

# Cost-Aware Bayesian Optimization with Adaptive Stopping via the Pandora's Box Gittins Index

Qian Xie 谢倩 (Cornell ORIE)

Job Talk

# Motivation: World of Optimization under Uncertainty

ML model training:

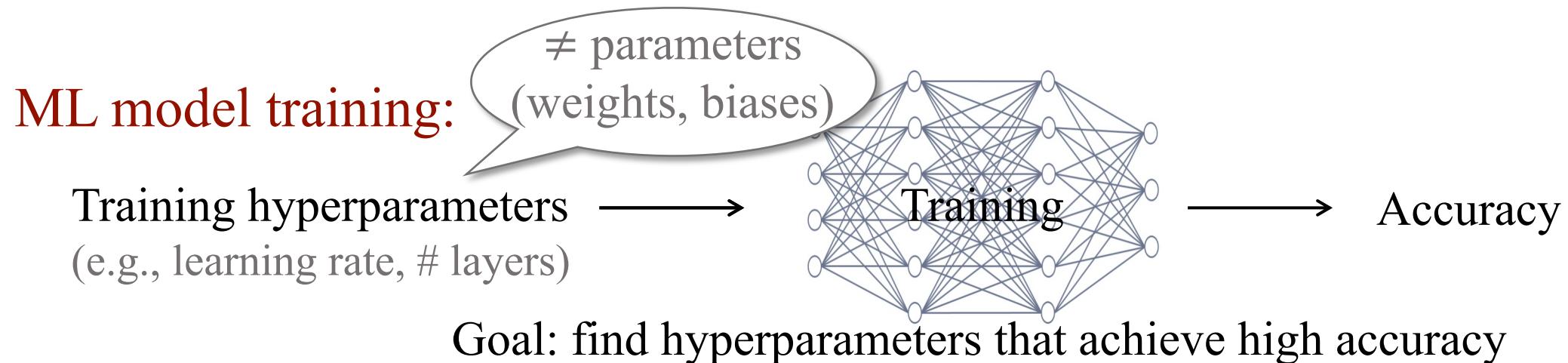
Training hyperparameters  $\longrightarrow$   
(e.g., learning rate, # layers)



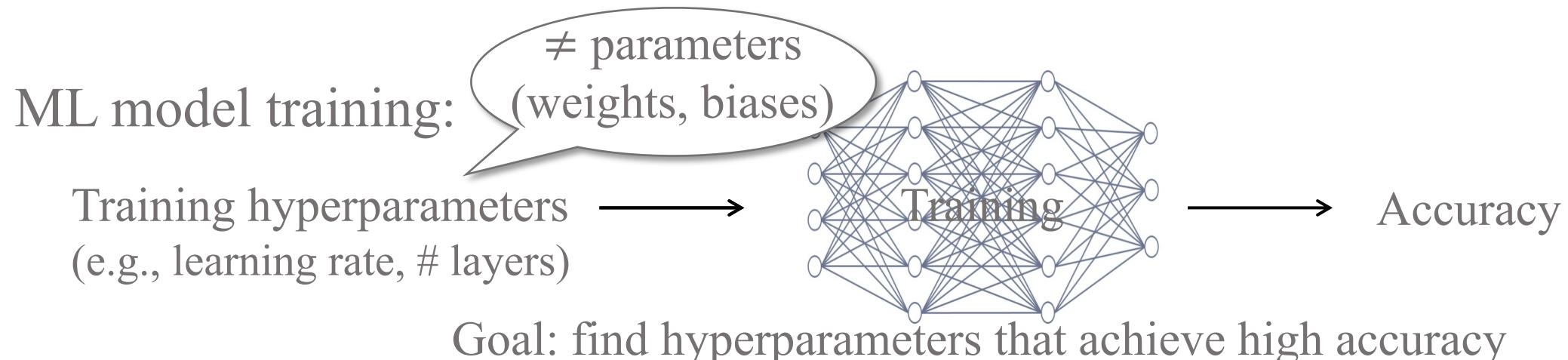
$\longrightarrow$  Accuracy

Goal: find hyperparameters that achieve high accuracy

# Motivation: World of Optimization under Uncertainty



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## Adaptive experimentation:



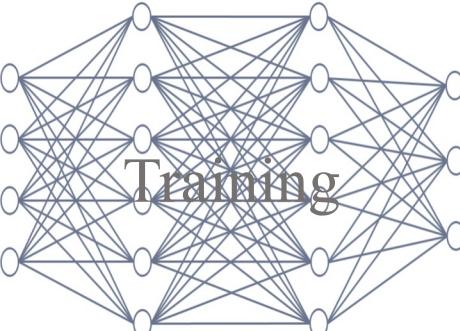
Goal: make decisions to achieve high revenue

# Motivation: World of Optimization under Uncertainty



Goal:  $\max_{x \in \mathcal{X}} f(x)$

ML model training:

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

Adaptive experimentation:

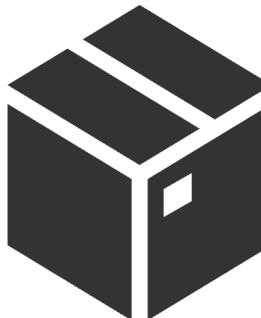
Decision/design variables  
(e.g., layout, pricing level)  $\longrightarrow$    $\longrightarrow$  Revenue

# Motivation: World of Optimization under Uncertainty

Black-box optimization:

(gradient-based methods not applicable)

Input  $x$   $\longrightarrow$



non-analytical &  
no gradient info

Observed outcome  $f(x)$

Goal:  $\max_{x \in \mathcal{X}} f(x)$

ML model training:

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



Accuracy

Adaptive experimentation:

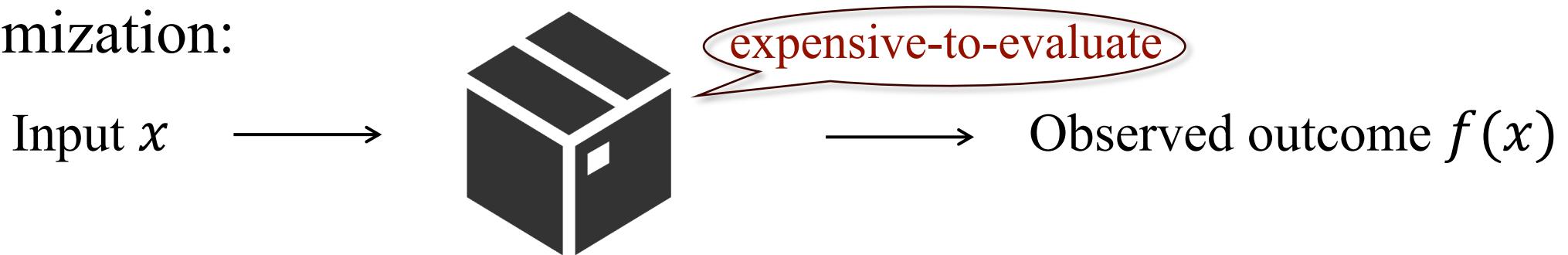
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Revenue

# Background: Black-Box Optimization

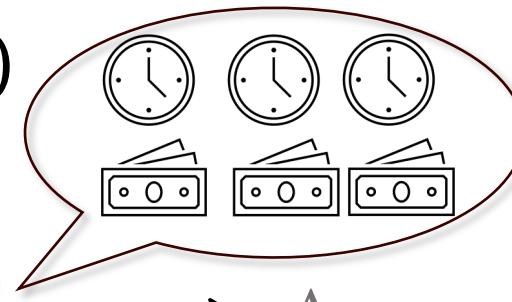
Black-box optimization:



ML model training:

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

Goal:  $\max_{x \in \mathcal{X}} f(x)$

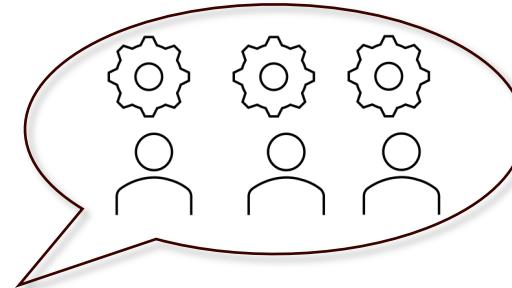
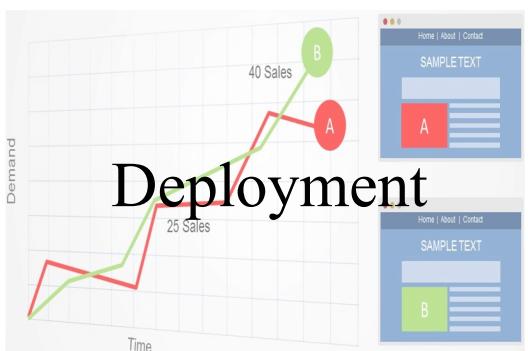


Training time

Compute credits

Adaptive experimentation:

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



Operational cost

User experience

# Background: Black-Box Optimization

Black-box optimization:

Input  $x$   $\longrightarrow$



expensive-to-evaluate

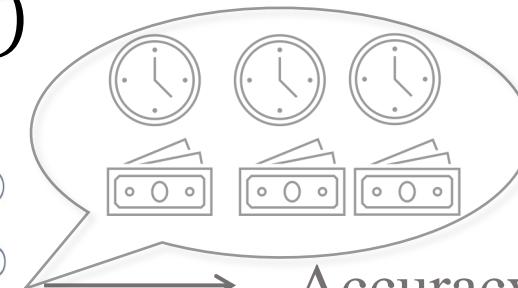
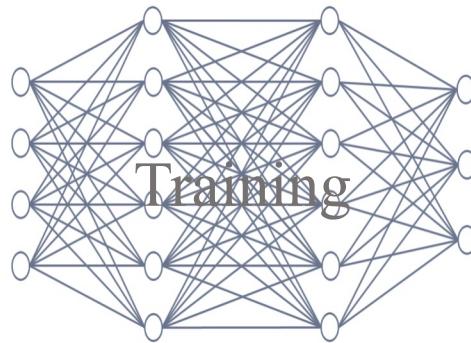
Goal:  $\mathbb{E} \max_{t=1,2,\dots,T} f(x_t)$

Observed outcome  $f(x)$

limited #evaluations

ML model training:

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

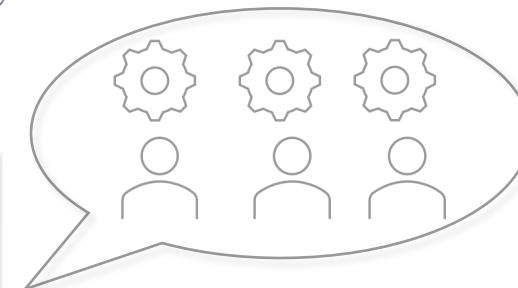


Training time

Compute credits

Adaptive experimentation:

