

NeurIPS'24 & INFORMS Data  
Mining Paper Competition Finalist

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

Qian Xie 谢倩 (Cornell ORIE)

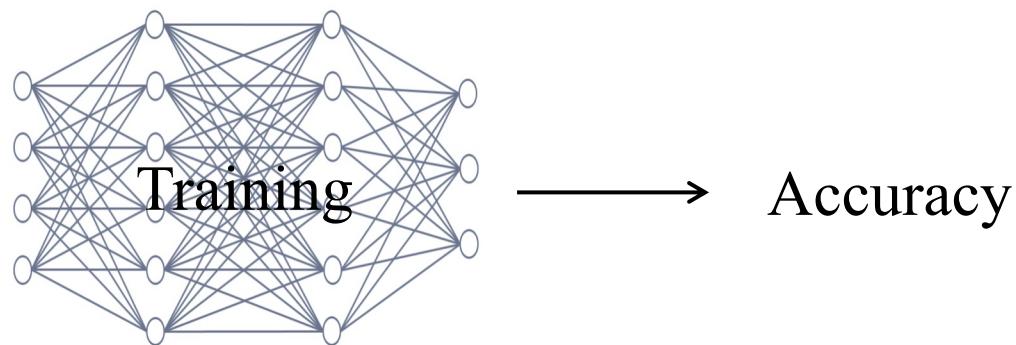
Joint work with Linda Cai (UC Berkeley), Theodore Brown (UCL), Raul Astudillo (MBZUAI), Peter Frazier, Alexander Terenin, and Ziv Scully (Cornell)

INFORMS Annual Meeting 2025 Job Market Showcase

# Motivation: World of Optimization under Uncertainty

ML model training:

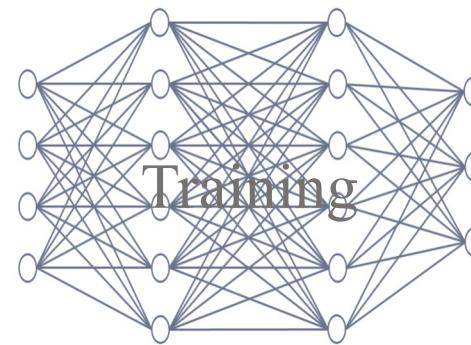
Training hyperparameters  
(e.g., learning rate, # layers)  $\longrightarrow$



# Motivation: World of Optimization under Uncertainty

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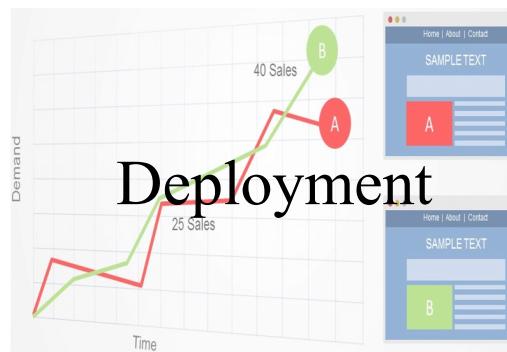
Training hyperparameters  
(e.g., learning rate, # layers)



Accuracy

Adaptive experimentation:

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



Revenue

# Motivation: World of Optimization under Uncertainty

Black-box optimization:

Input  $x$  →

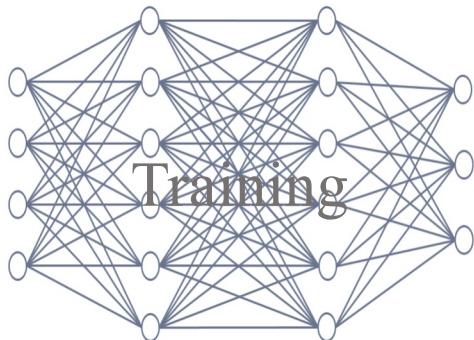


non-analytical &  
no gradient info

→ Performance metric  $f(x)$

ML model training:

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



→ Accuracy

Adaptive experimentation:

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



→ Revenue

# Motivation: World of Optimization under Uncertainty

Black-box optimization:

(gradient-based method not applicable)

Input  $x$   $\longrightarrow$

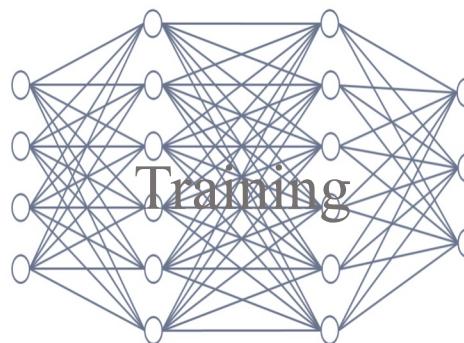


non-analytical &  
no gradient info

$\longrightarrow$  Observed outcome  $f(x)$

ML model training:

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



$\longrightarrow$  Accuracy

# Black-Box Optimization

Black-box optimization:

(gradient-based method not applicable)

Input  $x$  →



expensive-to-evaluate

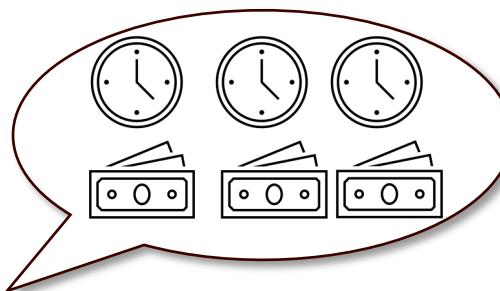
→ Observed outcome  $f(x)$

ML model training:

Training hyperparameters →  
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Training



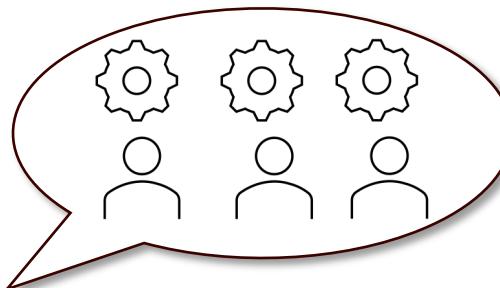
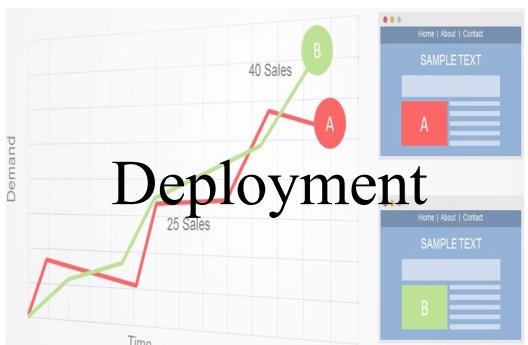
Training time

Compute credits

→ Accuracy

Adaptive experimentation:

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

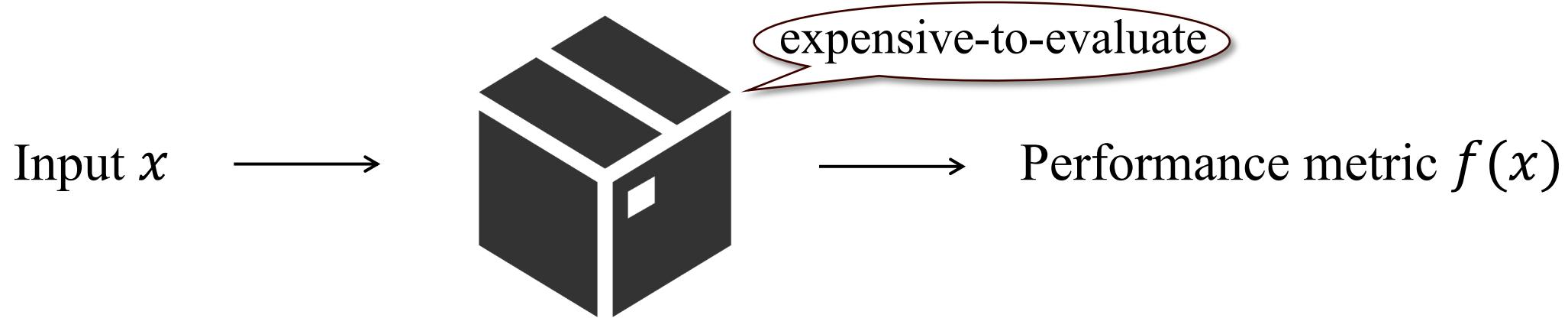


Operational cost

User experience

→ Revenue

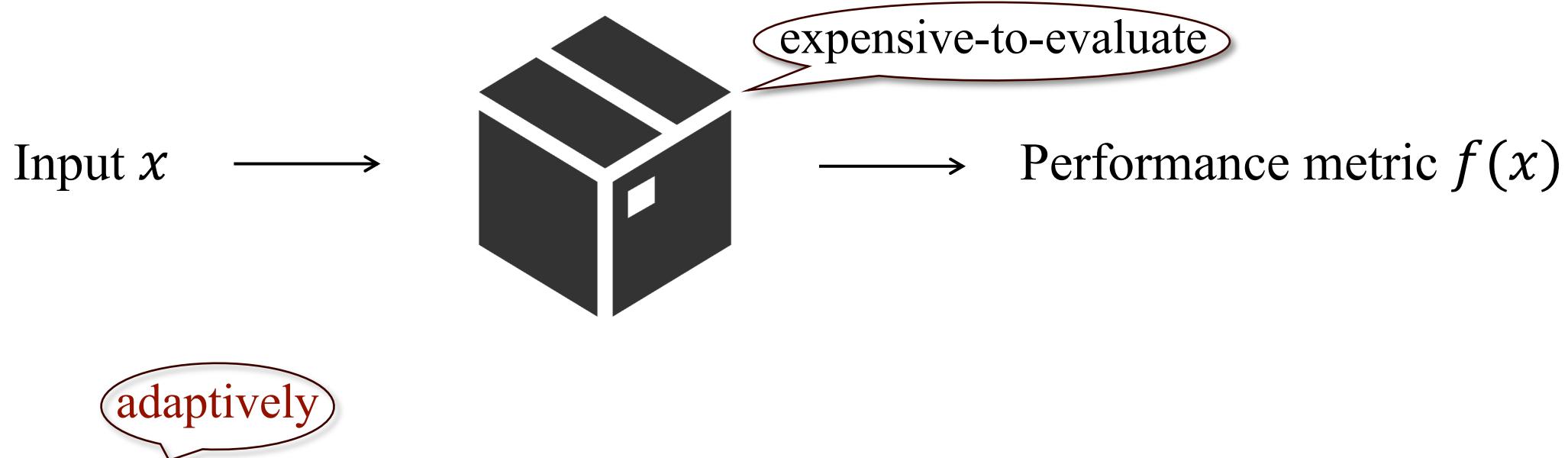
# Black-Box Optimization



**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



**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



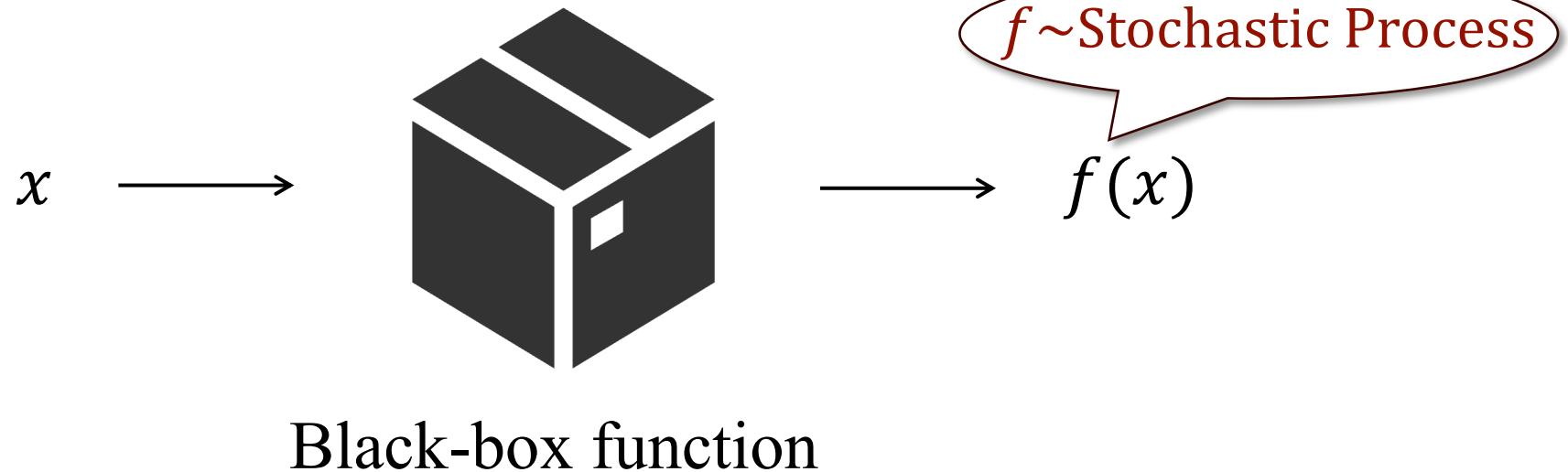
**High-level goal:** Choose  $x_1, \dots, x_T$  to maximize the expected best observed value

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Fewer #evaluations

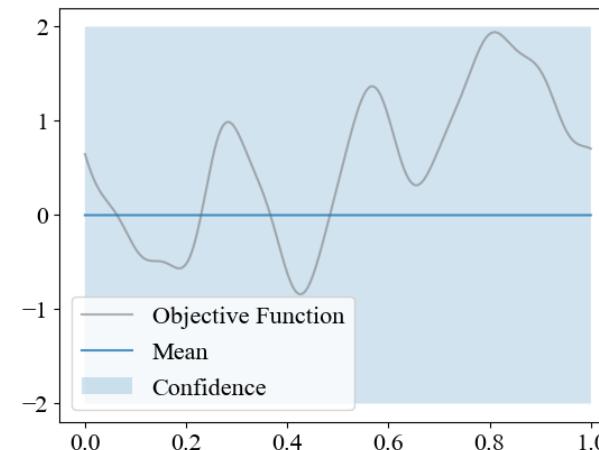
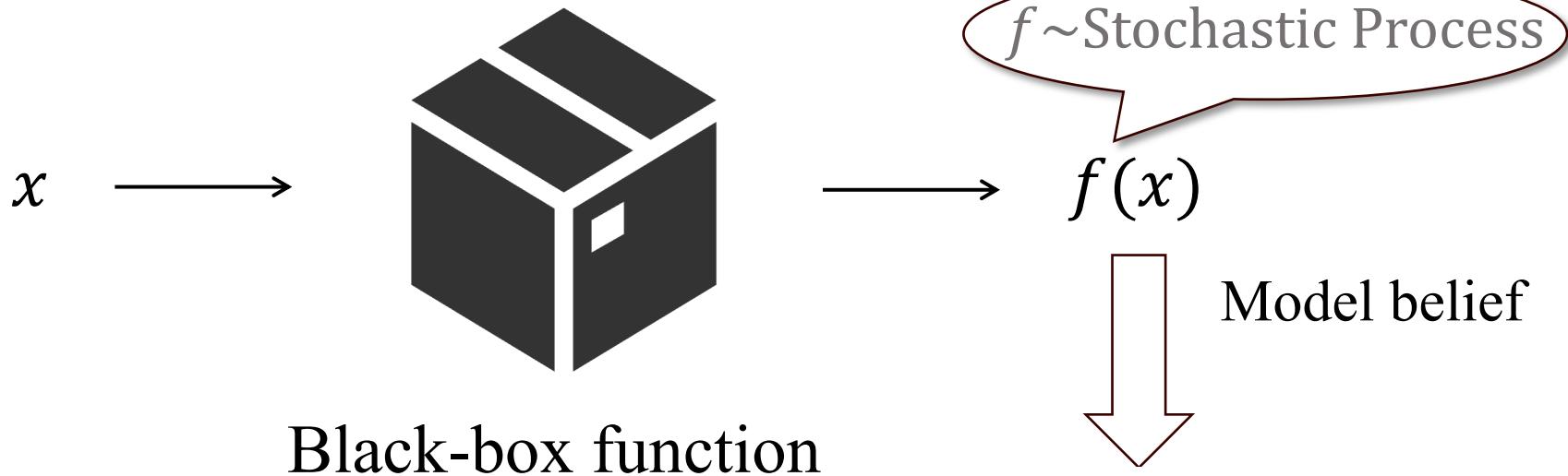
Efficient framework: Bayesian optimization

# Bayesian Optimization



# Bayesian Optimization

Time 0

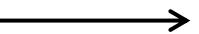


Probabilistic model  
(e.g., Gaussian process)

