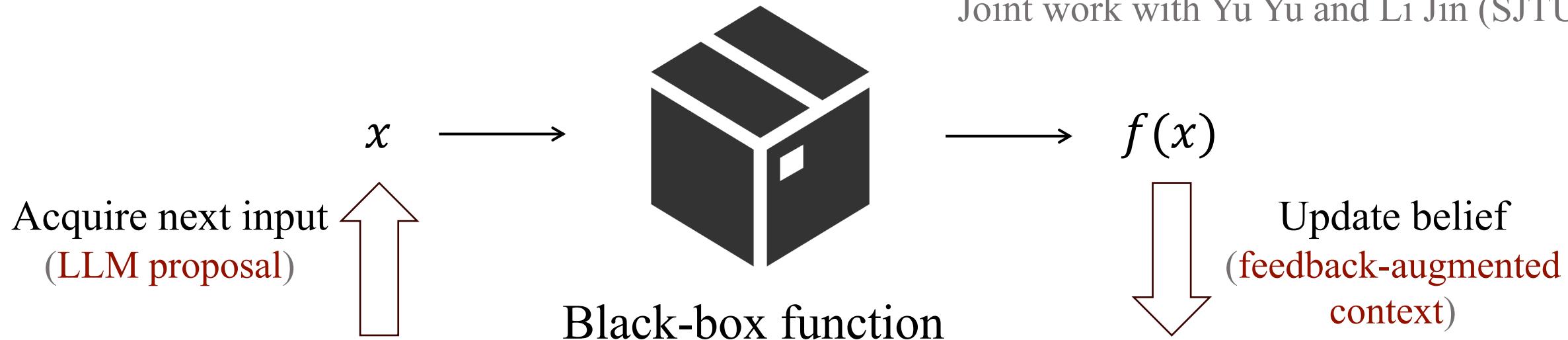
"Cost-aware Stopping for Bayesian  
Optimization." Under review.

# Recap: Bayesian Optimization



# Ongoing: LLM-Driven Black-Box Optimization

Joint work with Yu Yu and Li Jin (SJTU)

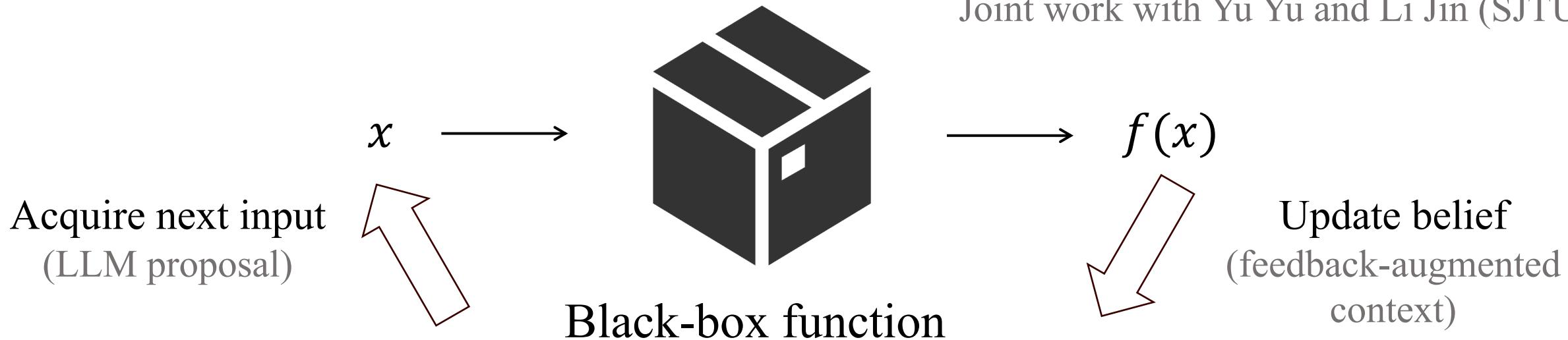


Acquisition function  
(e.g., Softmax sampling)

Probabilistic model  
(e.g., autoregressive model)

# Ongoing: LLM-Driven Black-Box Optimization

Joint work with Yu Yu and Li Jin (SJTU)



Large language model

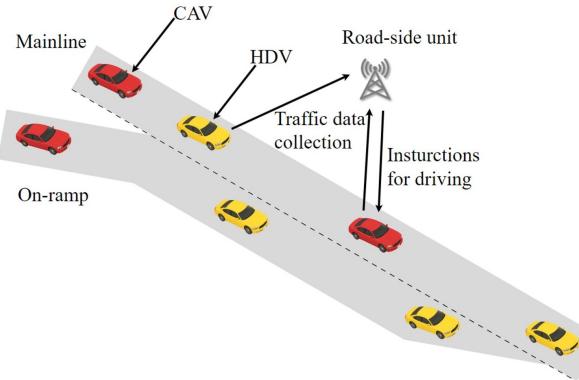
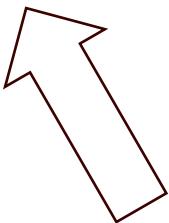
# Ongoing: LLM-Driven Black-Box Optimization

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)

Black-box function  
(RL training & evaluation)

Average speed

Update belief  
(feedback-augmented  
context)



Large language model

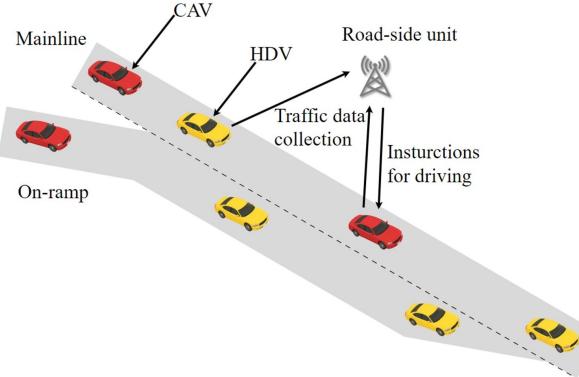
# Ongoing: LLM-Driven Black-Box Optimization

Mixed-autonomy traffic control:

(e.g., Transformer config)

RL state representation

Acquire next input  
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Joint work with Yu Yu and Li Jin (SJTU)

Black-box function  
(RL training & evaluation)



ChatGPT

★ Gemini



deepseek



Claude

Large language model

Average speed

Update belief  
(feedback-augmented  
context)

Can side info help?

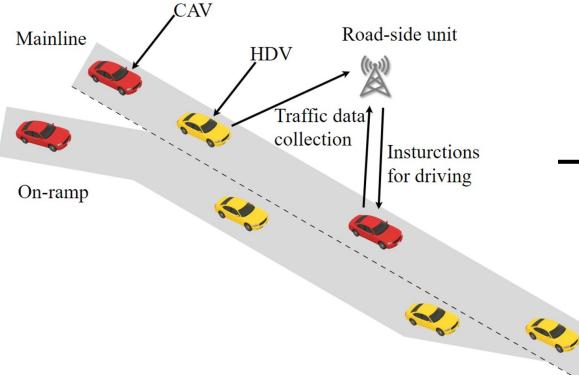
# Our LLM-Driven Method: Incorporate Side Info

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

Update belief  
(feedback-augmented  
context)

performance metric +  
representation quality

Black-box function  
(RL training & evaluation)



ChatGPT

Gemini



deepseek



Claude

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.