Decision/design variables  
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Operational cost

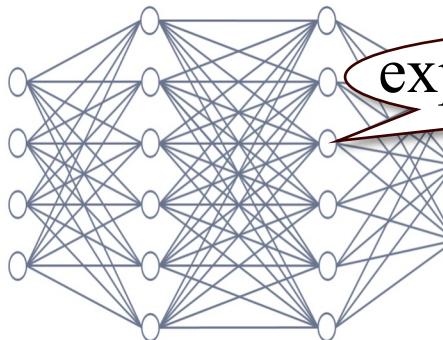
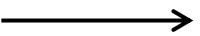
User experience

Revenue

# Naïve Non-Adaptive Approach: Grid Search

ML model training:

Training hyperparameters



expensive-to-evaluate

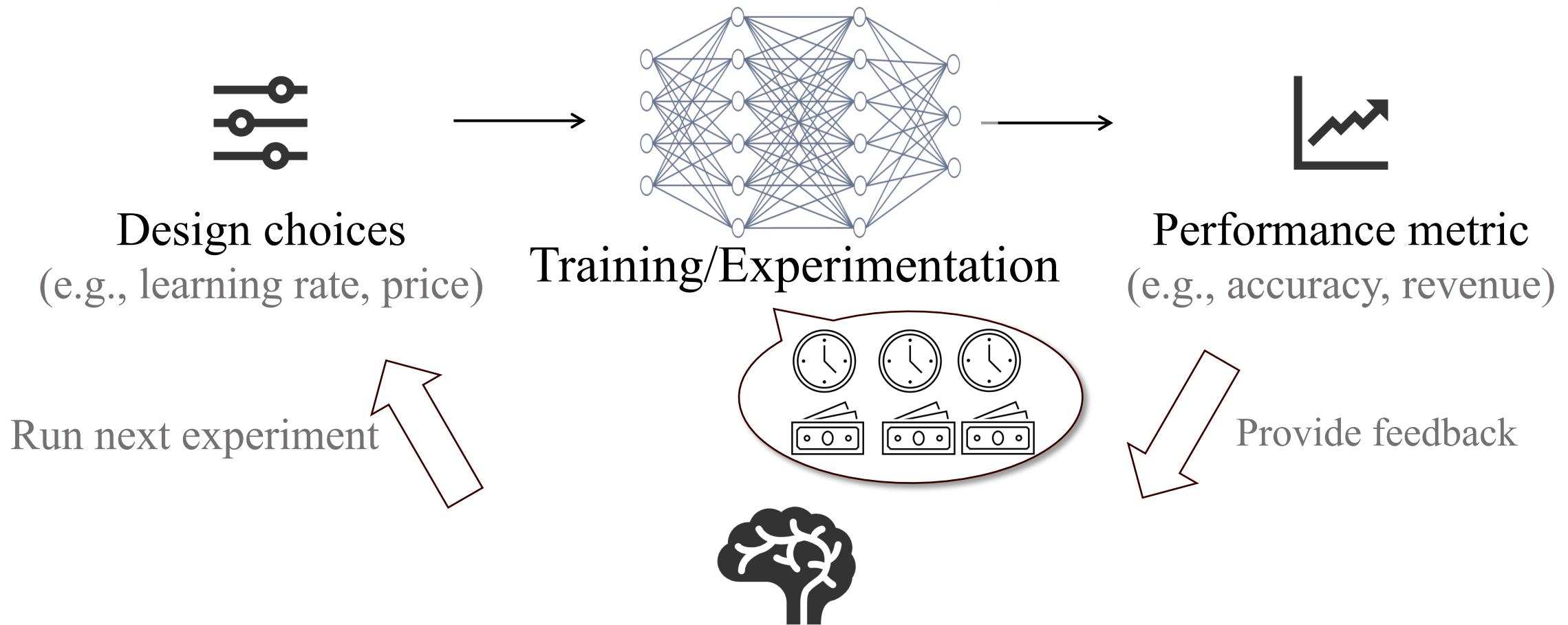
→ Accuracy

Goal: find hyperparameters that achieve high accuracy

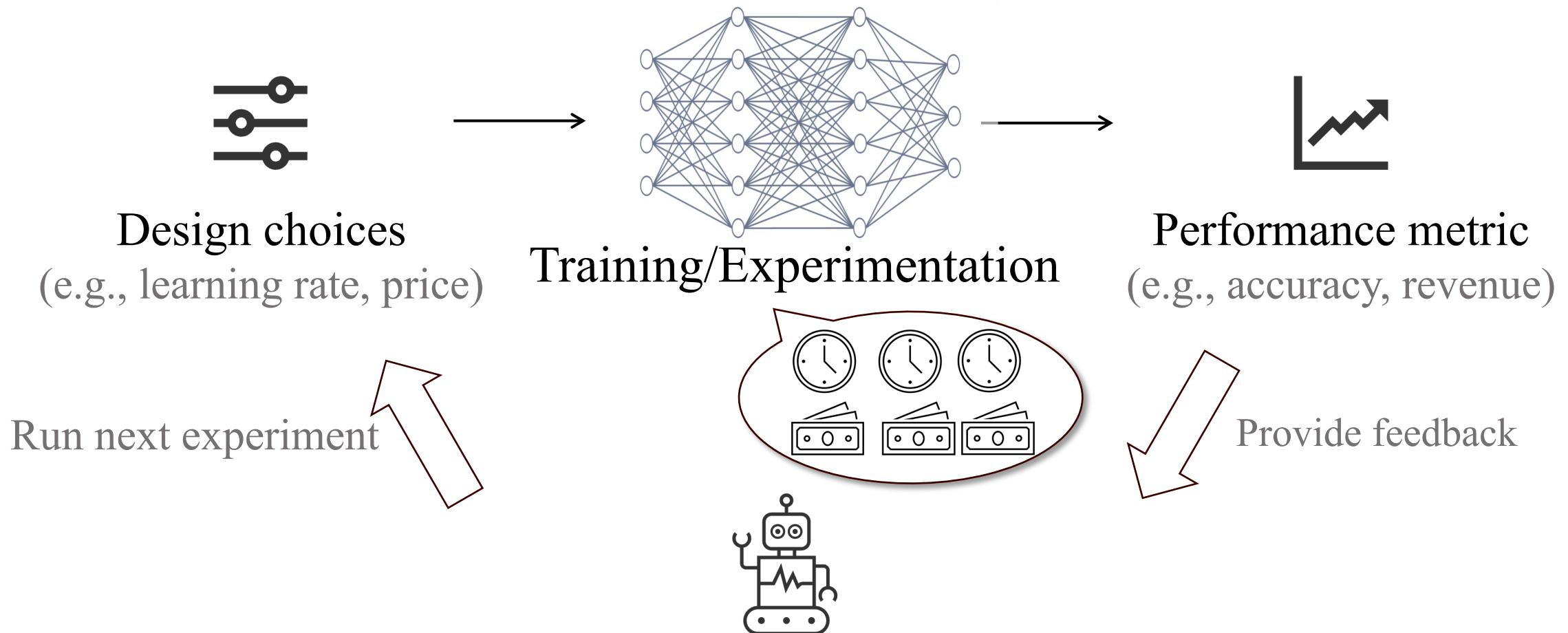
| Training hyperparameter | Range        | Number of Options |
|-------------------------|--------------|-------------------|
| Batch size              | [16, 512]    | 10                |
| Learning rate           | [1e-4, 1e-1] | 10                |
| Momentum                | [0.1, 0.99]  | 10                |
| Weight decay            | [1e-5, 1e-1] | 10                |
| Number of layers        | {1, 2, 3, 4} | 4                 |
| Max units per layer     | [64, 1024]   | 10                |
| Dropout                 | [0.0, 1.0]   | 10                |

40,000,000  
combinations!

# Naïve Adaptive Approach: Manual Tuning



# Data-Driven Adaptive Approaches



# Existing Umbrellas of Black-Box Optimization

## Naïve approaches:

- Grid search
- Random search
- Manual tuning

## Data-driven approaches:

- Local search
- Evolutionary algorithms
- Bayesian optimization
- Reinforcement learning
- LLM agent

# New Methods for Black-Box Optimization

## Naïve approaches:

- Grid search
- Random search
- Manual tuning

## Data-driven approaches:

- Local search
- Evolutionary algorithms
- Bayesian optimization ★
- Reinforcement learning ★
- LLM agent ★



## Contributions of new methods proposed in my work:

1. Novel connection to related decision problems
2. Principled decision rules
3. Competitive empirical performance



New methods under this umbrella

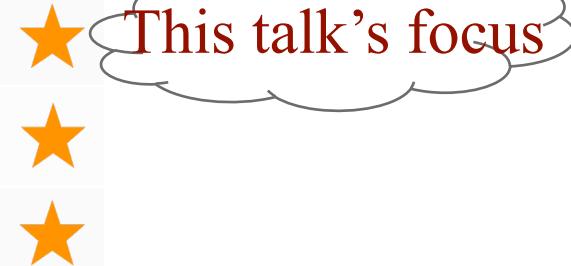
# New Methods for Black-Box Optimization

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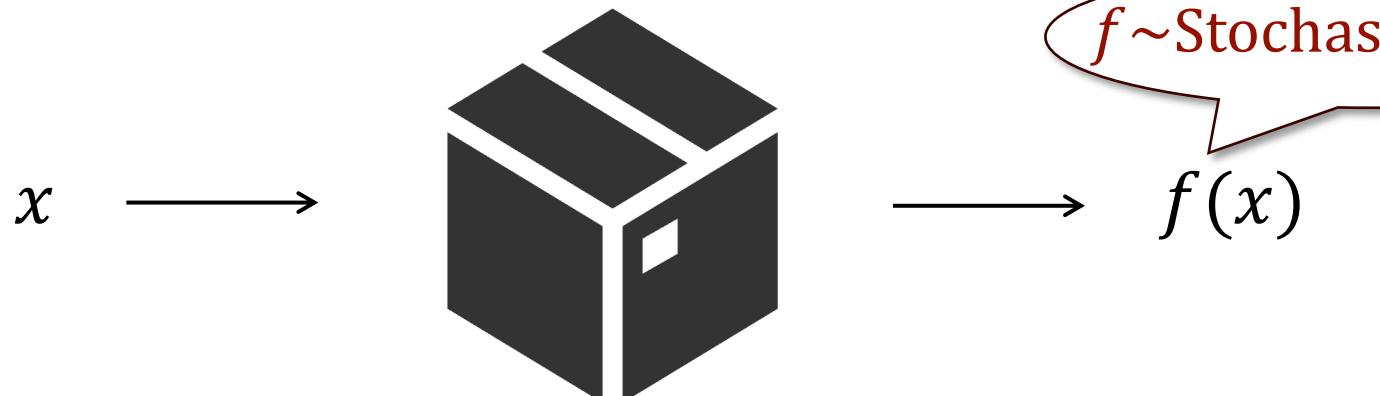
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New methods under this umbrella