# Bayesian Optimization

Time  $t$

$x_1, \dots, x_t$

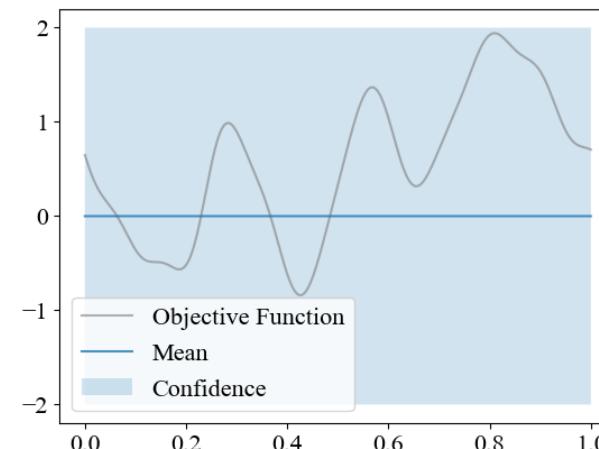


Black-box function

$f \sim \text{Stochastic Process}$

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

Model belief



Probabilistic model  
(e.g., Gaussian process)

# Bayesian Optimization

Time  $t$

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

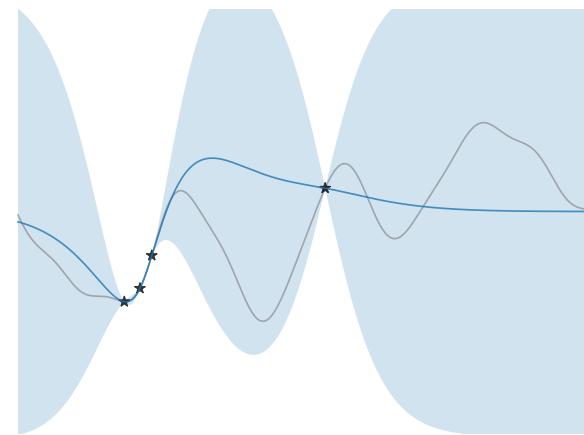


Black-box function

$f \sim \text{Stochastic Process}$

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

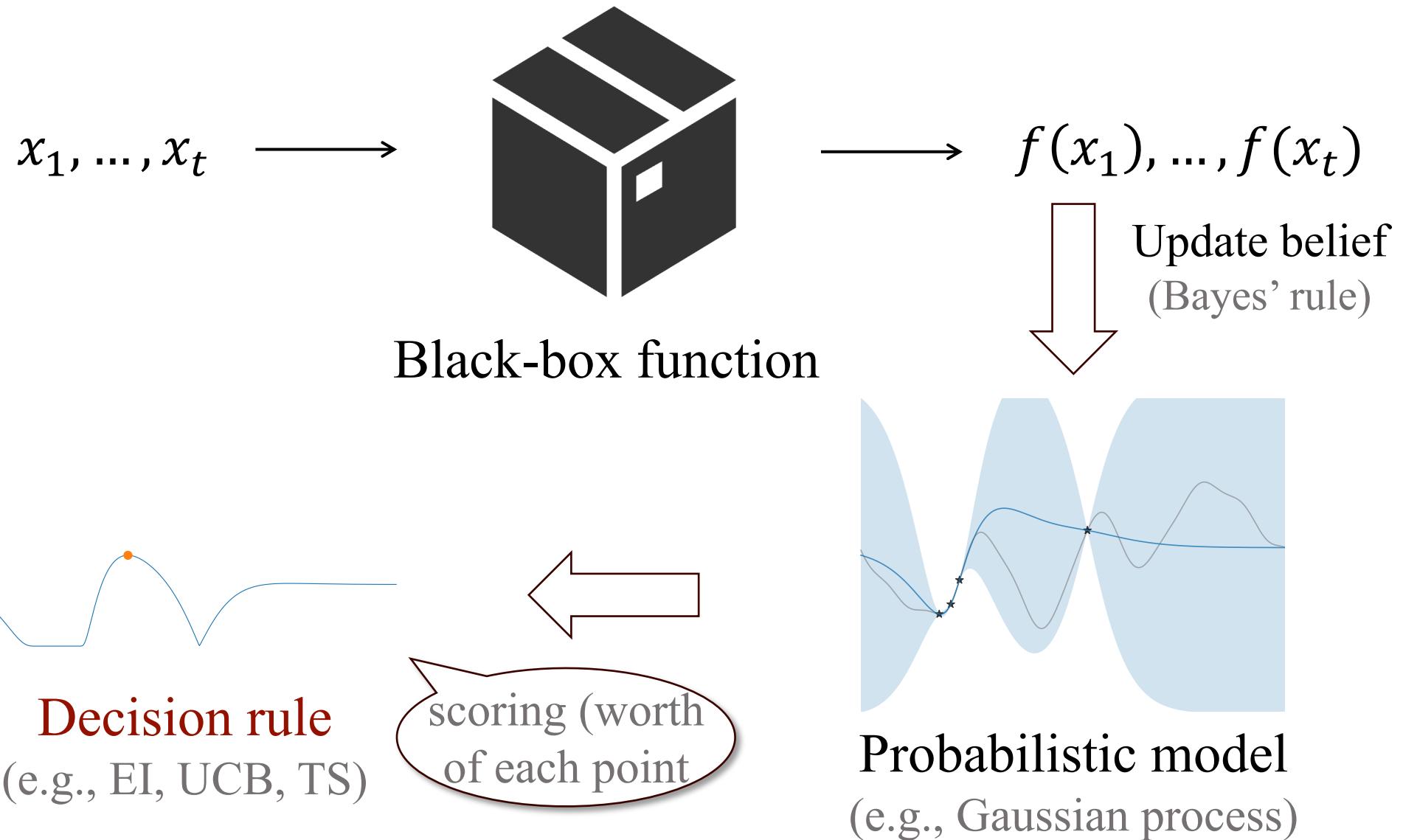
Update belief  
(Bayes' rule)



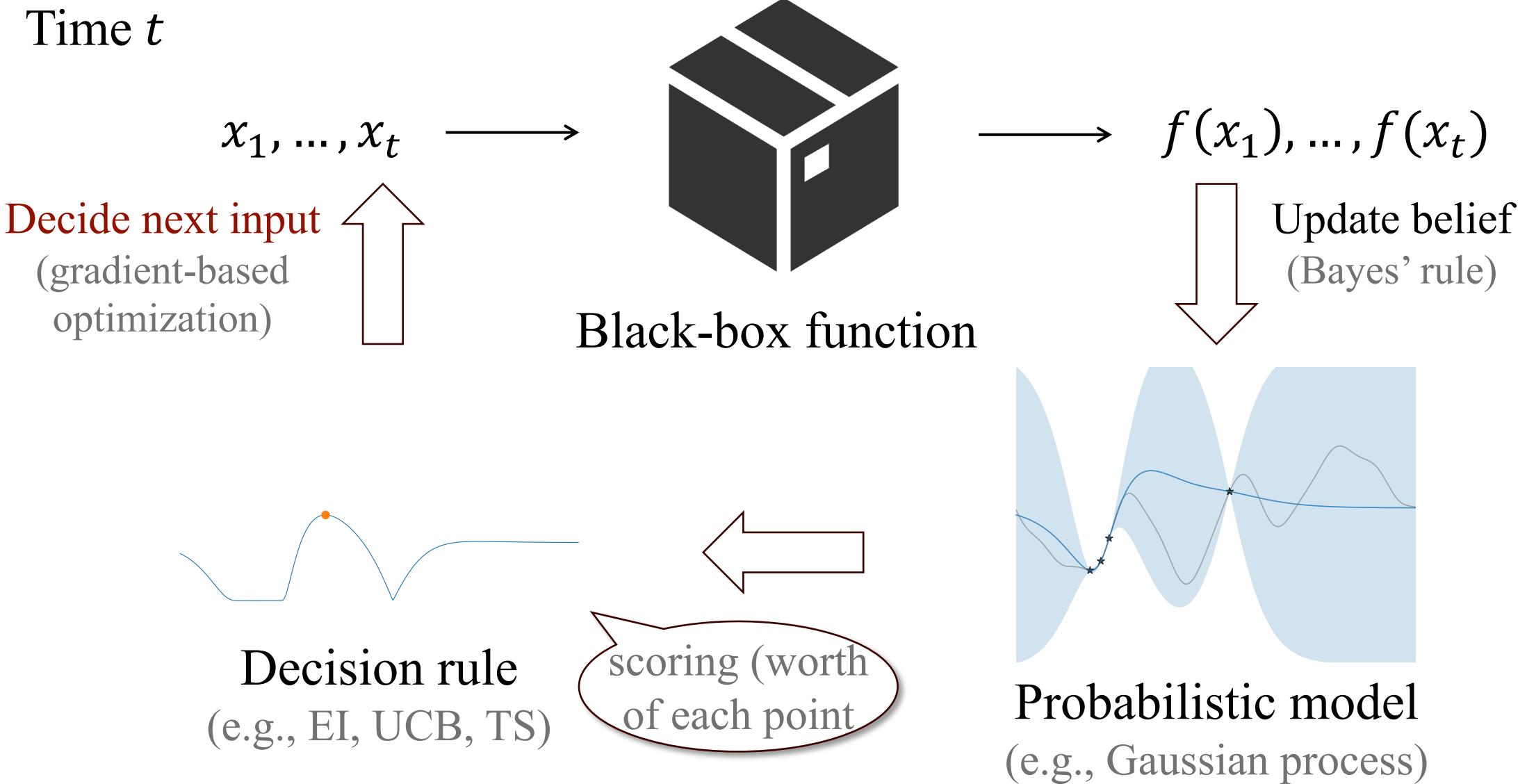
Probabilistic model  
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# Bayesian Optimization

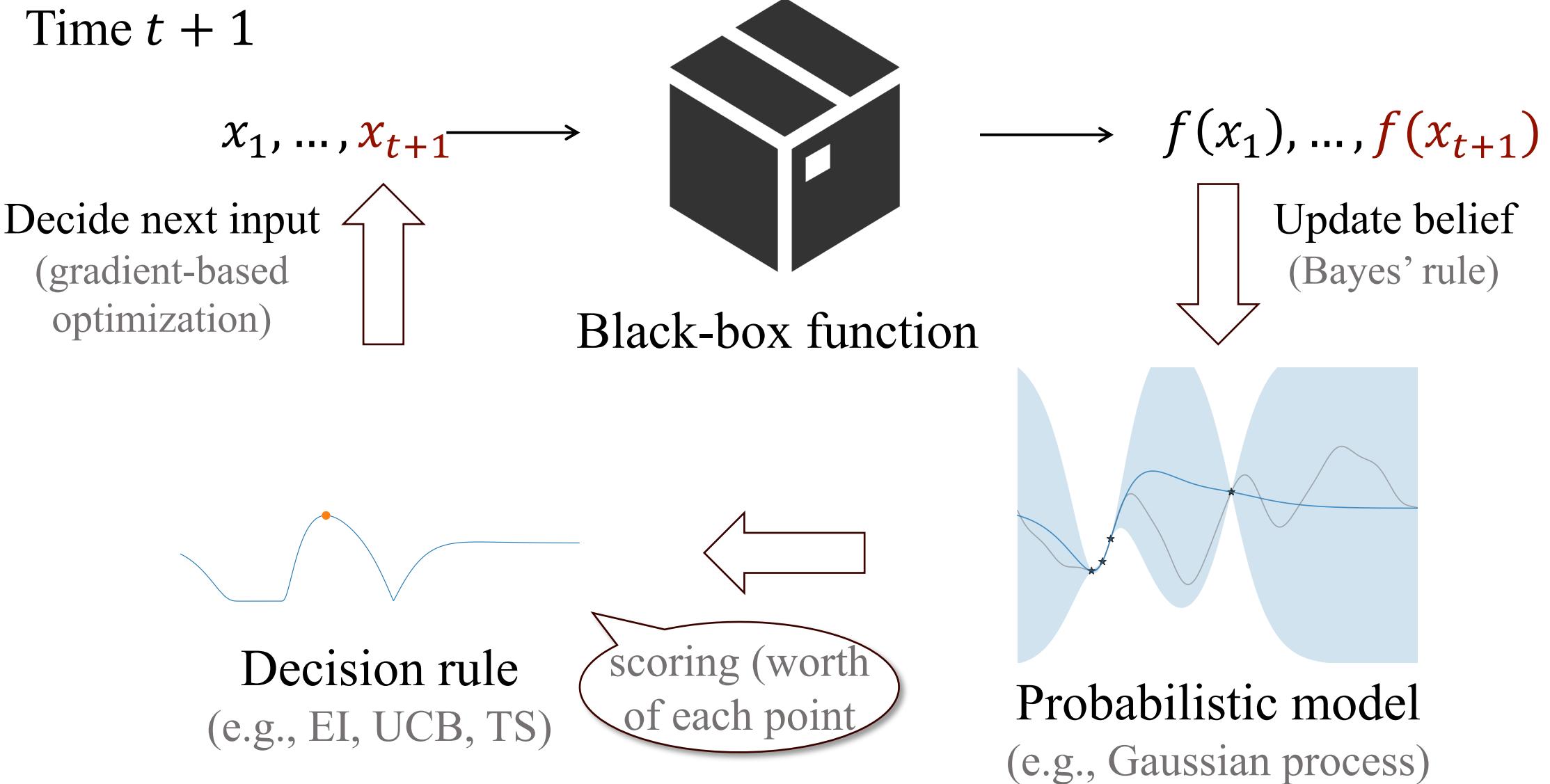
Time  $t$



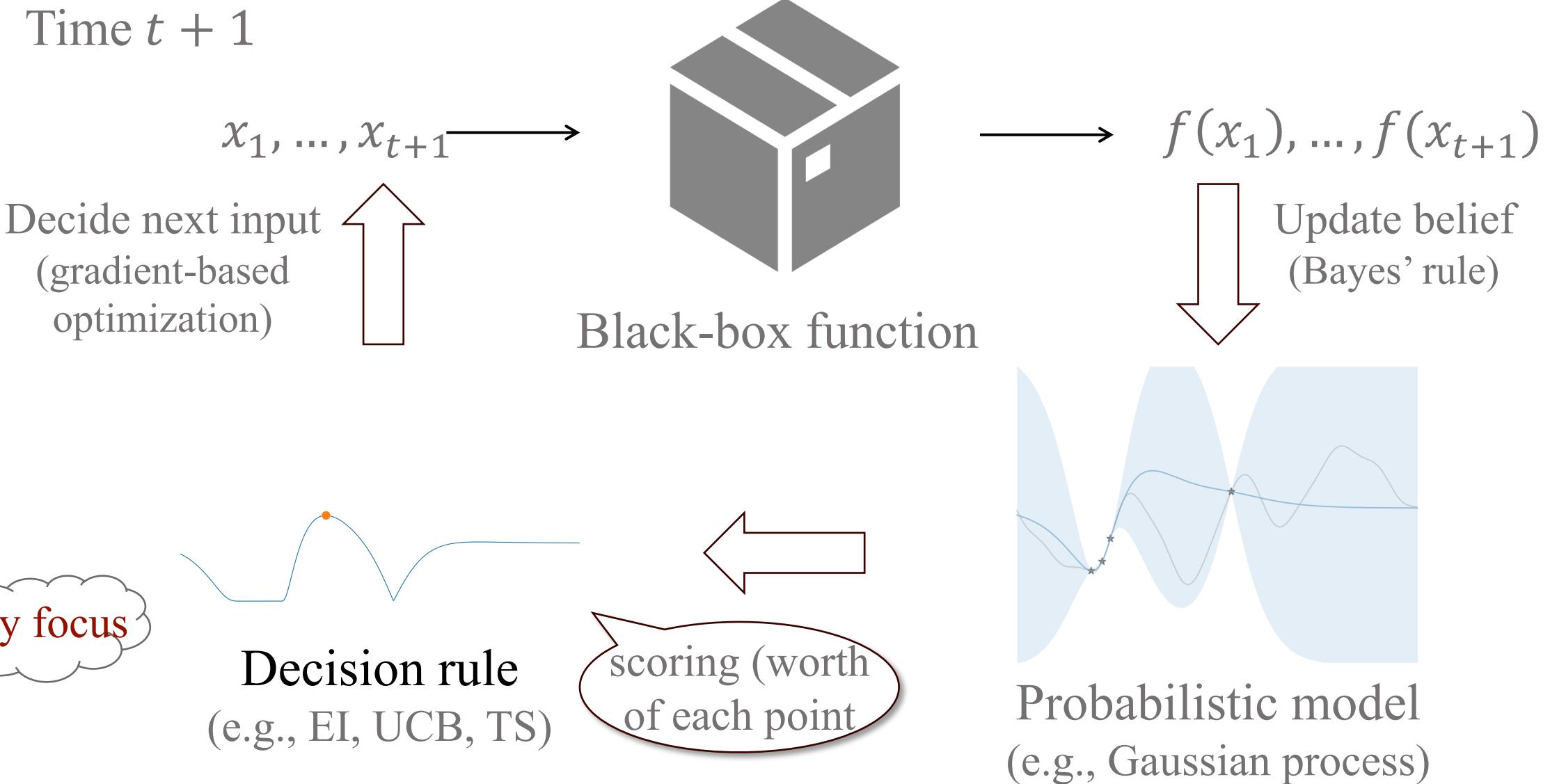
# Bayesian Optimization



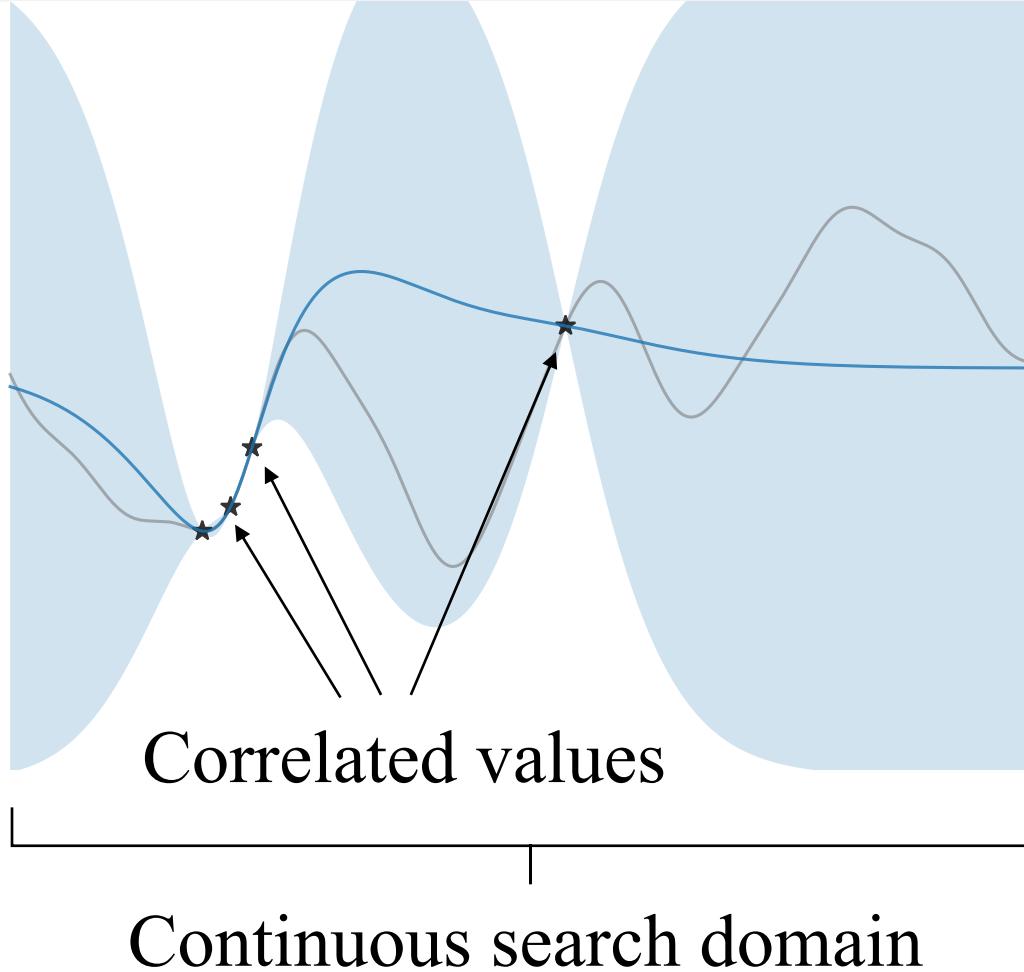
# Bayesian Optimization



# Bayesian Optimization



# Challenge in Decision Rule Design



Correlation & continuity  $\Rightarrow$  Intractable MDP  $\Rightarrow$  Optimal policy unknown

# Popular Decision Rule: Expected Improvement

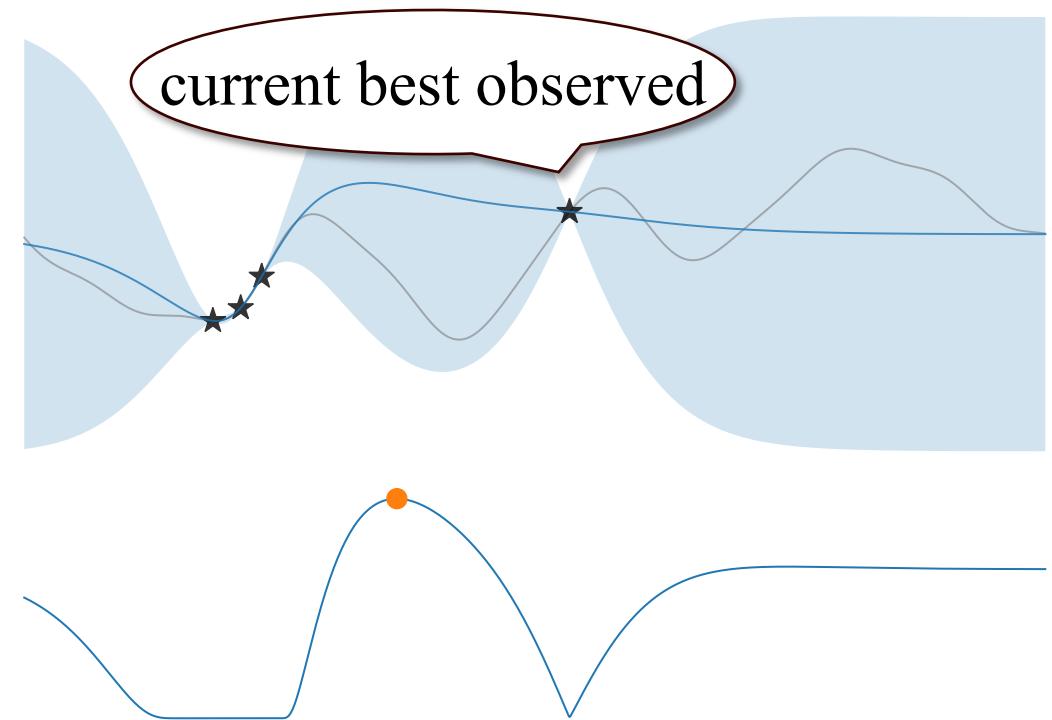
$$EI(x) = \mathbb{E}[\max(f(x) - y_{\text{best}}, 0) \mid x_1, \dots, x_t]$$

current best observed  
data  
“improvement”

$$x_{t+1} = \max_x EI_{f|D}(x; y_{\text{best}})$$

posterior distribution

One-step approximation to MDP



Expected improvement  $EI(x)$

# Popular Decision Rule: Expected Improvement

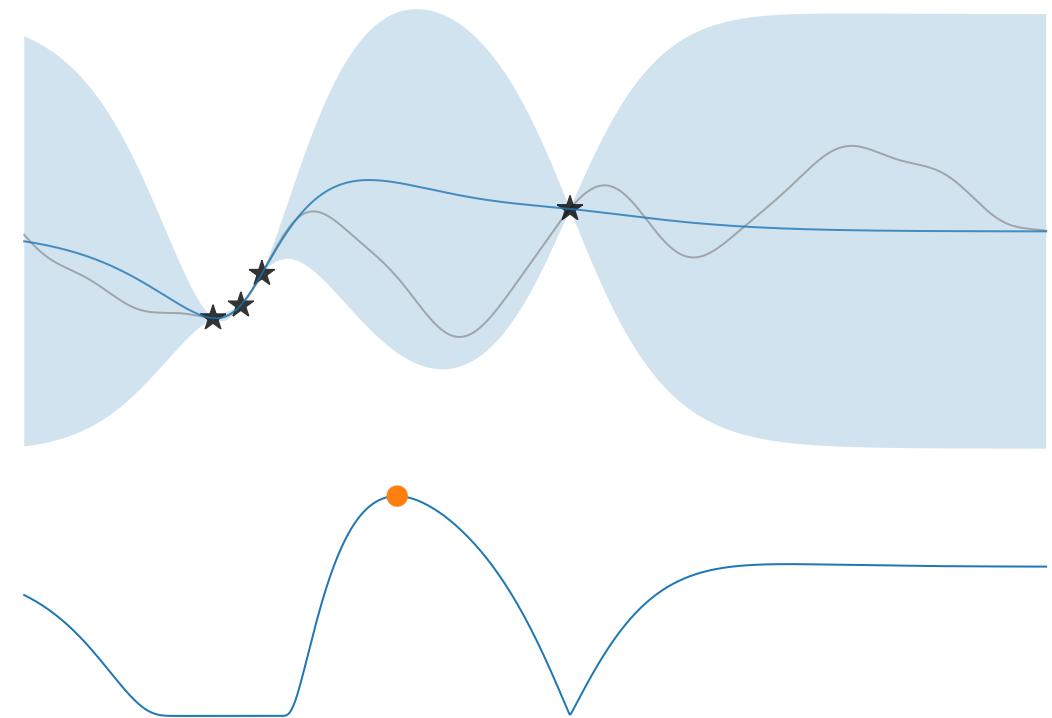
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One-step approximation to MDP

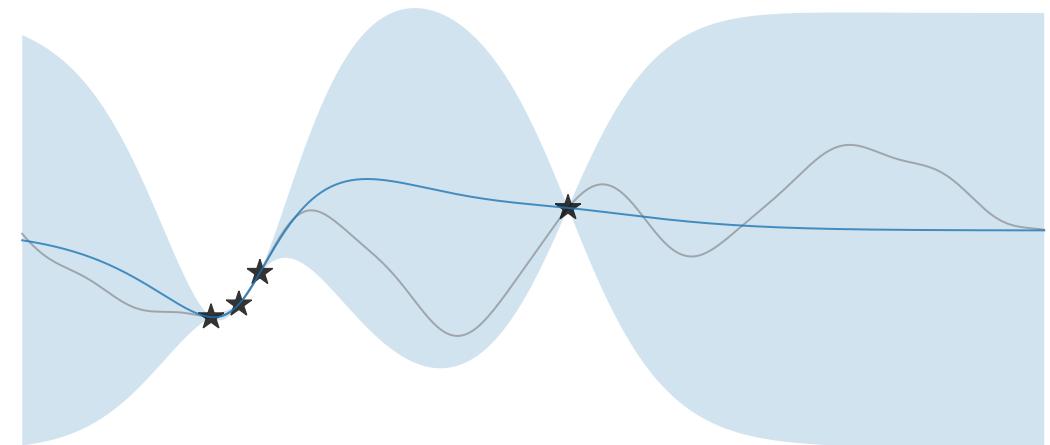


Expected improvement  $EI(x)$

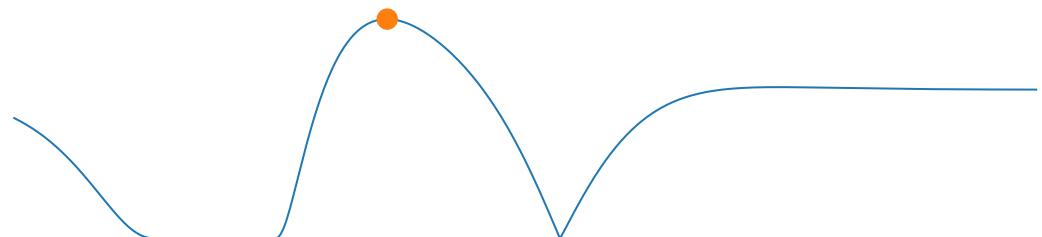
Improvement-based  
design principle

# Existing Design Principles

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



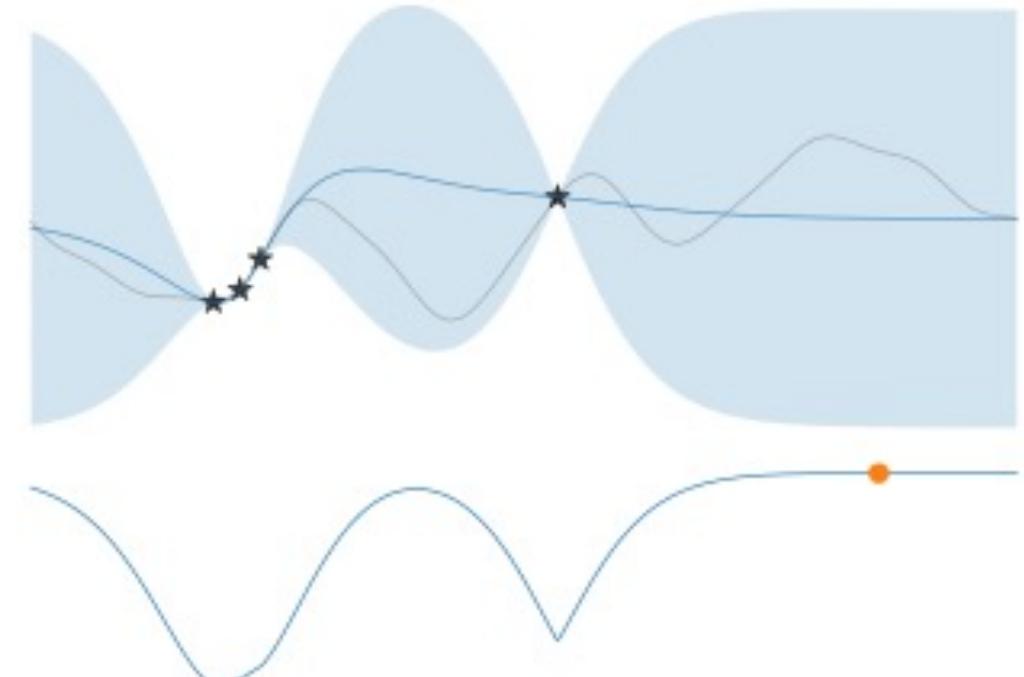
Expected improvement  $EI(x)$



Improvement-based  
design principle

# New Design Principle: Gittins Index

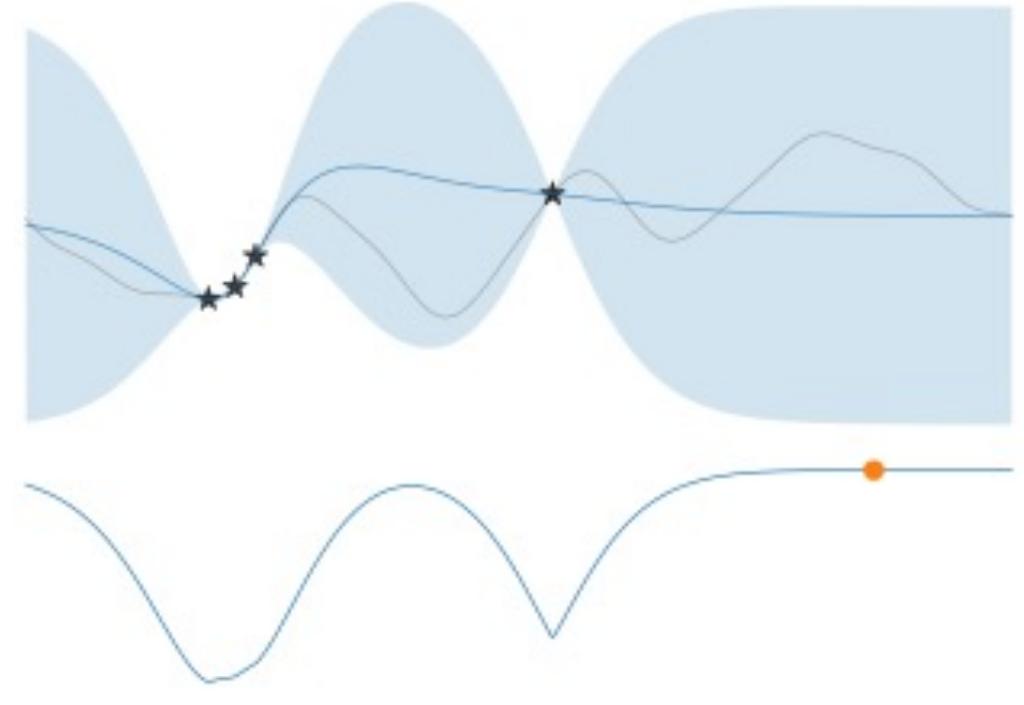
- Improvement-based (e.g., EI)
- Entropy-based
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- Thompson sampling (TS)
- **Gittins Index**



Gittins index  $GI(x)$

# New Design Principle: Gittins Index

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



Gittins index  $GI(x)$

? Why another principle?