# Bayesian Optimization

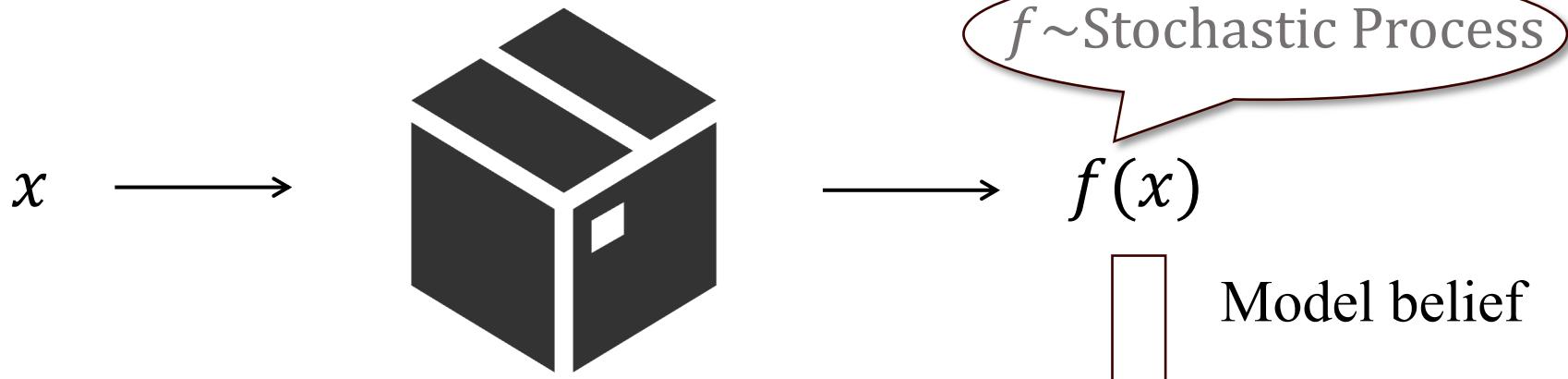


Black-box function

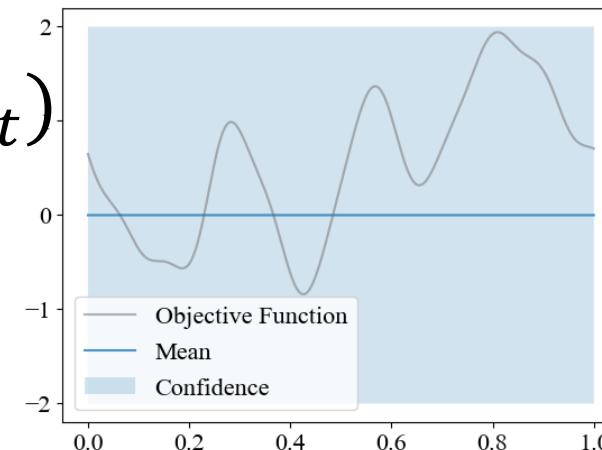
Goal:  $\max_{x \in \mathcal{X}} f(x)$

# Bayesian Optimization

Time 0



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

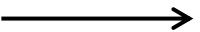


Probabilistic model  
(e.g., Gaussian process)

# Bayesian Optimization

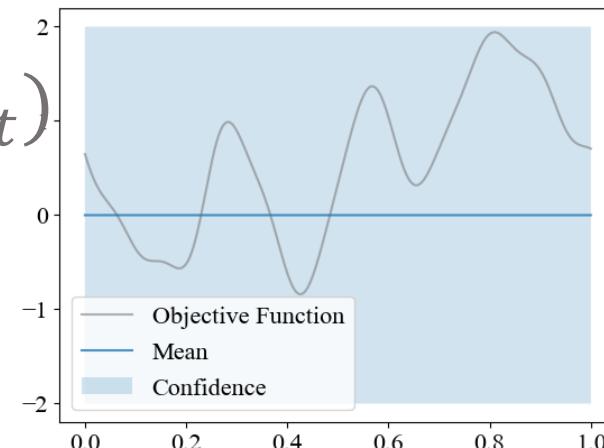
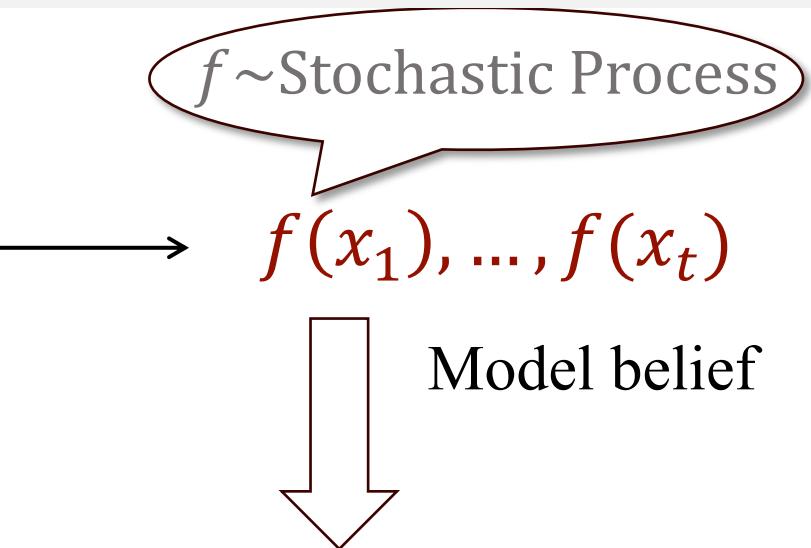
Time  $t$

$x_1, \dots, x_t$



Black-box function

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



Probabilistic model  
(e.g., Gaussian process)

# Bayesian Optimization

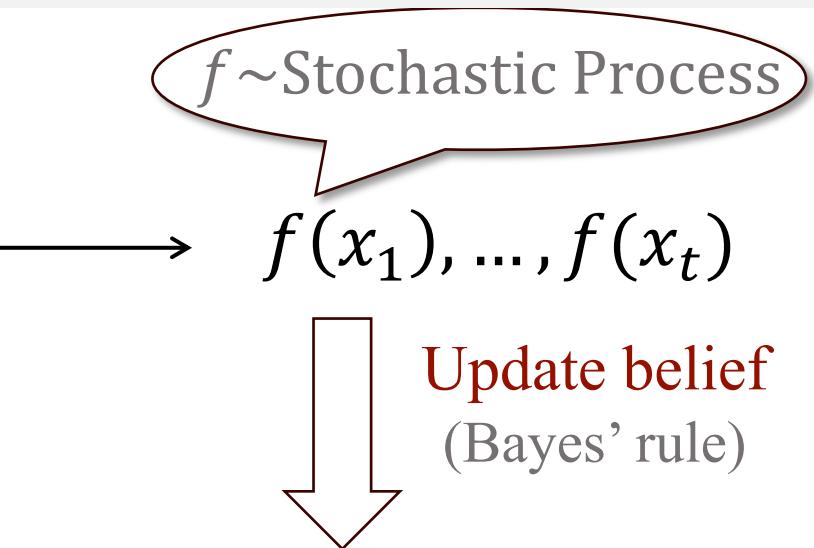
Time  $t$

$x_1, \dots, x_t$



Black-box function

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



Probabilistic model  
(e.g., Gaussian process)

# Bayesian Optimization

Time  $t$

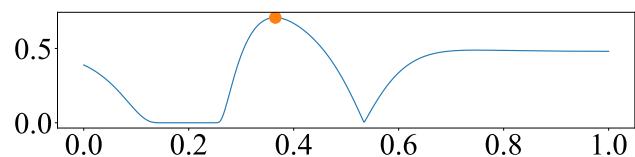
$x_1, \dots, x_t$



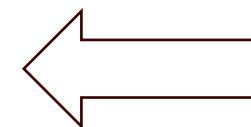
$f(x_1), \dots, f(x_t)$

Black-box function

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

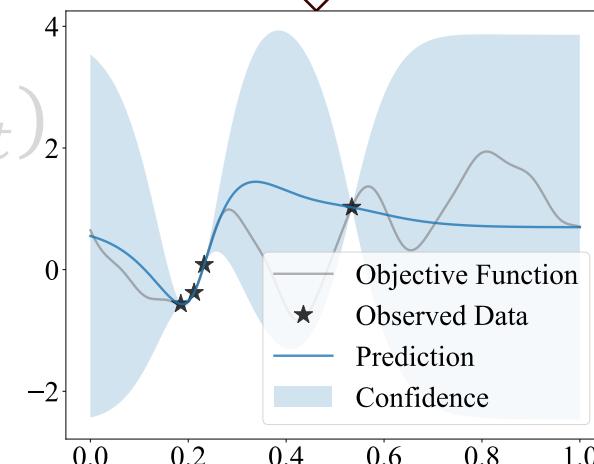


Decision rule  
(What to evaluate next)