# Our Contribution: Gittins Index Principle



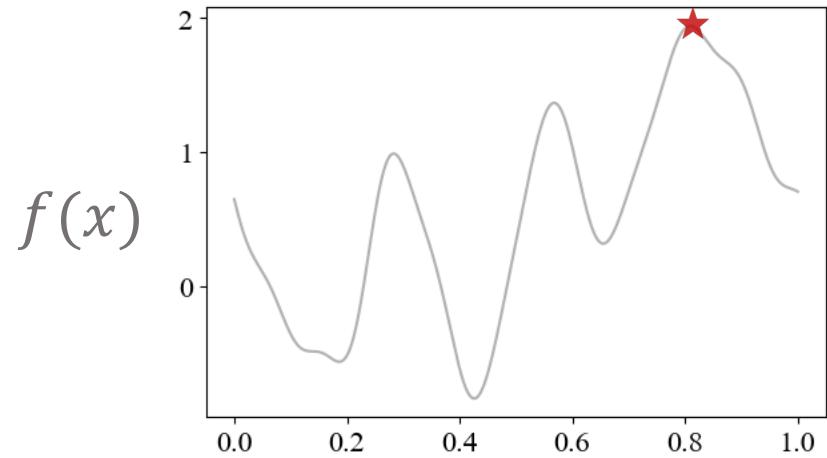
Why another principle?

1. Principled design via problem simplification
2. Natural incorporation of side info and flexibility
3. Competitive performance on benchmarks
4. Theoretical guarantees

# Our Contribution: Gittins Index Principle

1. Principled design via problem simplification
2. Natural incorporation of side info and flexibility
3. Competitive performance on benchmarks
4. Theoretical guarantees

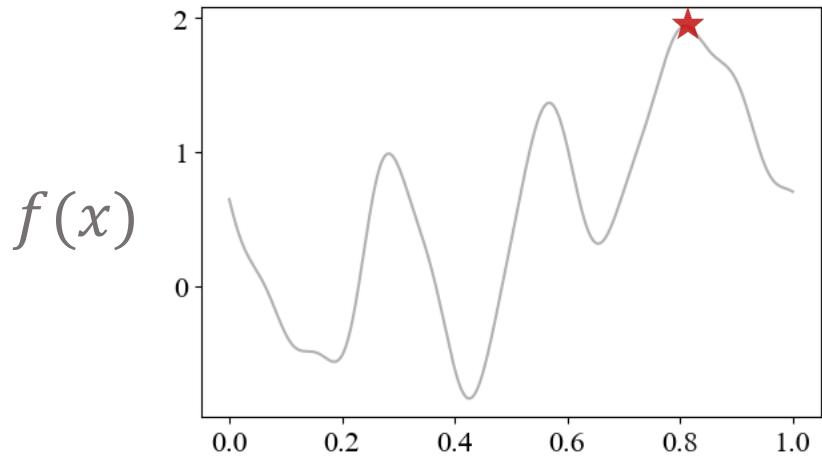
# Bayesian Optimization



Continuous

Correlated

# Bayesian Optimization



Continuous



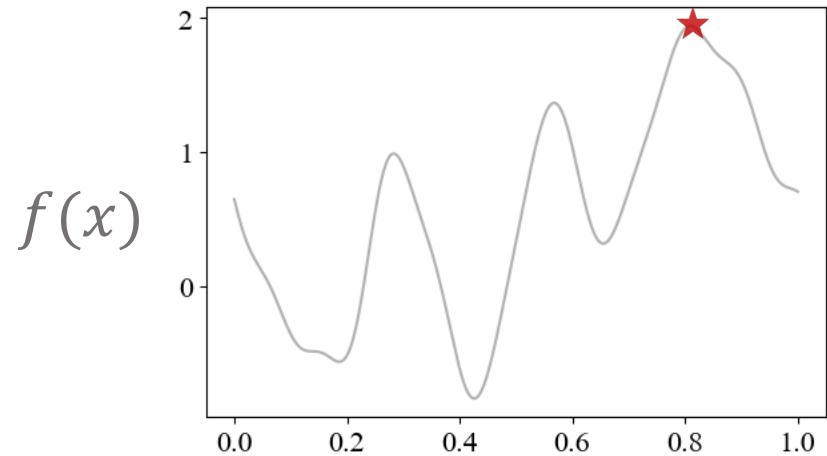
Discrete

Correlated



Independent

# Bayesian Optimization

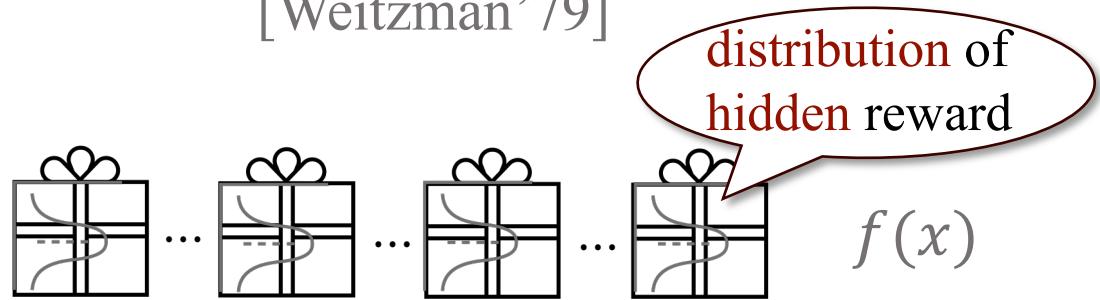


Continuous

Correlated

# Pandora's Box

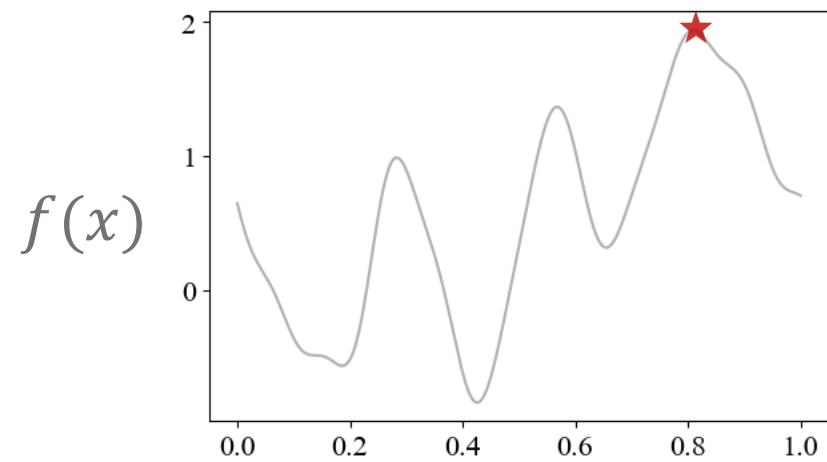
[Weitzman'79]



Discrete

Independent

# Bayesian Optimization

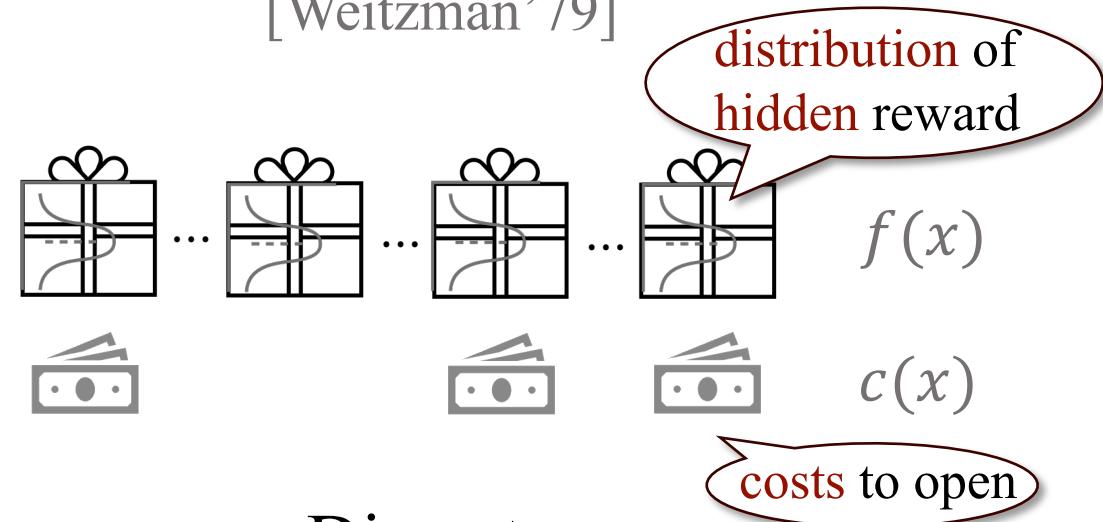


Continuous

Correlated

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[Weitzman'79]

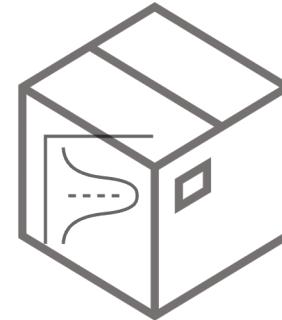
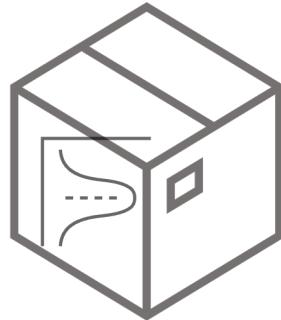
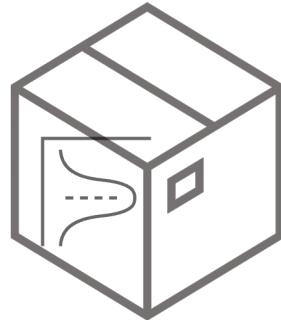
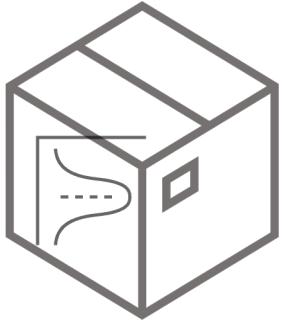


Discrete

Independent

# Pandora's Box

$t = 0$

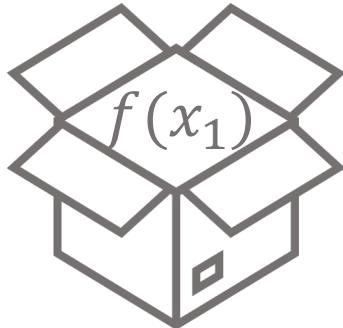


**High-level goal:** Choose box  $x_1, \dots, x_T$  to open to maximize the expected utility

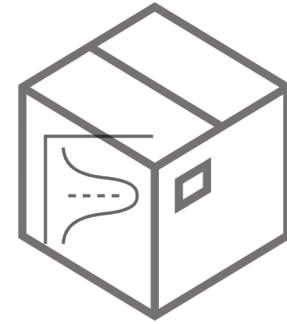
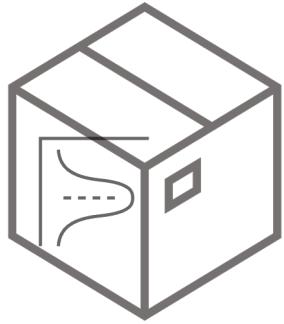
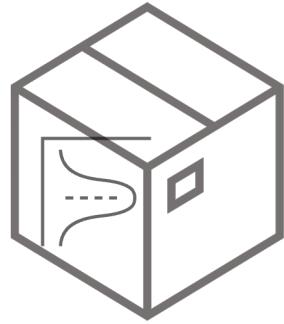
$$\mathbb{E} \max_{t=1,2,\dots,T} f(x_t) - \mathbb{E} \sum_{t=1}^T c(x_t)$$

# Pandora's Box

$t = 1$



$c(x_1)$

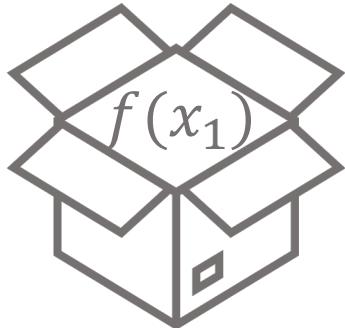


**High-level goal:** Choose box  $x_1, \dots, x_T$  to open to maximize the expected utility

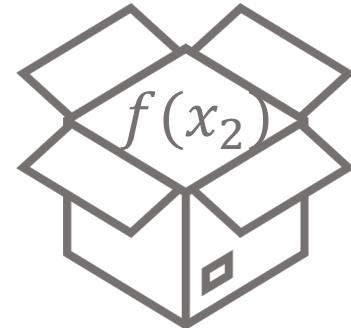
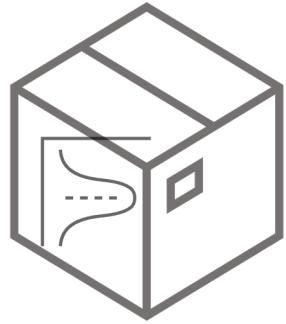
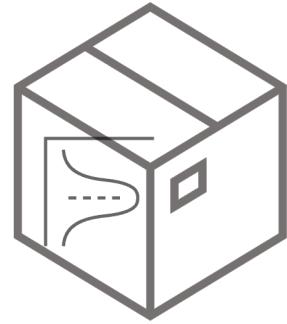
$$\mathbb{E} \max_{t=1,2,\dots,T} f(x_t) - \mathbb{E} \sum_{t=1}^T c(x_t)$$

# Pandora's Box

$t = 2$



$c(x_1)$



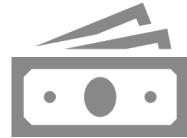
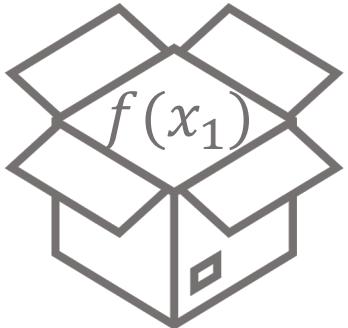
$c(x_2)$

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

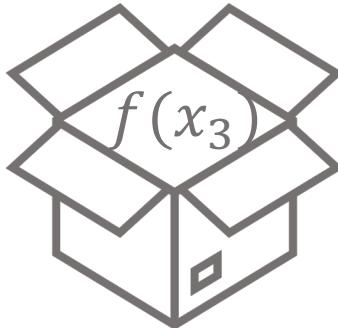
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# Pandora's Box

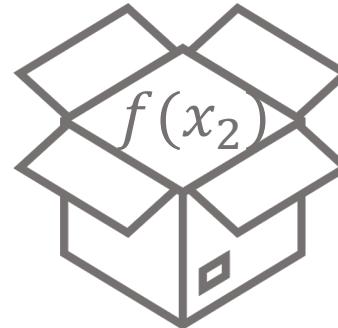
$t = 3$



$c(x_1)$



$c(x_3)$



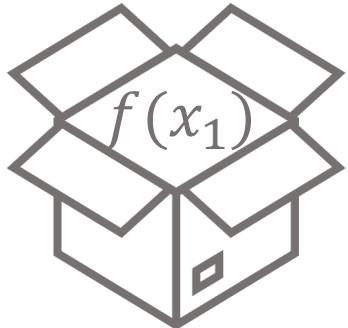
$c(x_2)$

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

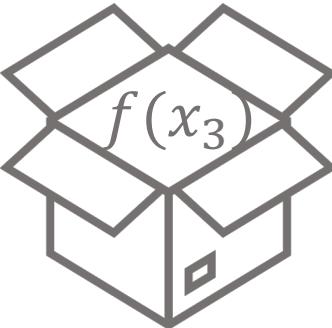
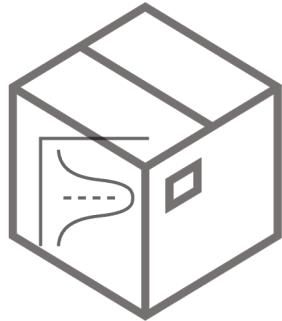
$$\mathbb{E} \max_{t=1,2,\dots,T} f(x_t) - \mathbb{E} \sum_{t=1}^T c(x_t)$$

# Pandora's Box

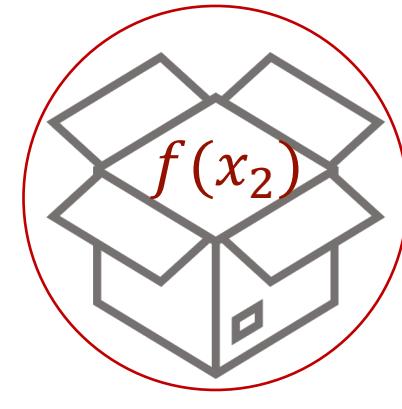
$t = T$ , stop



$c(x_1)$



$c(x_3)$

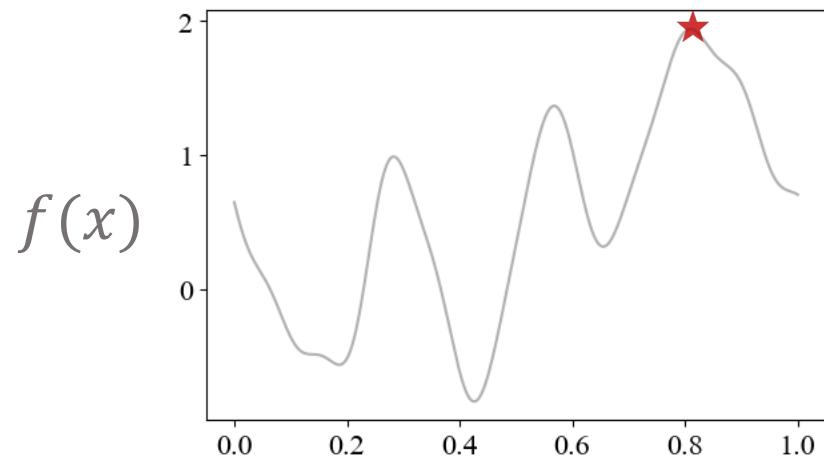


$c(x_2)$

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

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

# Bayesian Optimization

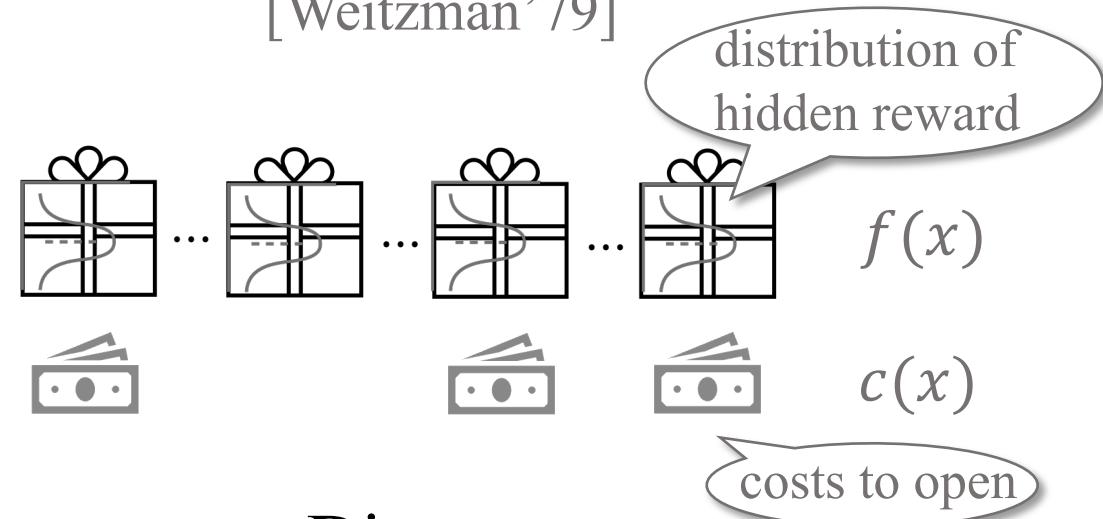


Continuous

Correlated

# Pandora's Box

[Weitzman'79]

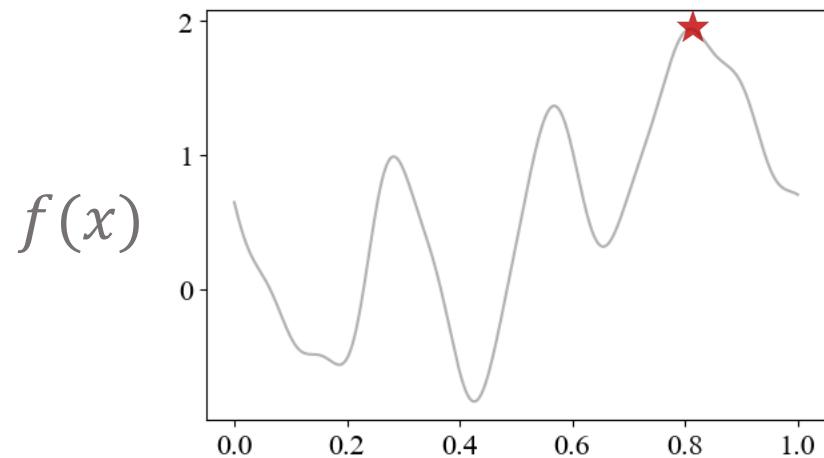


Discrete

Independent

Optimal policy: Gittins index

# Bayesian Optimization

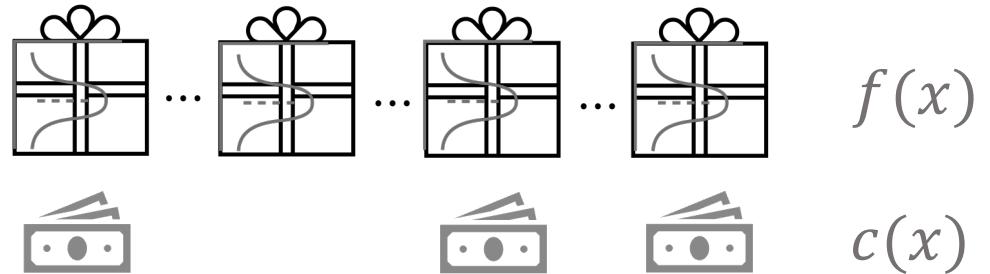


Continuous

Correlated

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[Weitzman'79]



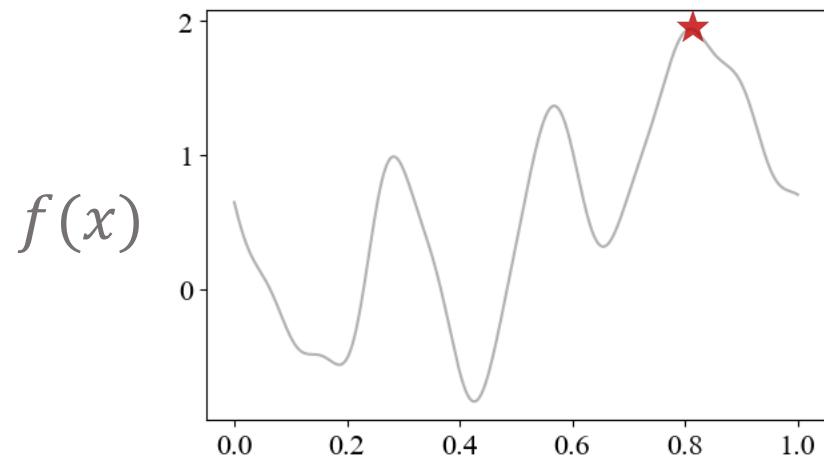
Discrete

Independent

How to translate?

Optimal policy: Gittins index

# Bayesian Optimization

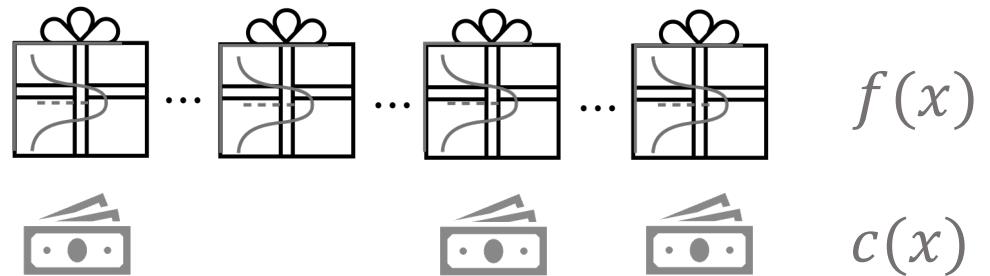


Continuous

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# Pandora's Box

[Weitzman'79]

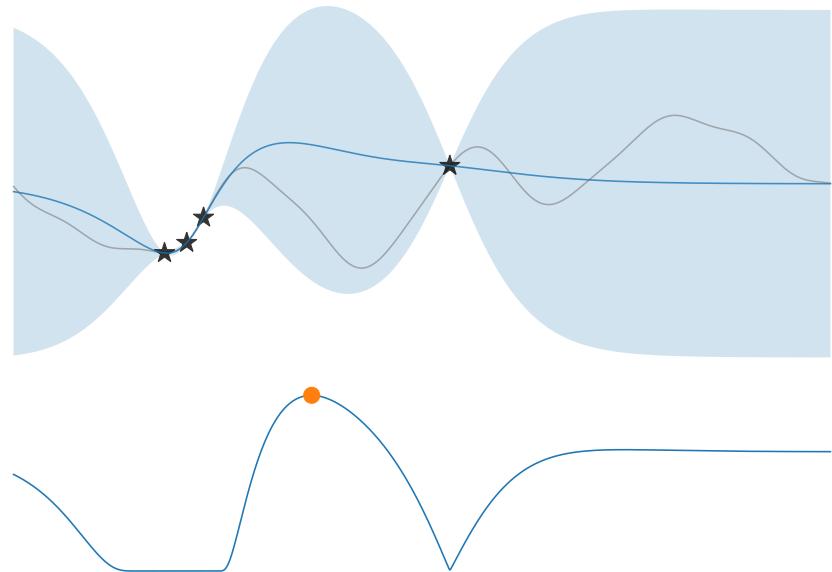


Discrete

Independent

Our policy:  $\text{GI}_{f|D}(x; c(x)) \leftarrow$  incorporate posterior  
take continuum limit      Optimal policy:  $\text{GI}_f(x; c(x))$

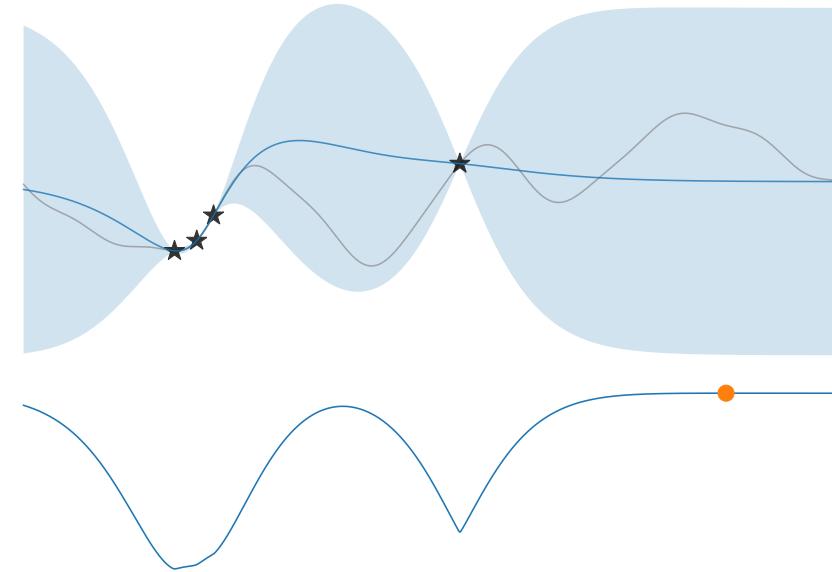
# Expected Improvement



$$\text{EI}_{f|D}(x; g) := \mathbb{E}[\max(f(x) - g, 0) | D]$$

Temporal simplification to MDP

# Gittins Index



$$\text{GI}_{f|D}(x) = g \text{ s.t. } \text{EI}_{f|D}(x; g) = c(x)$$

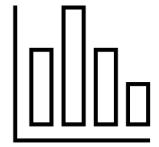
Spatial simplification to MDP

# Our Contribution: Gittins Index Principle

Joint work with Ziv Scully and Alexander Terenin et al.

1. Principled design via problem simplification
2. Natural incorporation of side info and flexibility
3. Competitive performance on benchmarks
4. Theoretical guarantees

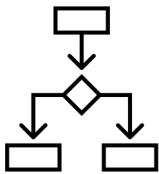
# Under-explored Side Info and Flexibility



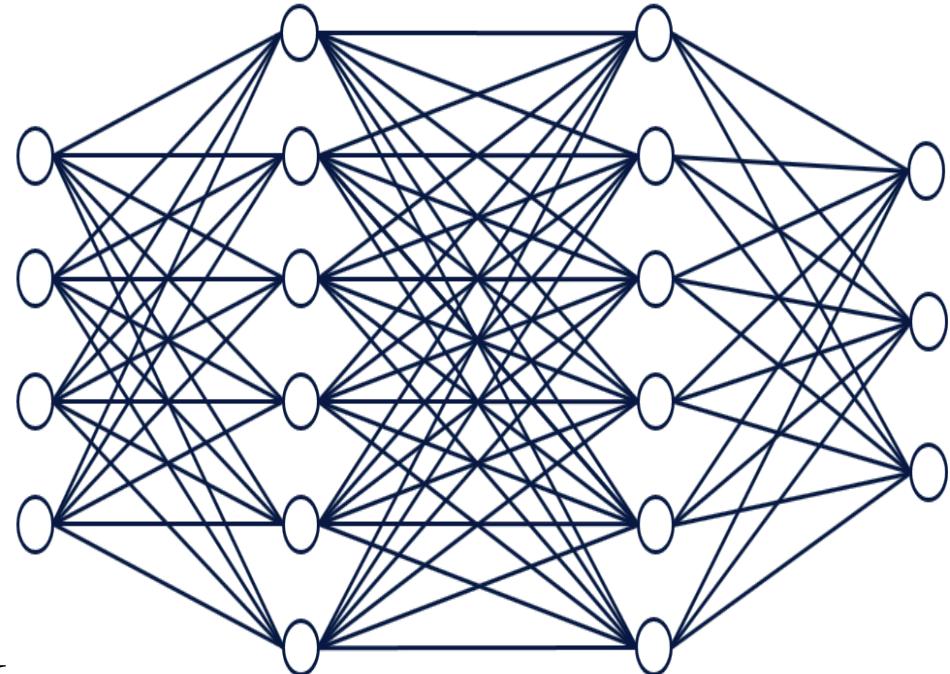
Varying evaluation costs



Smart stopping time



Observable multi-stage feedback



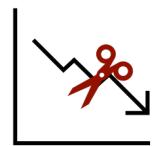
# How does existing principle incorporate them?



Varying evaluation costs

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

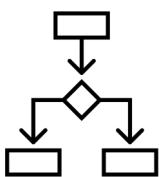
Why not subtraction?



Smart stopping time

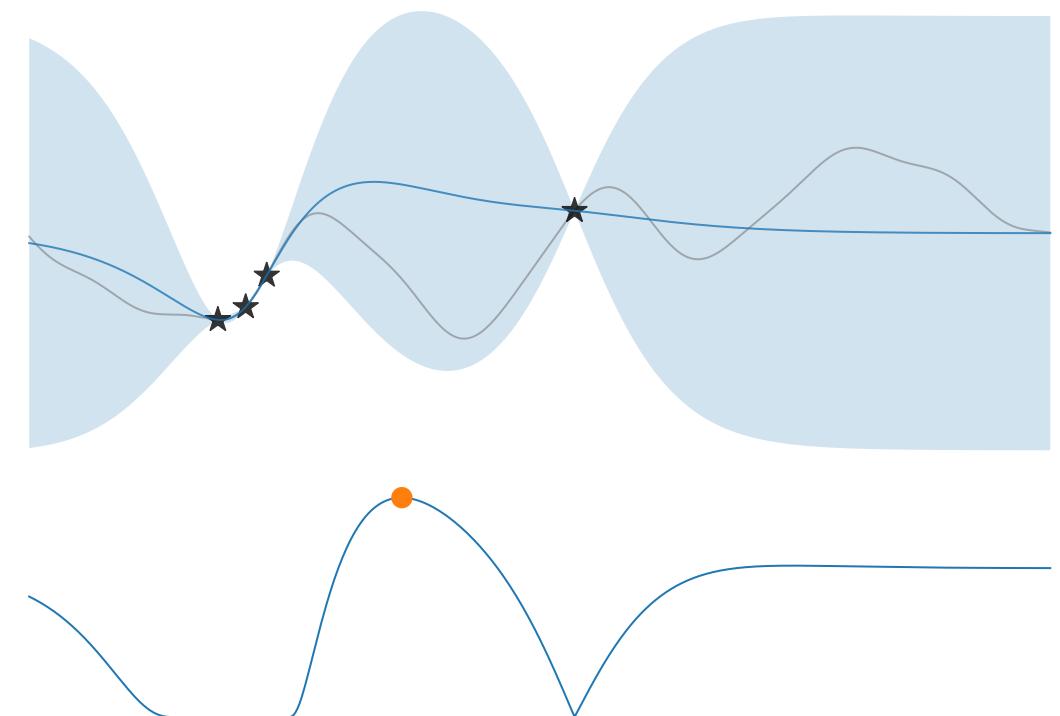
$$EI(x) \leq \theta$$

Which threshold?