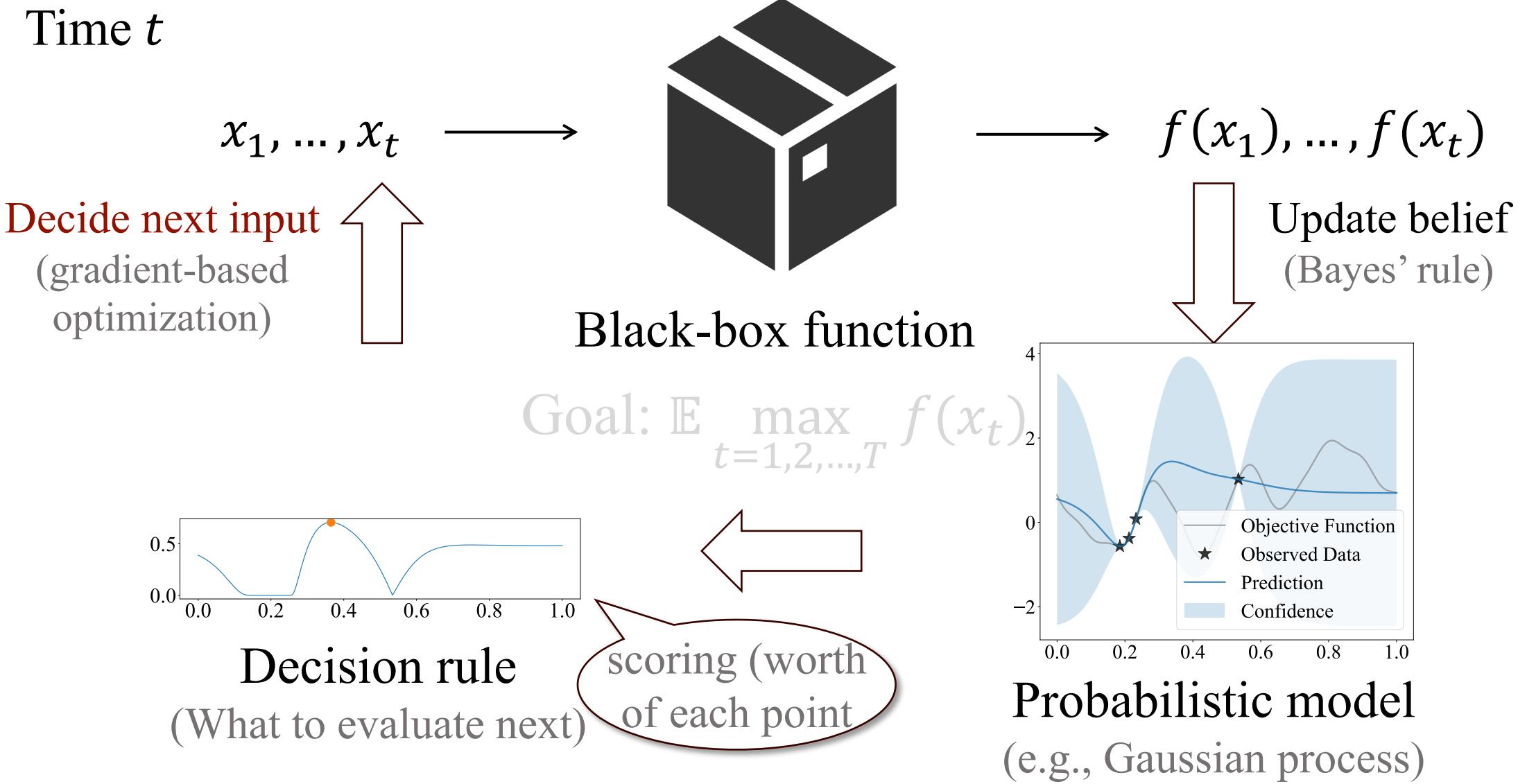
scoring (worth  
of each point)

Update belief  
(Bayes' rule)



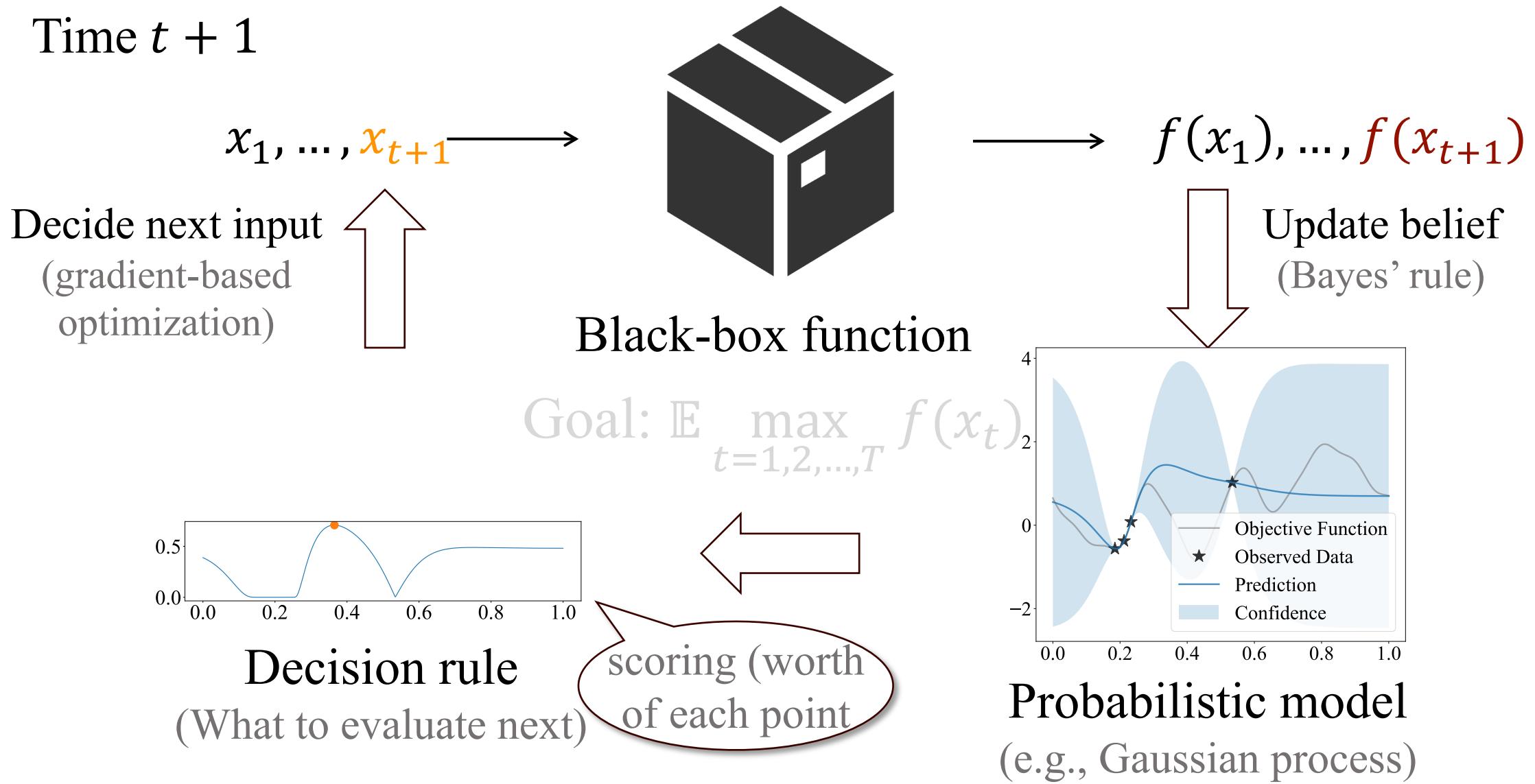
Probabilistic model  
(e.g., Gaussian process)

# Bayesian Optimization



# Bayesian Optimization

Time  $t + 1$



# Bayesian Optimization

Time  $t + 1$

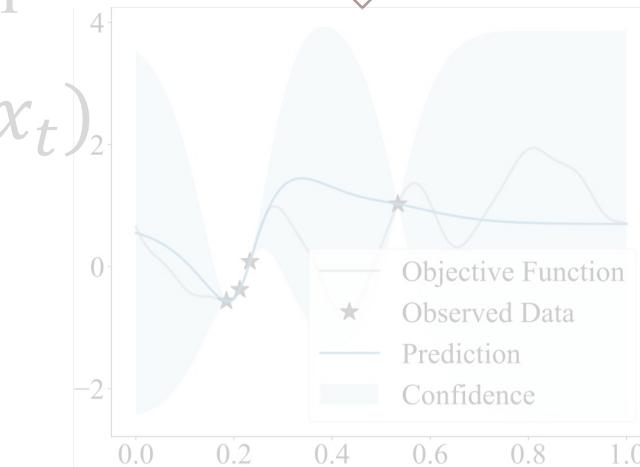
$x_1, \dots, x_{t+1} \longrightarrow$

Decide next input  
(gradient-based  
optimization)



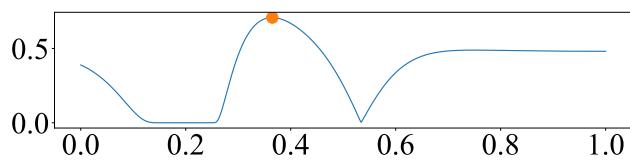
$f(x_1), \dots, f(x_{t+1})$

Update belief  
(Bayes' rule)



Black-box function

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

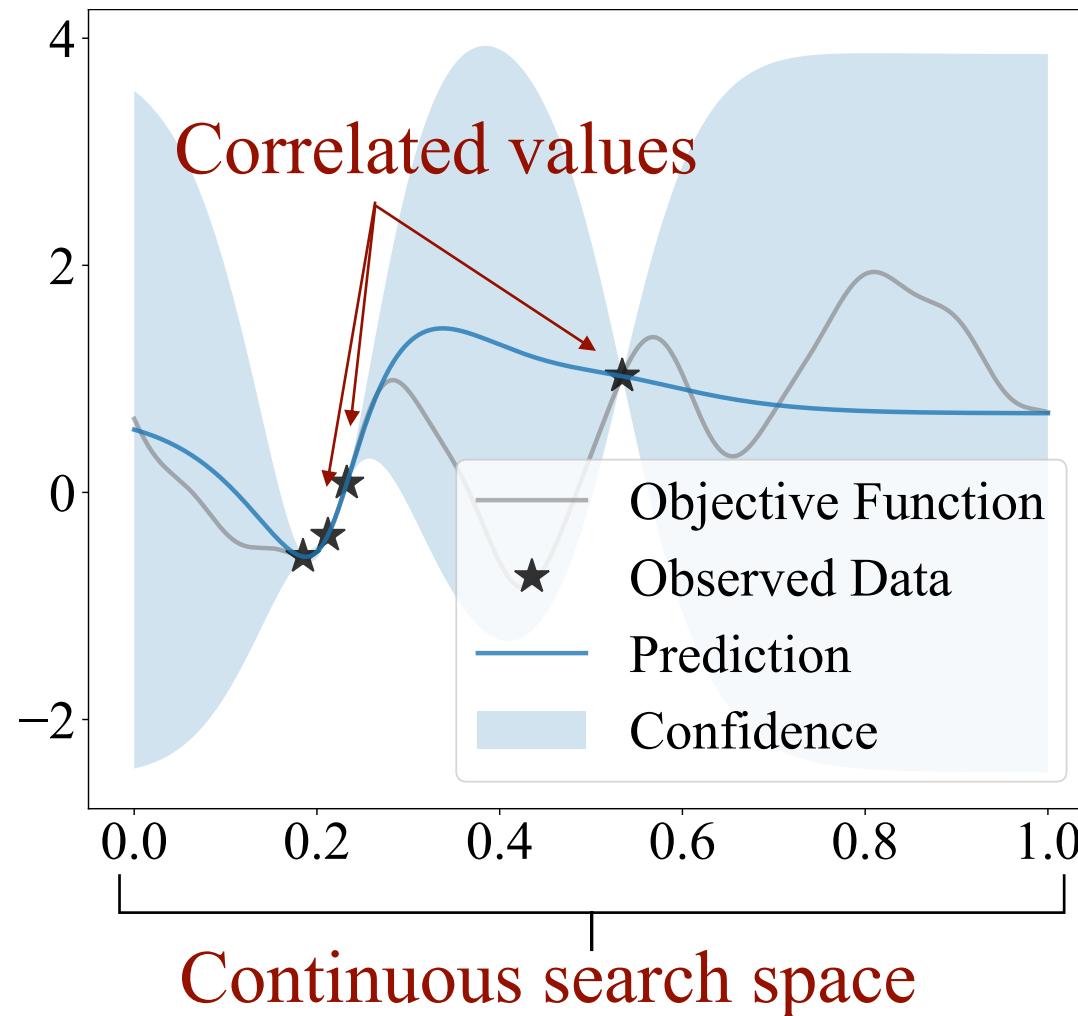


Decision rule  
(What to evaluate next)

scoring (worth  
of each point)

Probabilistic model  
(e.g., Gaussian process)

# Challenges in Decision Rule Design



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

# Popular Decision Rule: Expected Improvement

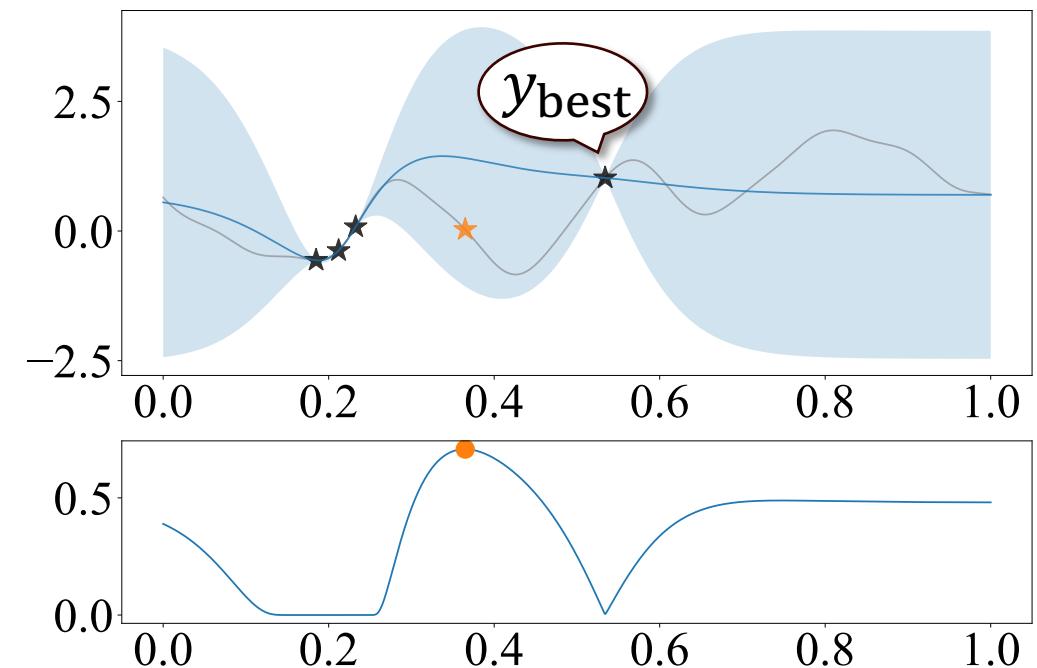
$$EI(x) = \mathbb{E}[\max(f(x) - y_{\text{best}}, 0) | x_1, \dots, x_t]$$

current best observed  
data  $D$   
“improvement”

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

posterior distribution

One-step approximation to MDP



Expected improvement  $EI(x)$

# Popular Decision Rule: Expected Improvement

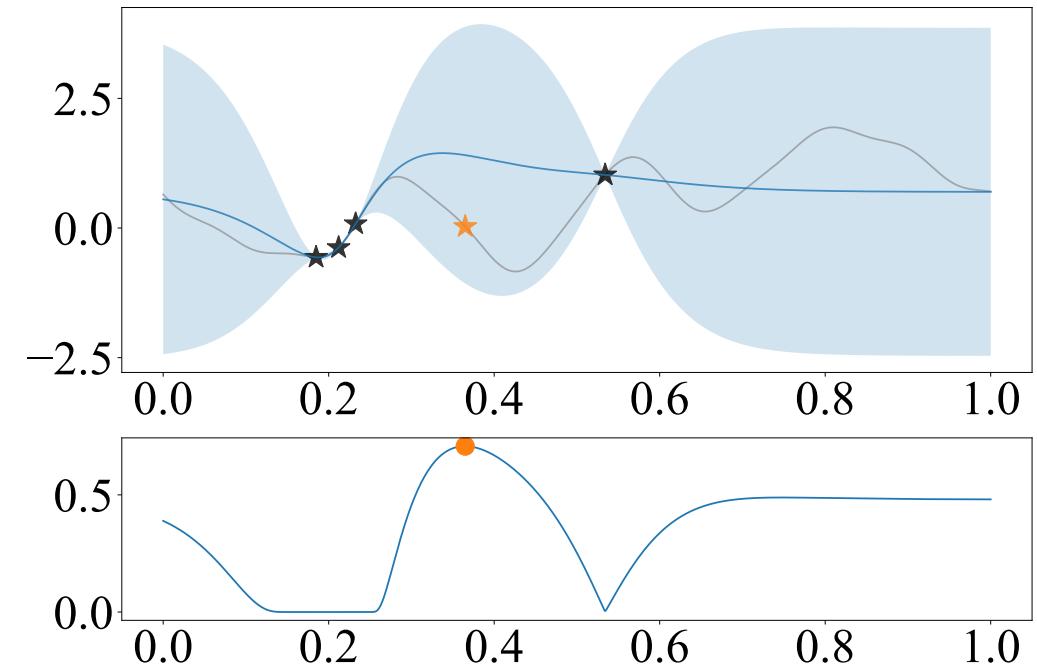
$$EI(x) = \mathbb{E}[\max(f(x) - y_{\text{best}}, 0) \mid x_1, \dots, x_t]$$

current best observed  
data  $D$   
“improvement”