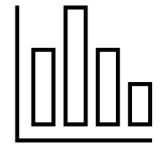
Observable multi-stage feedback

?

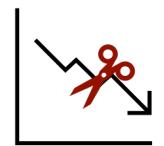


Expected improvement  $EI(x)$

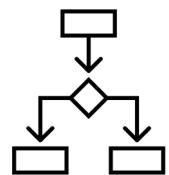
# Under-explored Side Info and Flexibility



Varying evaluation costs



Smart stopping time

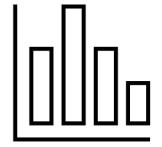


Observable multi-stage feedback



New design principle:  
**Gittins index**

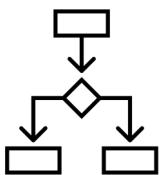
# Why Gittins index?



Varying evaluation costs



Smart stopping time



Observable multi-stage feedback

New design principle:  
Gittins index

**Optimal** in related sequential  
decision problems

# Why Gittins index?



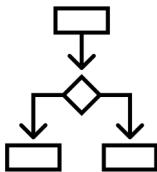
Varying evaluation costs

Features in **Pandora's box**



Smart stopping time

Features in **Pandora's box**

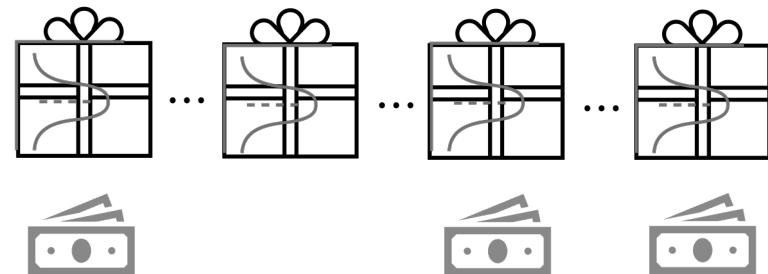


Observable multi-stage feedback



New design principle:  
Gittins index

Optimal in related sequential  
decision problems

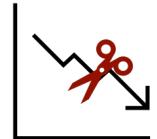


# Why Gittins index?



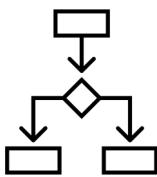
Varying evaluation costs

Features in Pandora's box



Smart stopping time

Features in Pandora's box

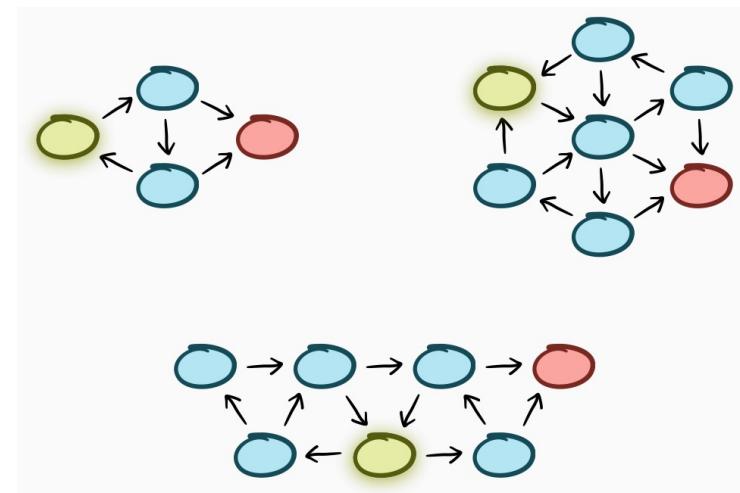


Observable multi-stage feedback

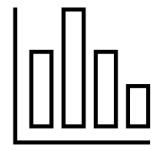
Features in Markov chain selection

New design principle:  
Gittins index

Optimal in related sequential  
decision problems

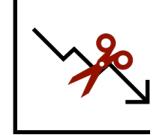


# Why Gittins index?



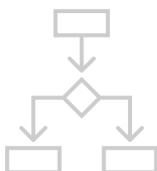
Varying evaluation costs

Features in Pandora's box



Smart stopping time

Features in Pandora's box



Observable multi-stage feedback

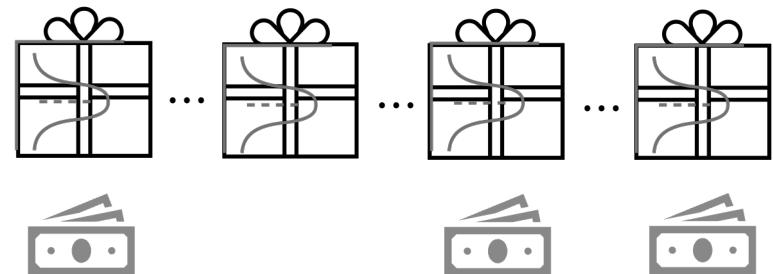
Features in Markov chain selection



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

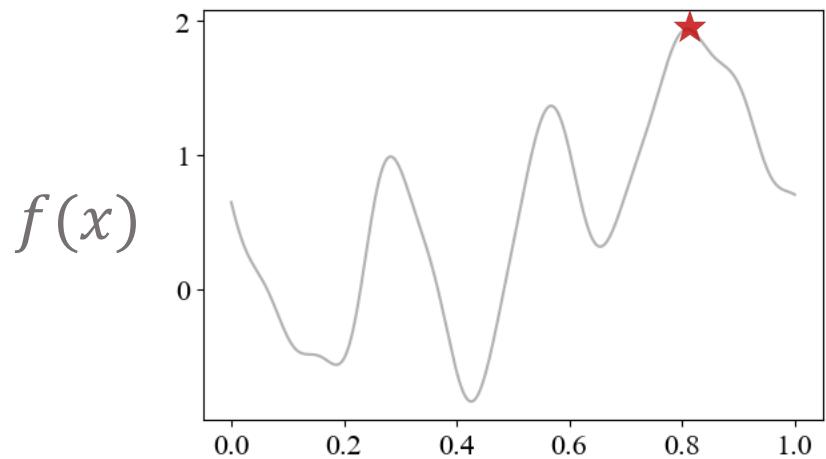
New design principle:  
Gittins index

Optimal in related sequential  
decision problems



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

# Bayesian Optimization



Continuous

Correlated

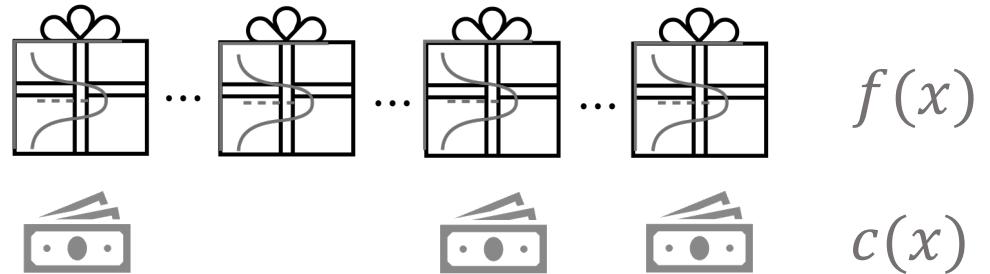
Fixed-iteration

Expected best-observed value

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

# Pandora's Box

[Weitzman'79]



Discrete

Independent

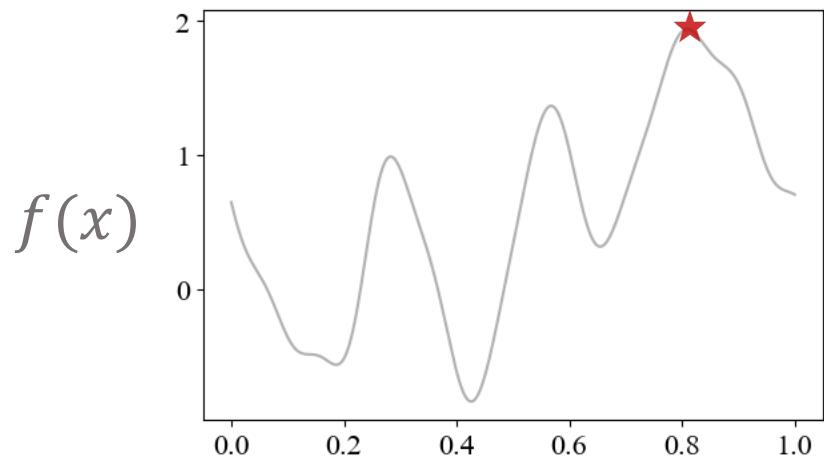
Flexible-stopping

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]



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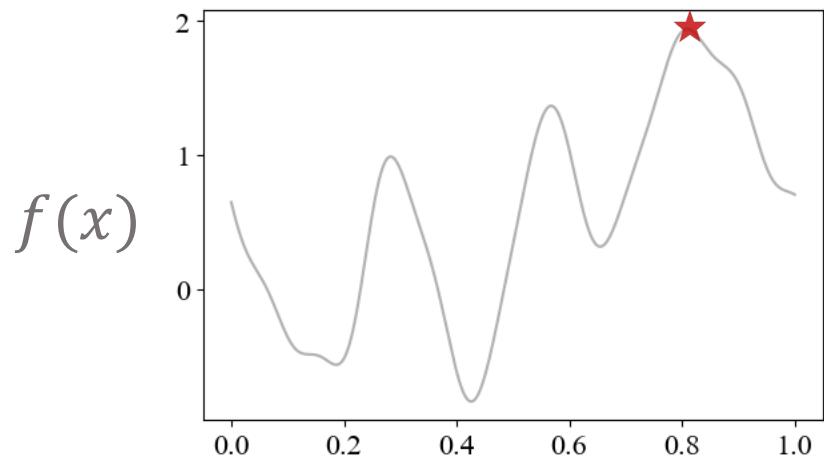
Flexible-stopping

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

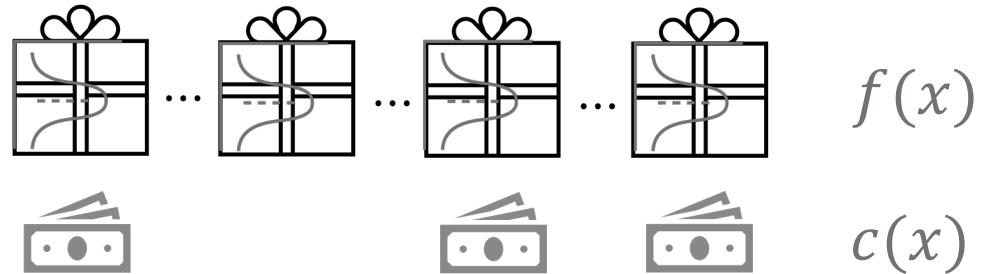
Fixed-iteration

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

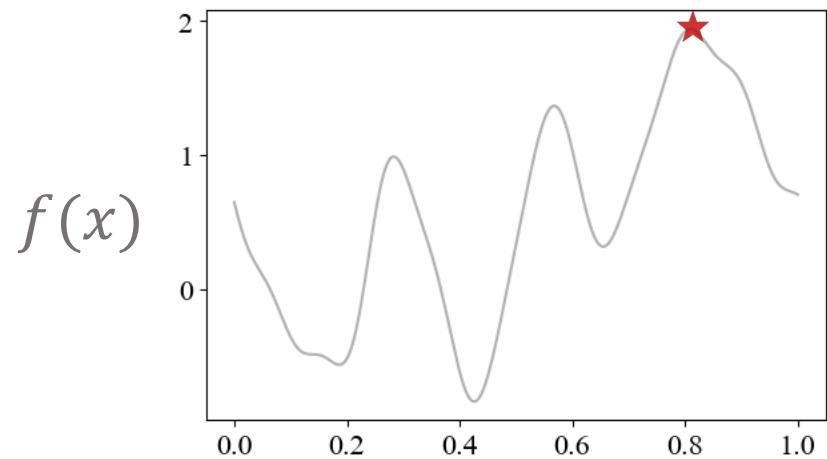
Flexible-stopping

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

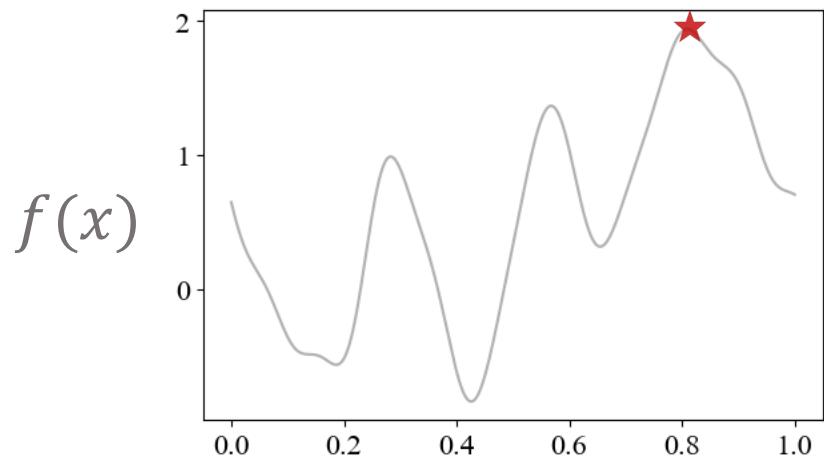
Flexible-stopping

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]

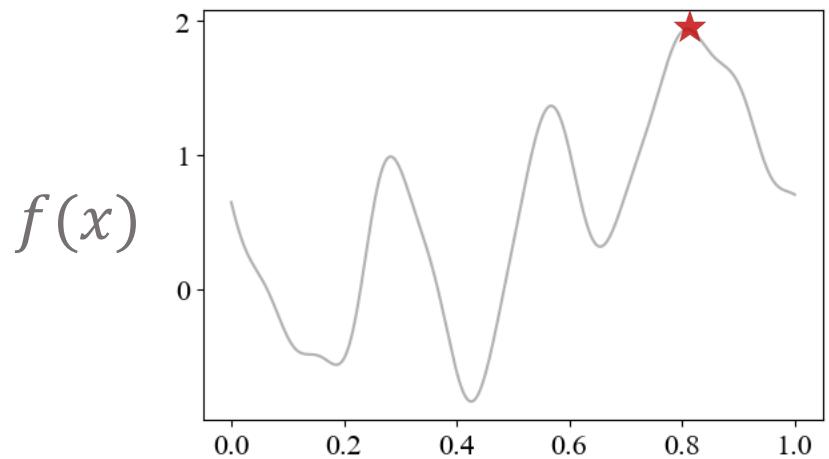


Discrete

Independent

Flexible-stopping  
Expected cost-adjusted regret

# Bayesian Optimization



Continuous

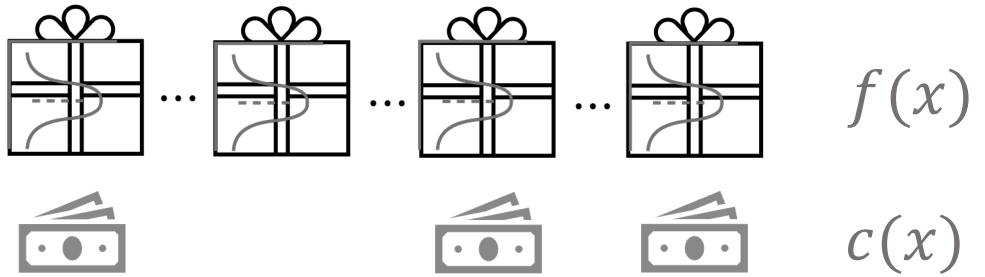
Correlated

Fixed-budget / Flexible-stopping

Expected (cost-adjusted) regret

# Pandora's Box

[Weitzman'79]



Discrete

Independent

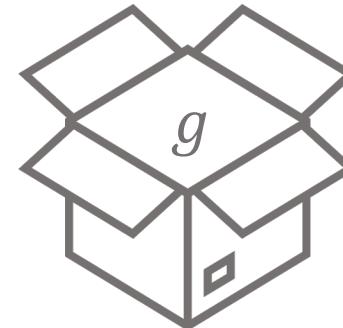
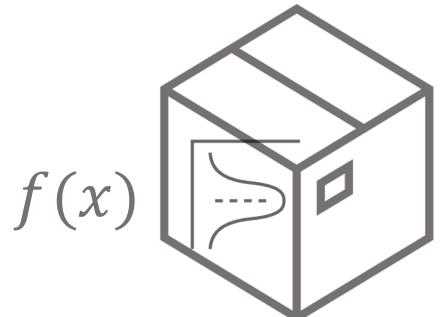
Flexible-stopping

Expected cost-adjusted regret

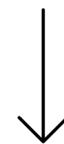
Optimal policy: Gittins index

# Optimal Policy: Gittins Index

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



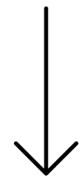
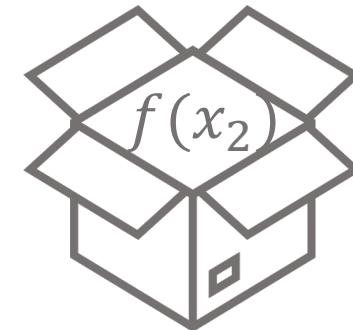
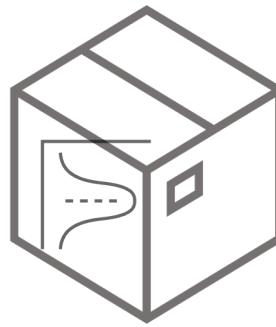
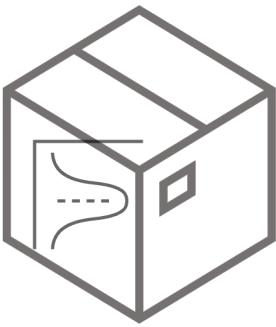
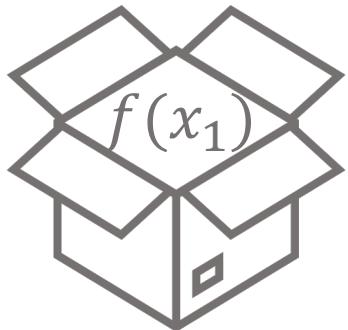
$$\text{GI}_f(x; c(x))$$



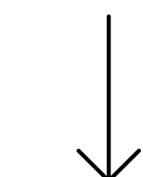
$$g$$

# Optimal Policy: Gittins Index

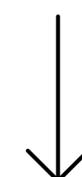
Step 2: Open the box with highest index if it is closed



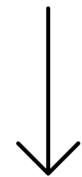
$$f(x_1)$$



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



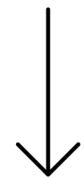
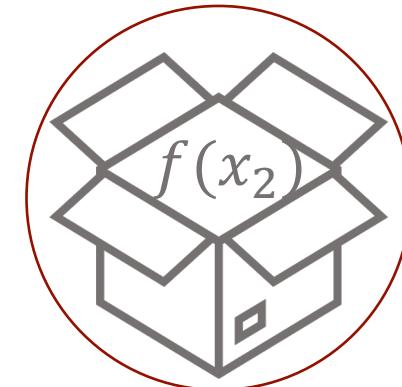
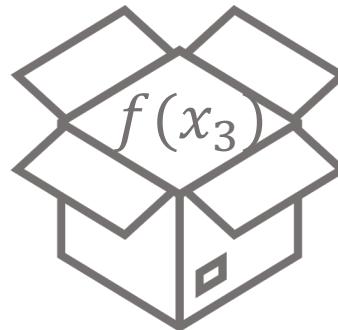
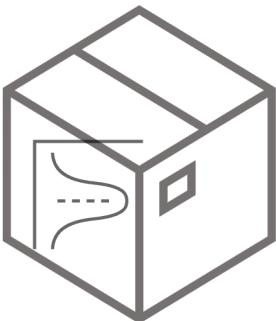
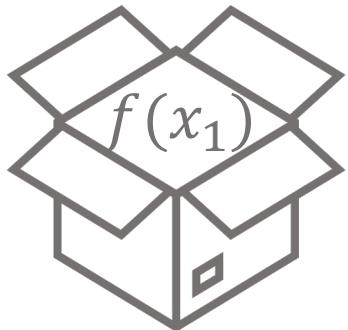
$$\text{GI}_f(x'; c(x'))$$



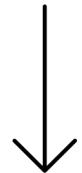
$$f(x_2)$$

# Optimal Policy: Gittins Index

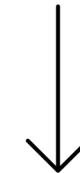
Step 2': Select the box with highest index if it is opened and stop



$$f(x_1)$$



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



$$f(x_3)$$



$$f(x_2)$$

# Expected Improvement vs Gittins Index



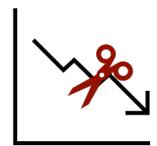
Varying evaluation costs

$$\text{EI}(x)/c(x)$$

Why not subtraction?

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

naturally incorporates costs



Smart stopping time

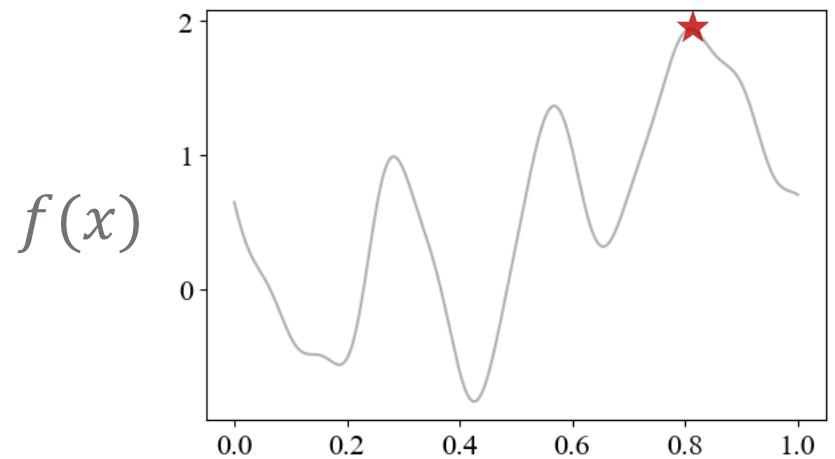
$$\text{EI}(x) \leq \theta$$

Which threshold?

$$\max_x \text{GI}(x; c(x)) \leq y_{\text{best}} \\ \Leftrightarrow \max_x \text{EI}(x)/c(x) \leq 1$$

derived shared stopping rule

# Bayesian Optimization



Continuous

Correlated

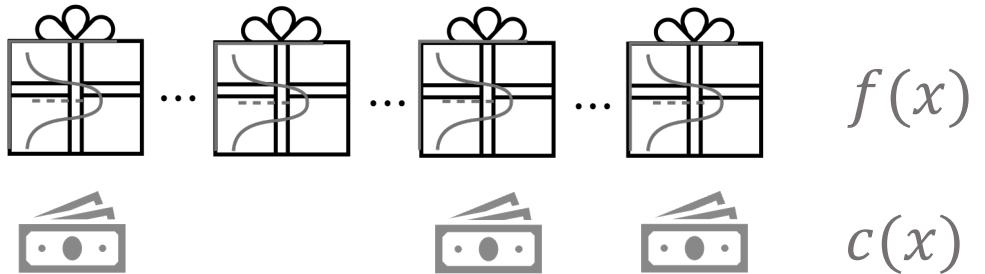
Fixed-budget / Flexible-stopping

Expected (cost-adjusted) regret

Is Gittins index good?

# Pandora's Box

[Weitzman'79]



Discrete

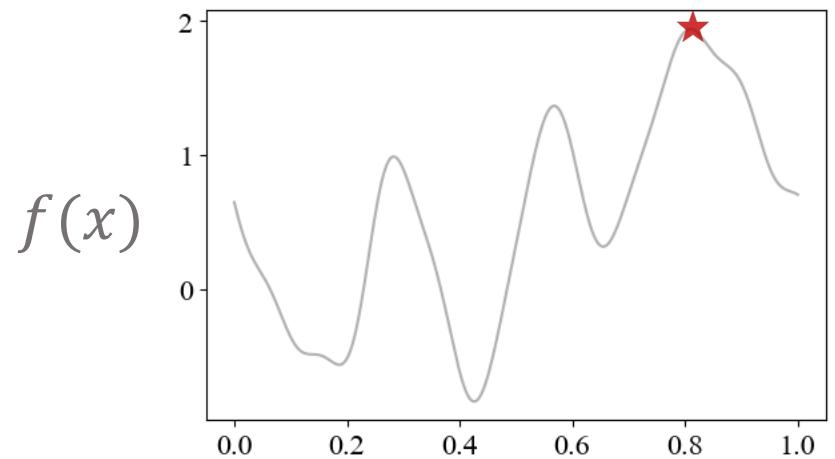
Independent

Flexible-stopping

Expected cost-adjusted regret

Gittins index is optimal

# Bayesian Optimization



Continuous

Correlated

Fixed-budget / Flexible-stopping

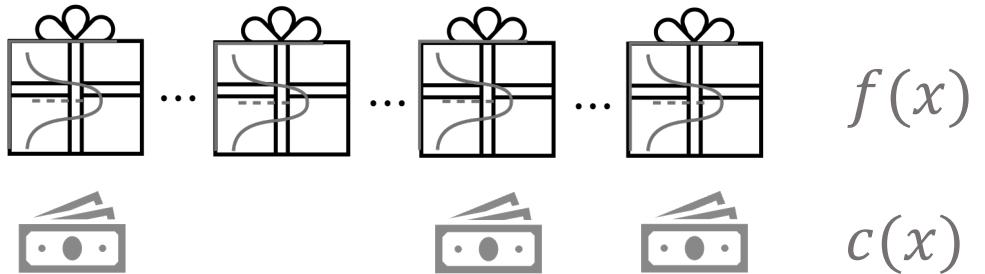
Expected (cost-adjusted) regret

Is Gittins index good?

empirically

# Pandora's Box

[Weitzman'79]



Discrete

Independent

Flexible-stopping

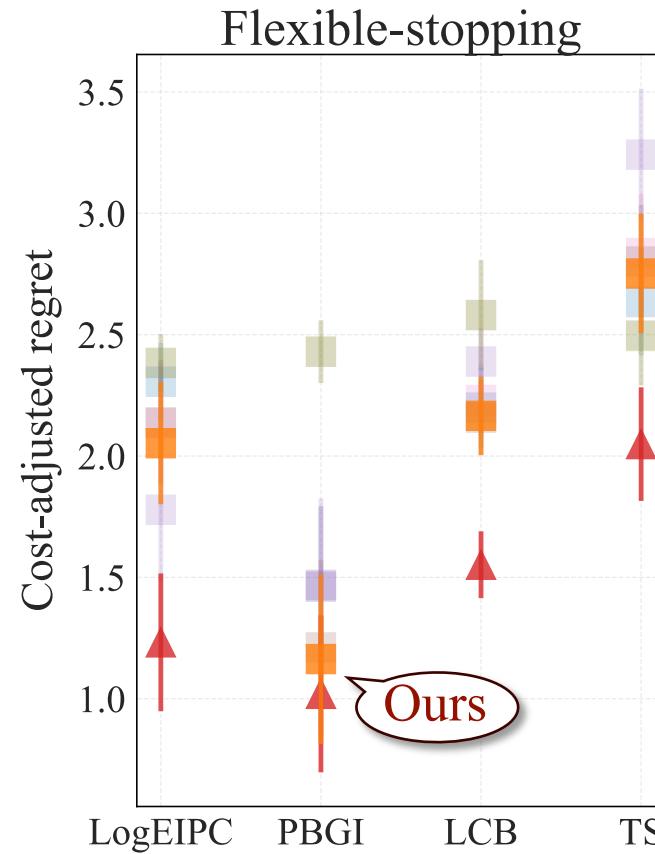
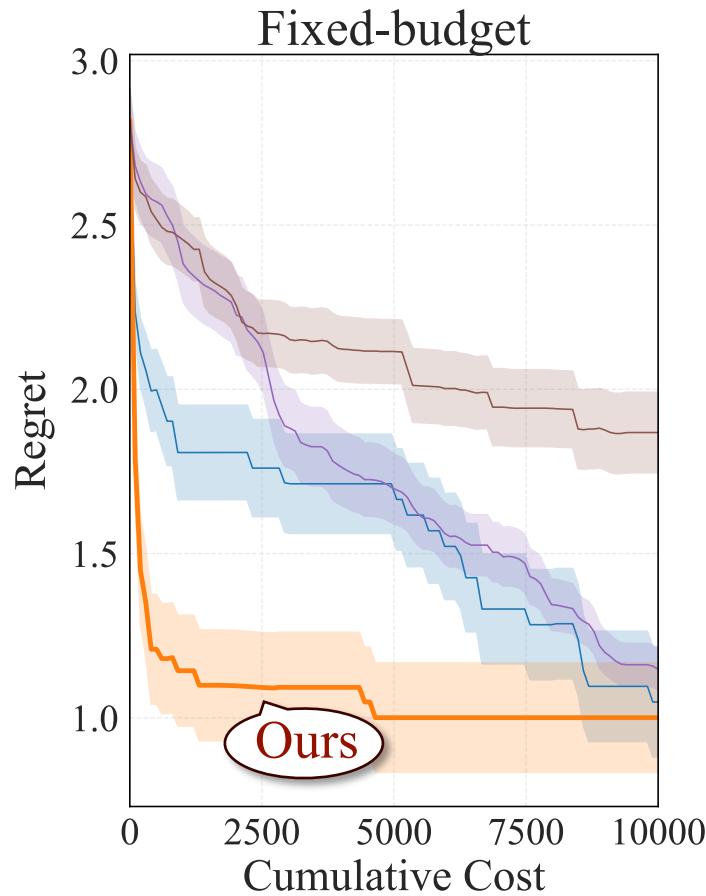
Expected cost-adjusted regret

Gittins index is optimal

# Our Contribution: Gittins Index Principle

1. Principled design via problem simplification
2. Natural incorporation of side info and flexibility
3. Competitive performance on benchmarks
4. Theoretical guarantees

# Gittins Index vs Baselines on AutoML Benchmark

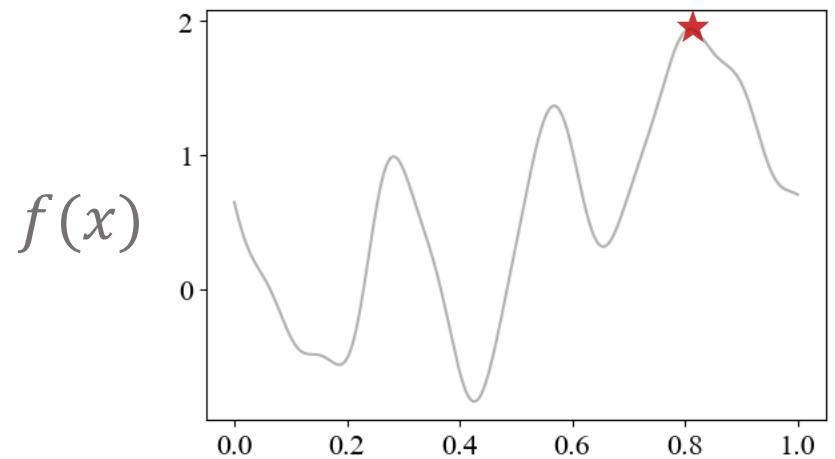


Lower the better

LogEIPC	LCB	PBGI/LogEIPC	SRGap-med	GSS	PRB
PBGI	TS	LogEIPC-med	UCB-LCB	Convergence	Hindsight

Bound on achievable performance

# Bayesian Optimization



Continuous

Correlated

Fixed-budget / Flexible-stopping

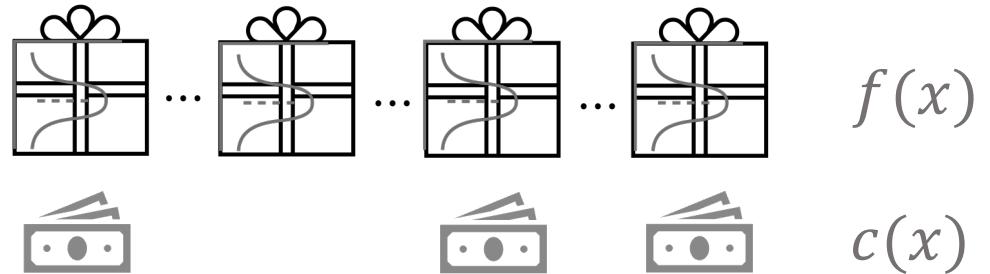
Expected (cost-adjusted) regret

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

Joint work with Ziv Scully and Alexander Terenin et al.