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

posterior distribution

One-step approximation to MDP

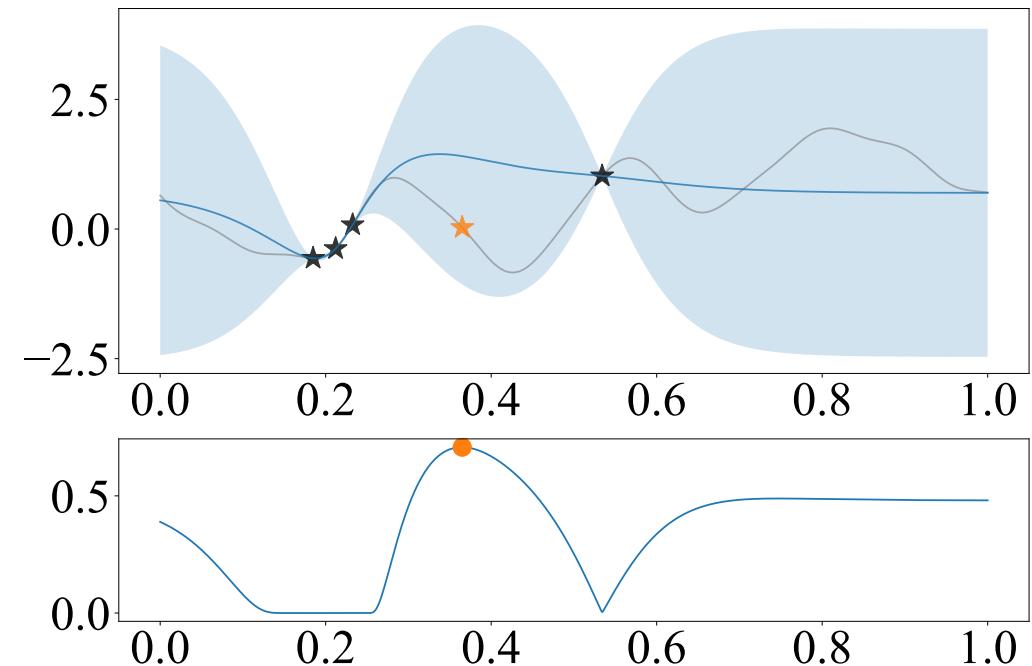


Expected improvement  $EI(x)$

Improvement-based  
design principle

# Existing Design Principles

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

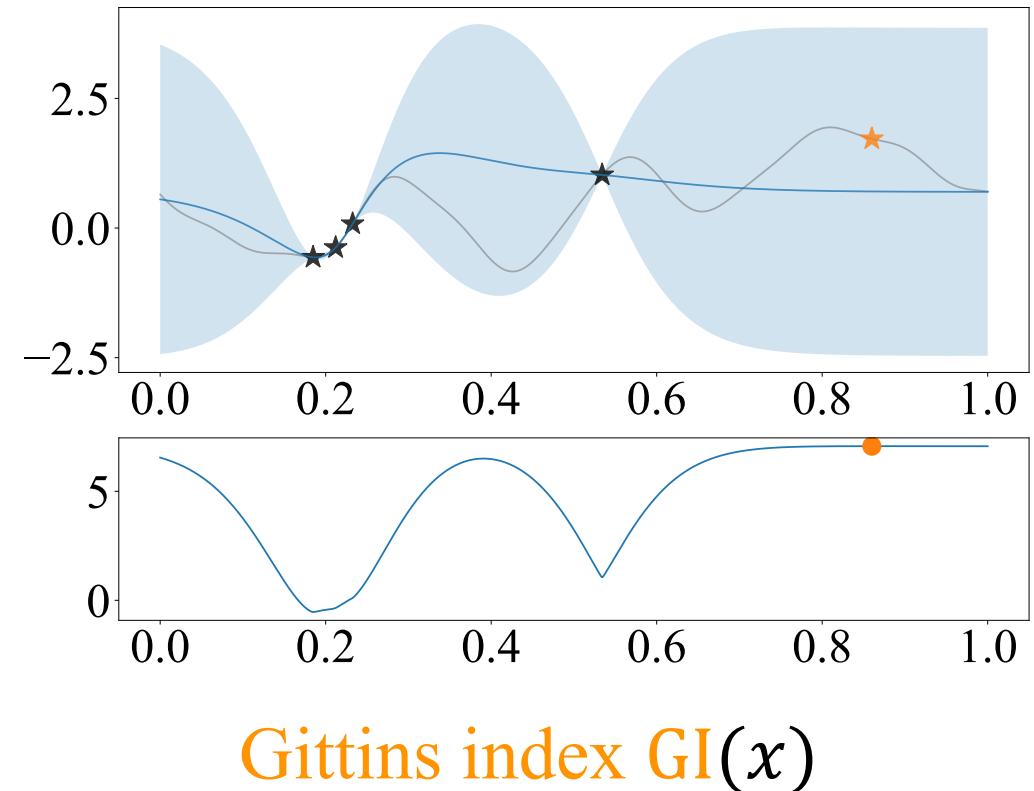


Expected improvement  $EI(x)$

Improvement-based  
design principle

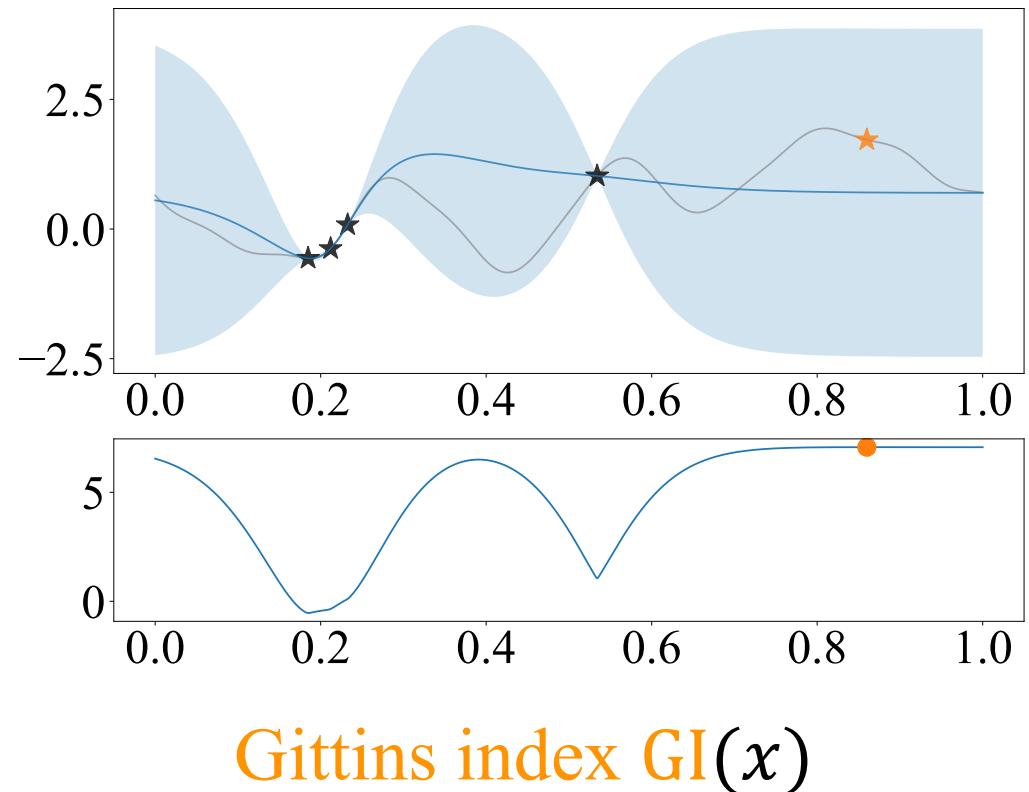
# New Design Principle: Gittins Index

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



# New Design Principle: Gittins Index

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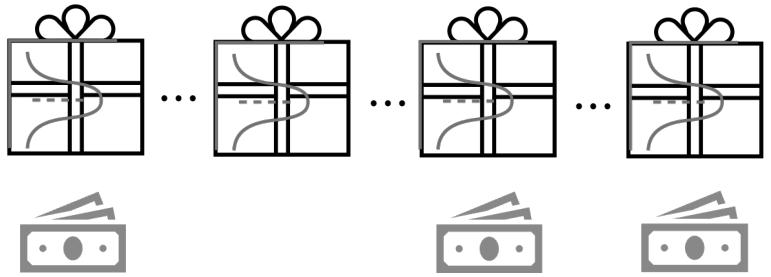


Gittins index  $GI(x)$

? Why another principle?

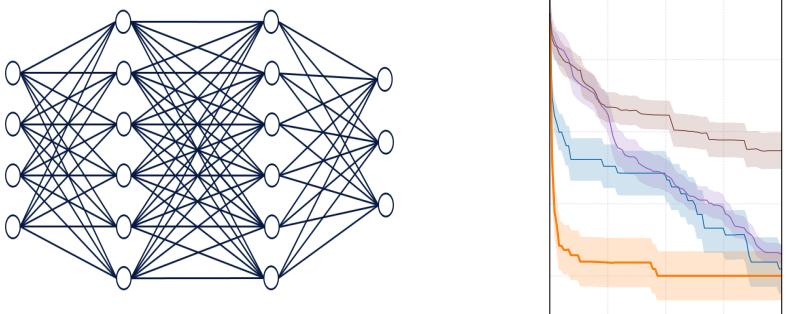
# Our Contribution: Gittins Index Principle

## Novel connection



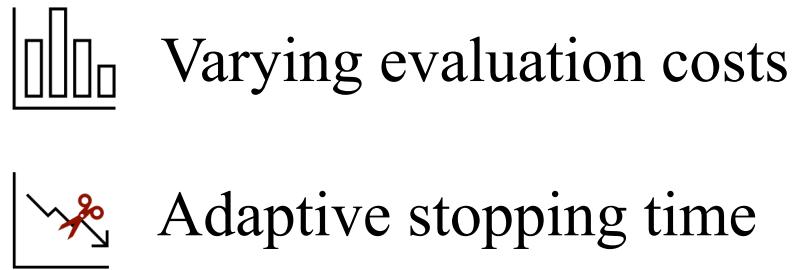
Link to **Pandora's Box** problem  
& **Gittins index** theory

## Competitive empirical performance



Interests from practitioners (e.g., Meta)

## Principled decision rules



Unified framework for  
selection and stopping

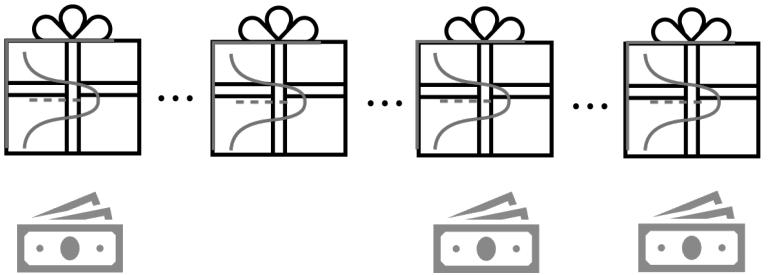
## Future potential

- Best-prompt identification
- Adaptive response sampling
- Chain-of-thought selection

Application to **efficient LLM**

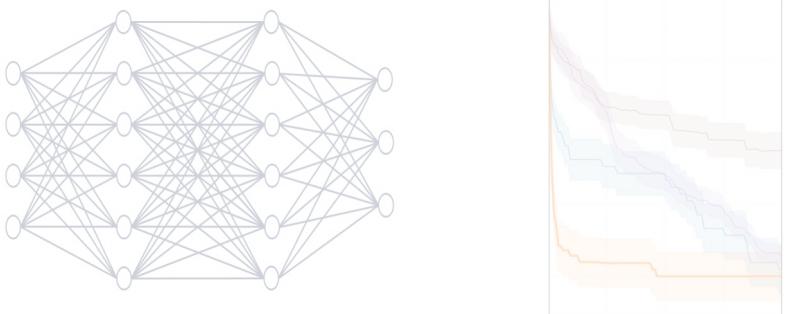
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Link to **Pandora's Box** problem  
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Interests from practitioners (e.g., Meta)

Principled decision rules



Unified framework for cost-aware selection and stopping

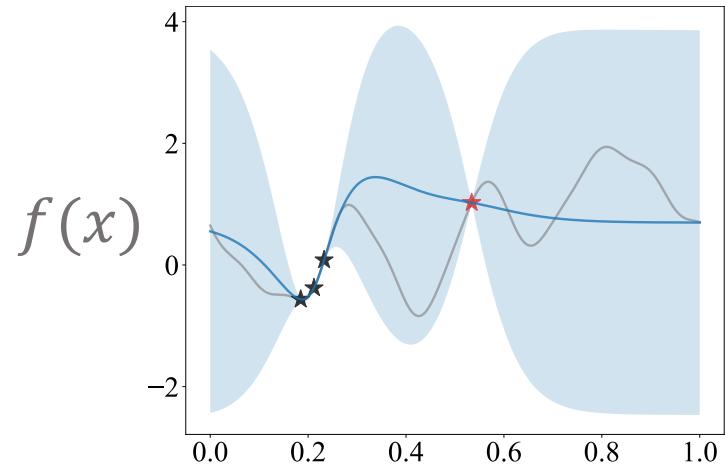
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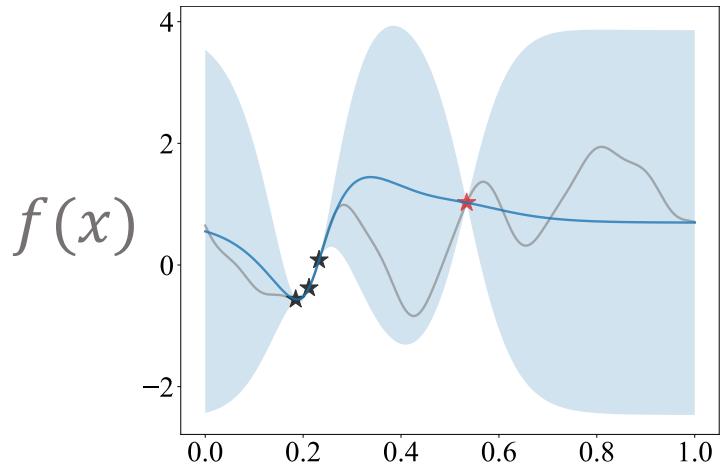
# Bayesian Optimization



Continuous search space

Correlated function values

# Bayesian Optimization



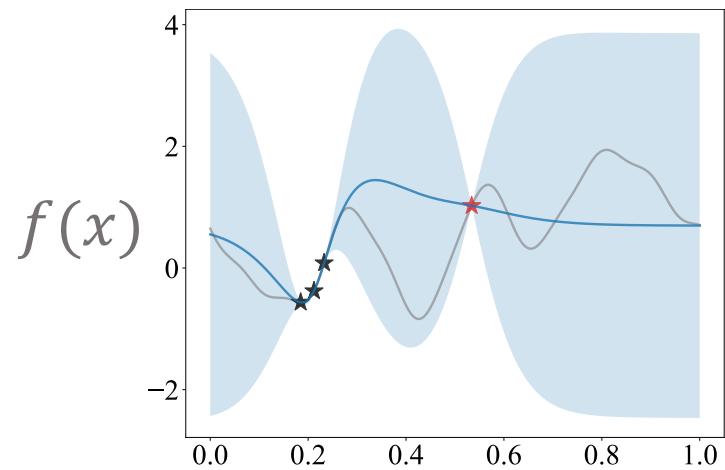
Continuous search space  $\Rightarrow$

Discrete

Correlated function values  $\Rightarrow$

Independent

# Bayesian Optimization



Continuous search space

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# Pandora's Box

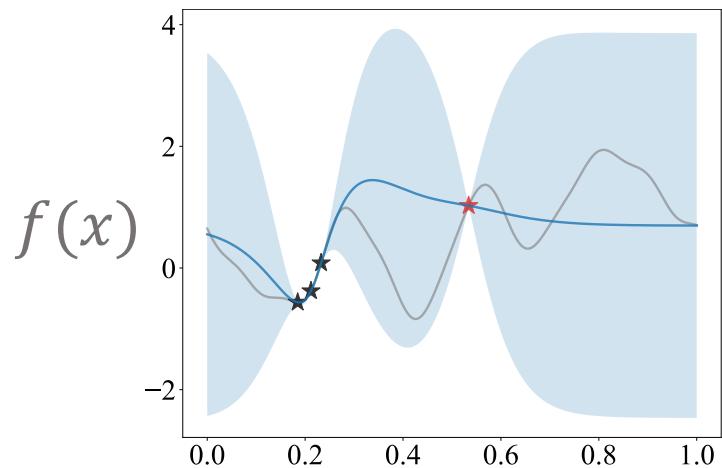
[Weitzman'79]