1. Principled design via problem simplification
2. Natural incorporation of side info and flexibility
3. Competitive performance on benchmarks
4. Theoretical guarantees

# Theoretical Guarantee and Empirical Validation

Theorem (Safeguard Guarantee)

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

or LogEIPC

cost-adjusted regret

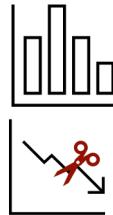
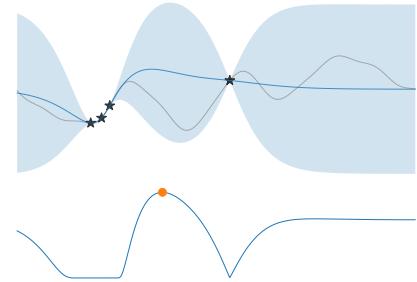
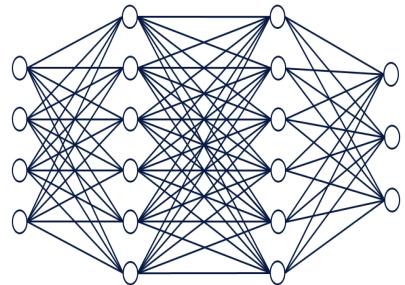
## Implication:

- 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.



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

## Studied problem

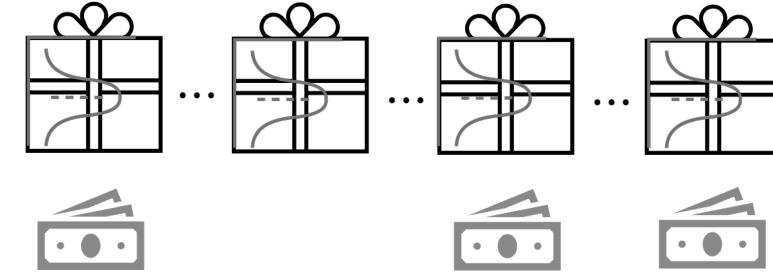


Varying evaluation costs



Adaptive stopping time

## Key idea



Link to Pandora's Box problem  
& Gittins index theory

## Impact



BoTorch



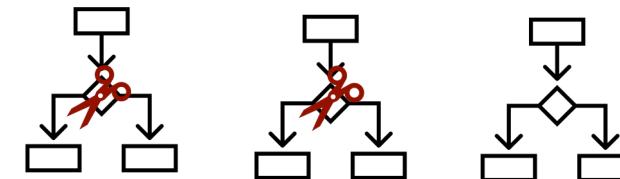
Ax

Competitive empirical performance &  
interests from practitioners



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

## Ongoing work

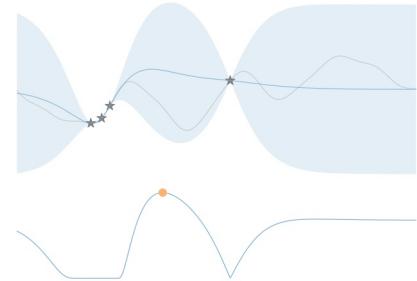
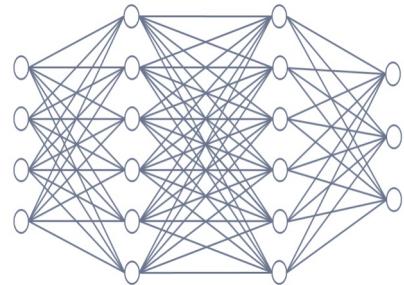


Sharper theoretical guarantees & black-  
box optimization w/ multi-stage feedback



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

# Studied problem

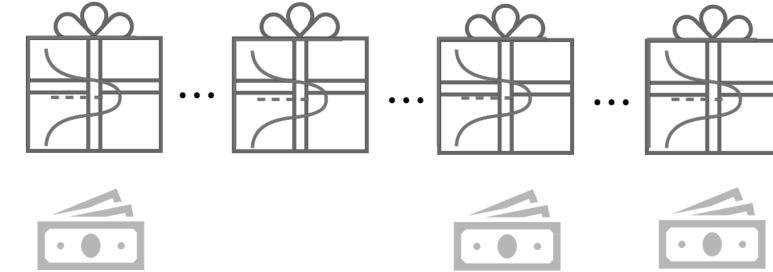


Varying evaluation costs



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



ChatGPT



deepseek

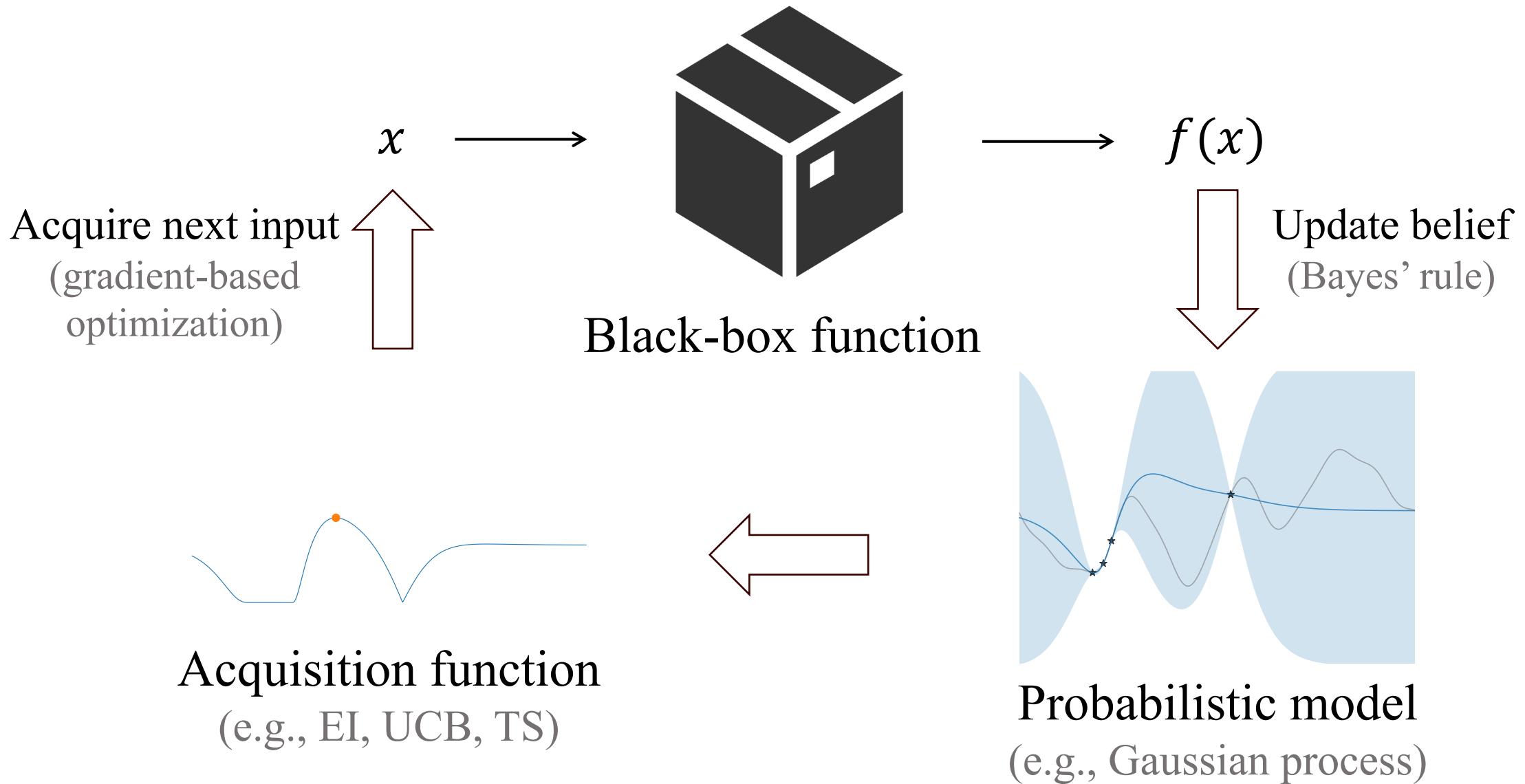


## LLM-driven black-box optimization

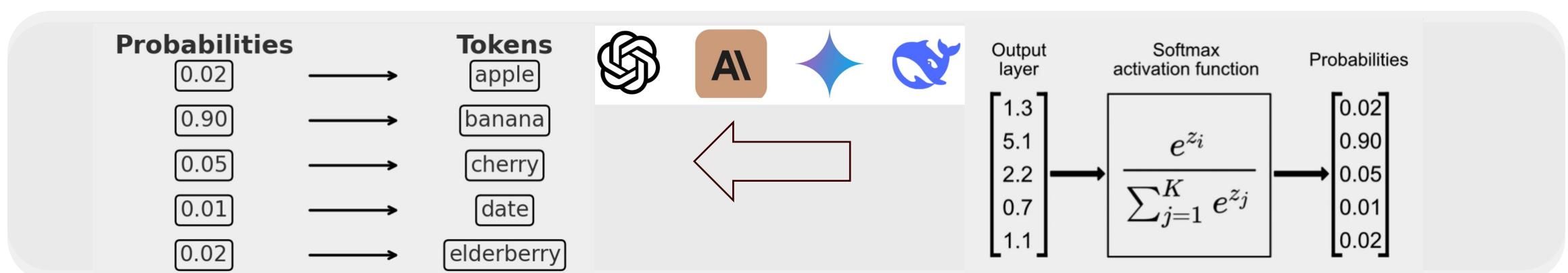
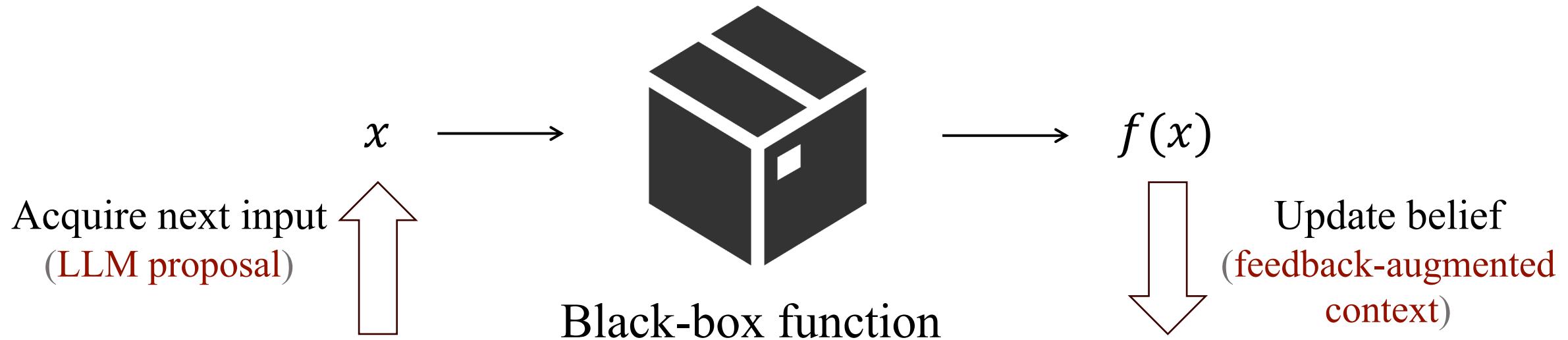


"Cost-aware Stopping for Bayesian  
Optimization." Under review.

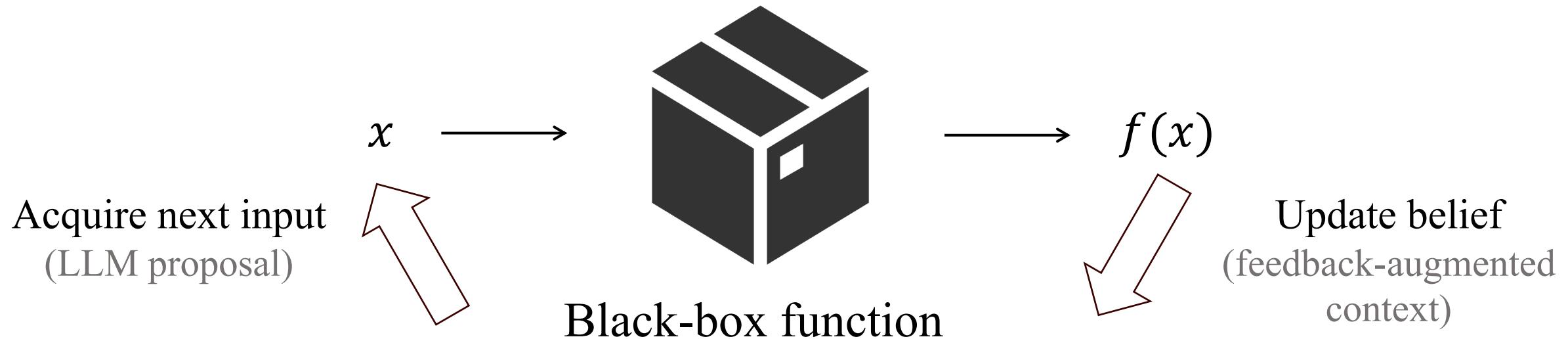
# Recap: Bayesian Optimization



# Ongoing: LLM-Driven Black-Box Optimization



# Ongoing: LLM-Driven Black-Box Optimization



ChatGPT

Gemini



deepseek Claude

Large language model

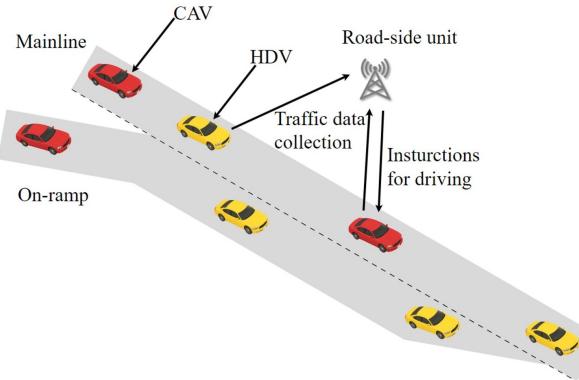
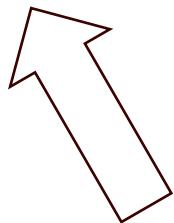
# Ongoing: LLM-Driven Black-Box Optimization

Mixed-autonomy traffic control:

(e.g., Transformer config)

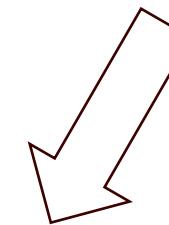
RL state representation

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)



ChatGPT

Gemini



deepseek Claude

Large language model

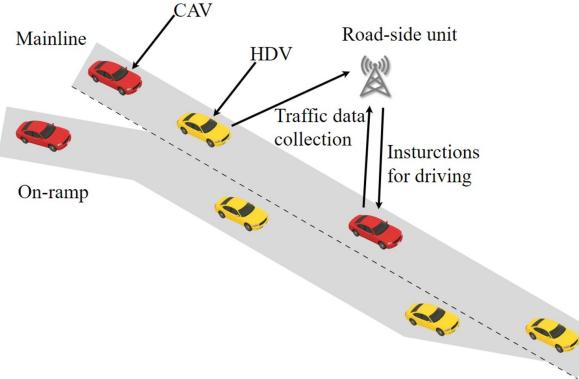
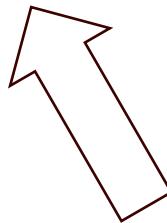
# Ongoing: LLM-Driven Black-Box Optimization

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)

Can side info help?

Black-box function  
(RL training & evaluation)



ChatGPT

Gemini



deepseek



Claude

Large language model

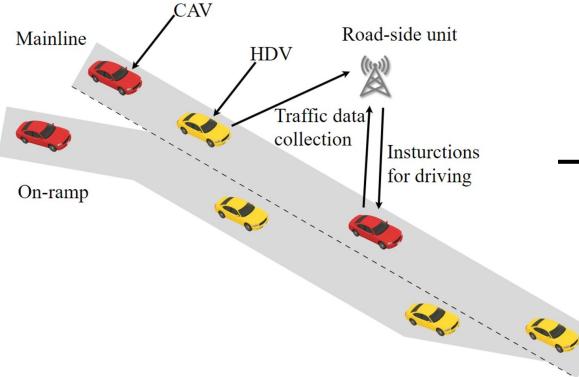
# Our LLM-Driven Method: Incorporate Side Info

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)

Black-box function  
(RL training & evaluation)



ChatGPT



deepseek



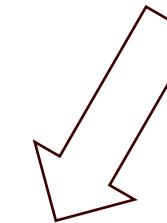
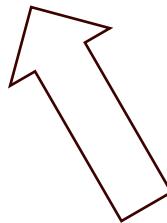
Claude

Large language model

Average speed

Update belief  
(feedback-augmented context)

performance metric +  
representation quality



# 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.