Discrete

Independent

# Bayesian Optimization

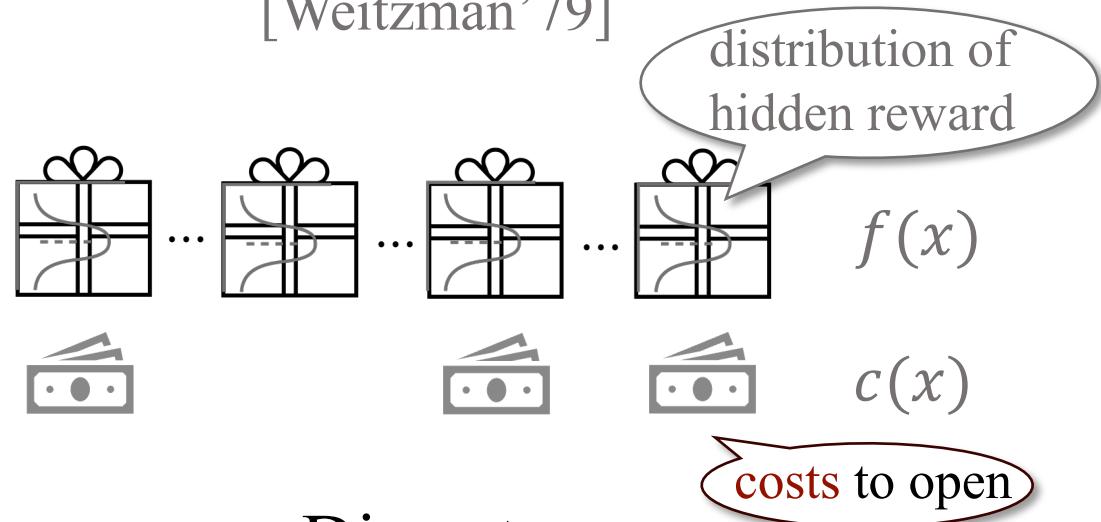


Continuous search space

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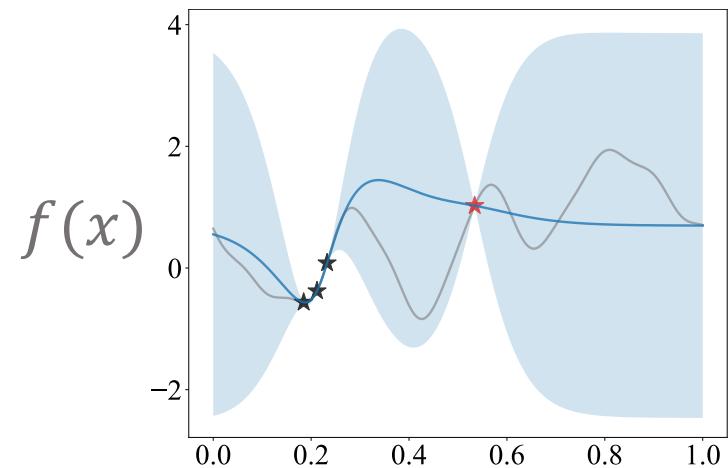
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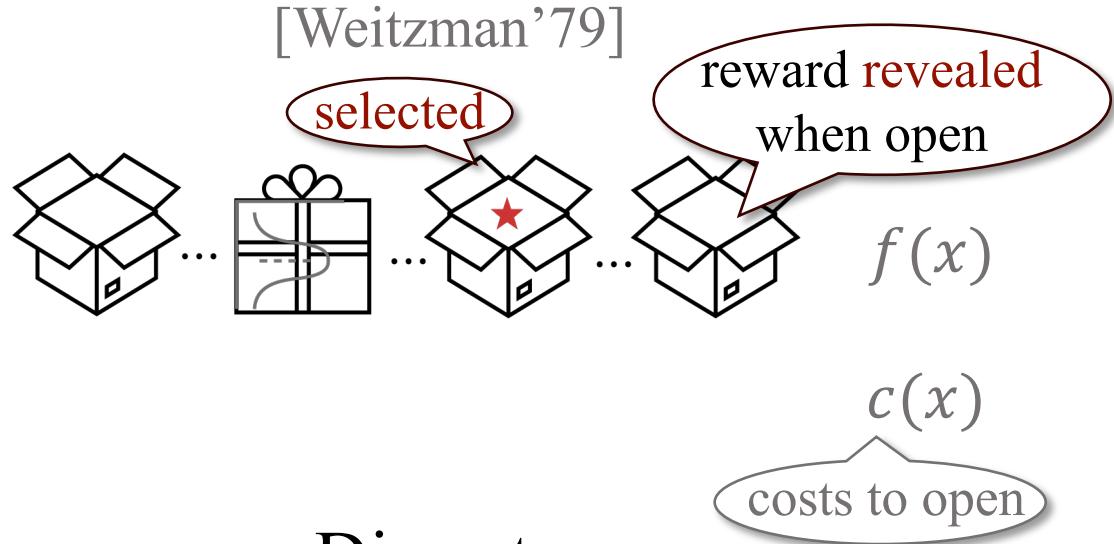
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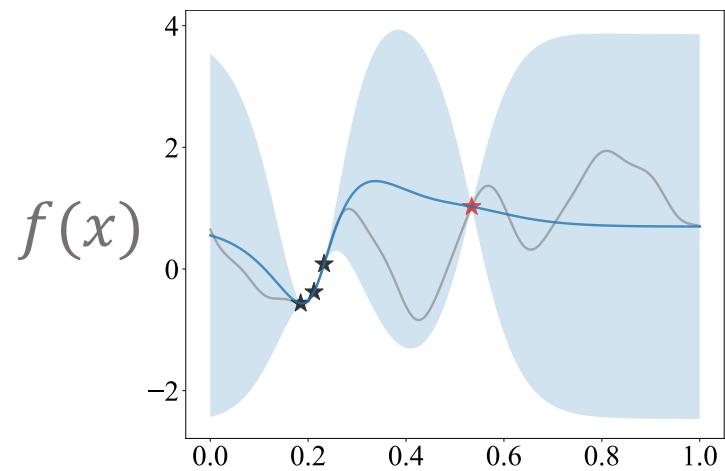
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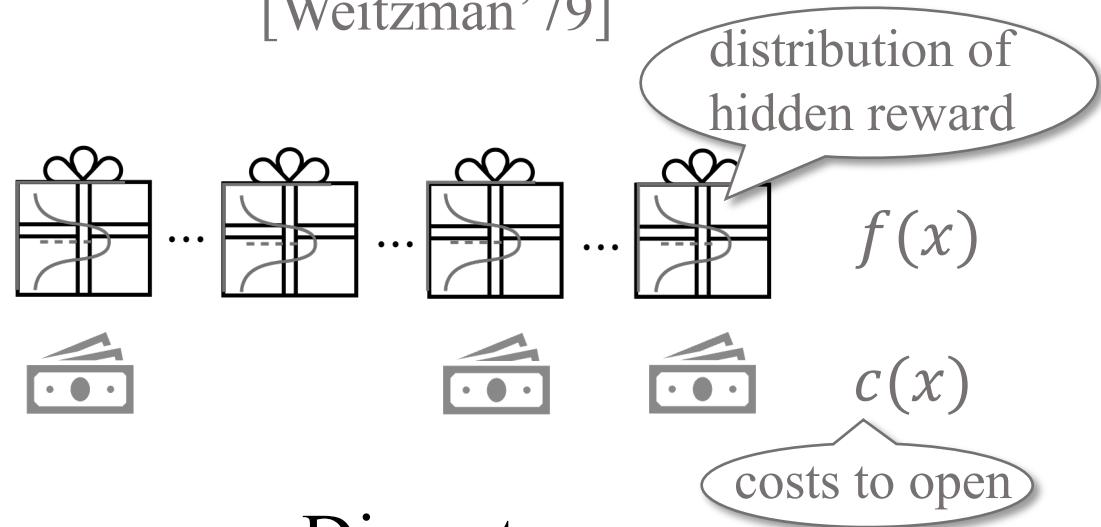


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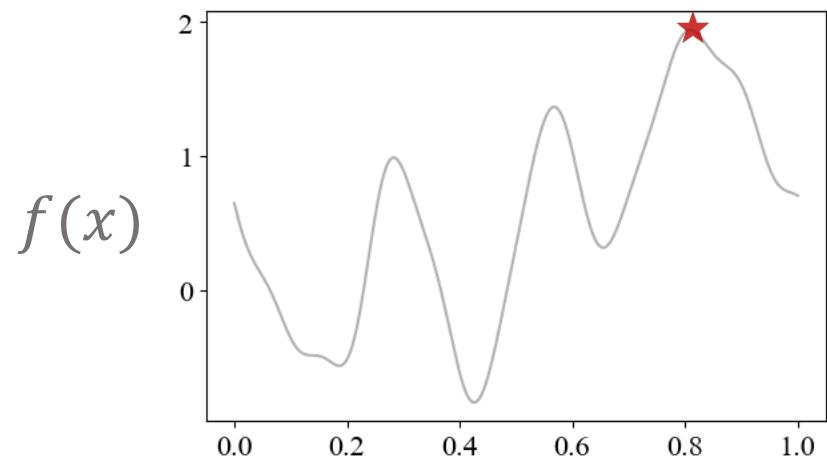


Discrete

Independent

Optimal policy: Gittins index

# Bayesian Optimization

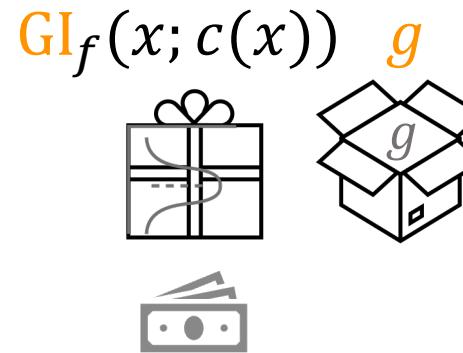


Continuous

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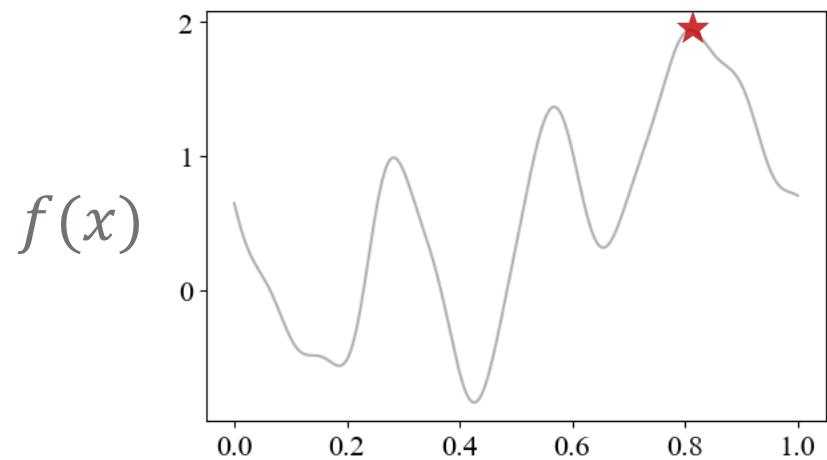


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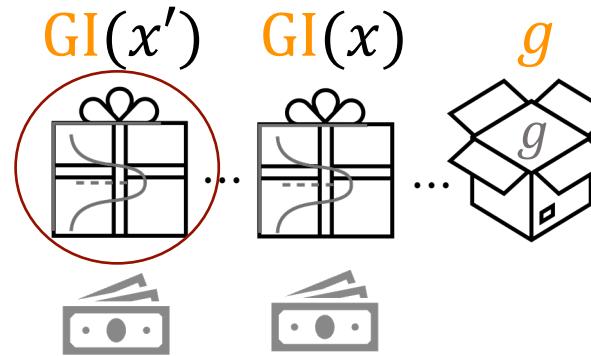


Continuous

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# Pandora's Box

[Weitzman'79]



Discrete

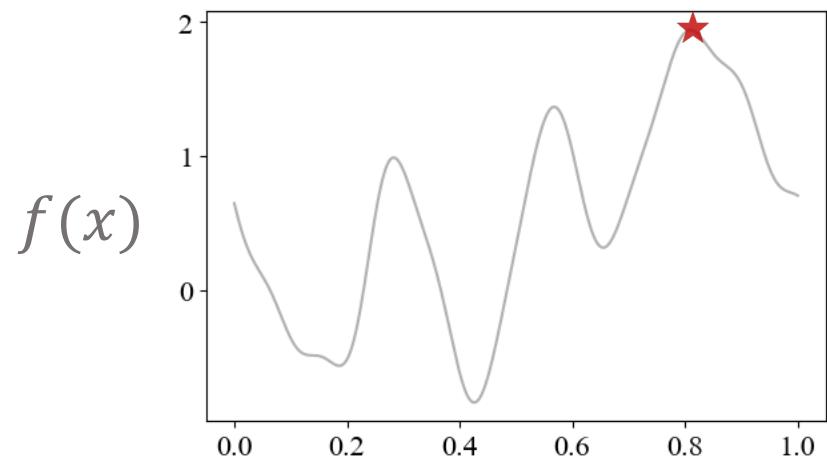
Independent

Step 2: Act on the box with the **highest** index

- *Closed*: open it
- *Opened*: select & stop

Optimal policy: **Gittins index**

# Bayesian Optimization

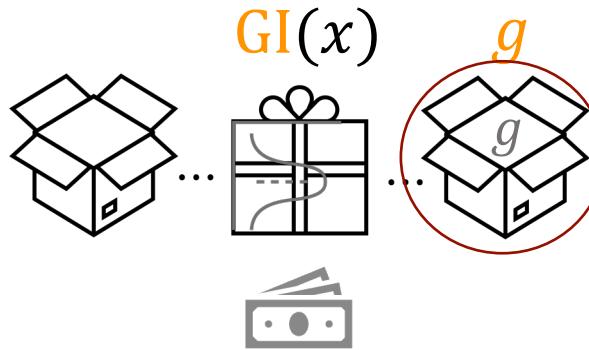


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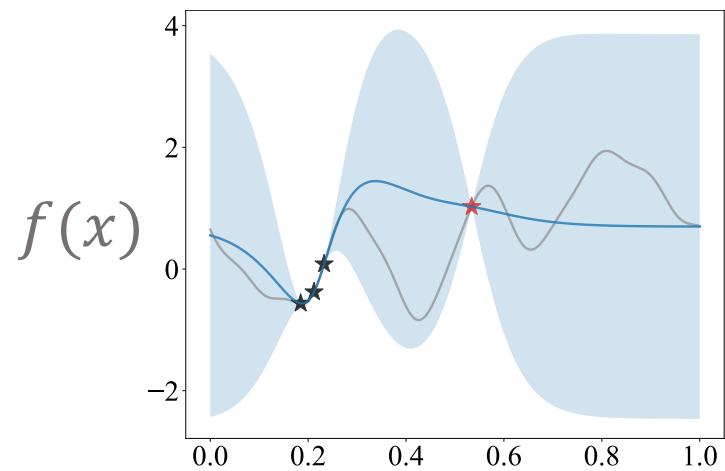
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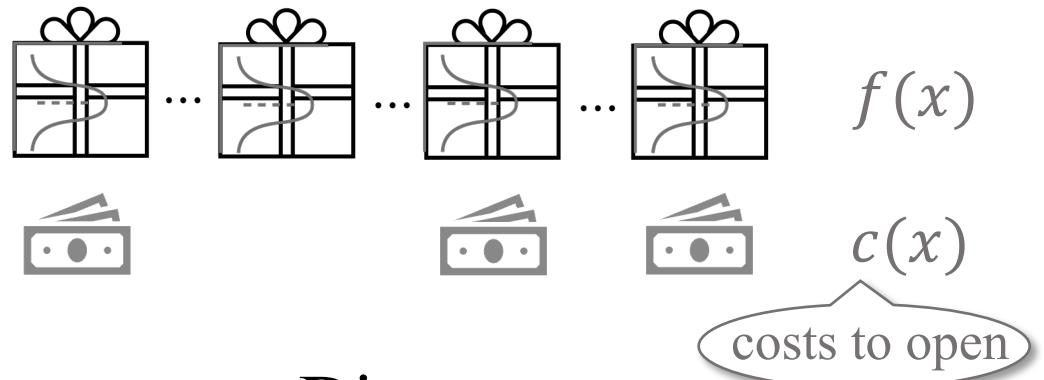


Continuous search space

Correlated function values

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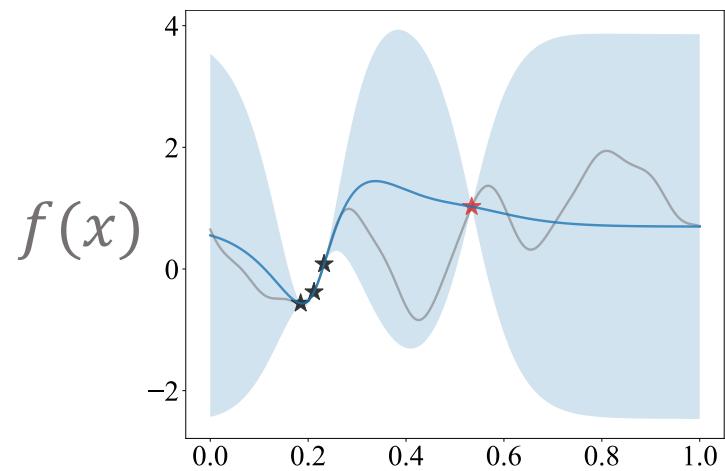
Discrete

Independent

How to translate?

Optimal policy: Gittins index

# Bayesian Optimization

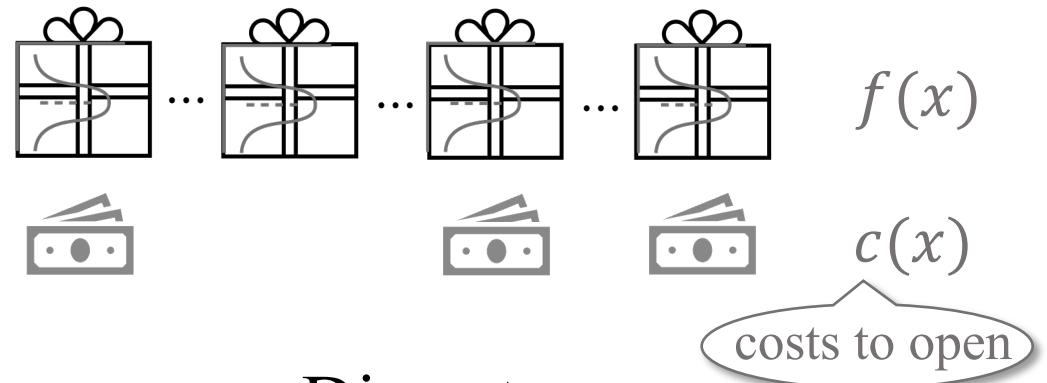


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[Weitzman'79]



Discrete

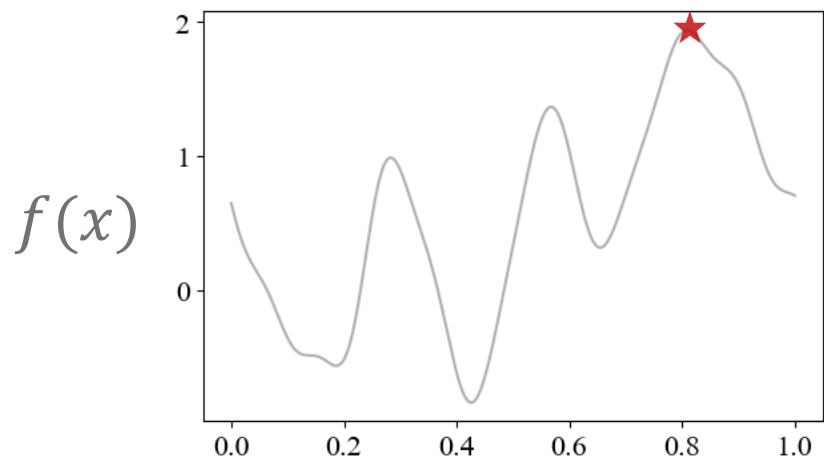
Independent

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

incorporate posterior  
take continuum limit

New!

# Bayesian Optimization



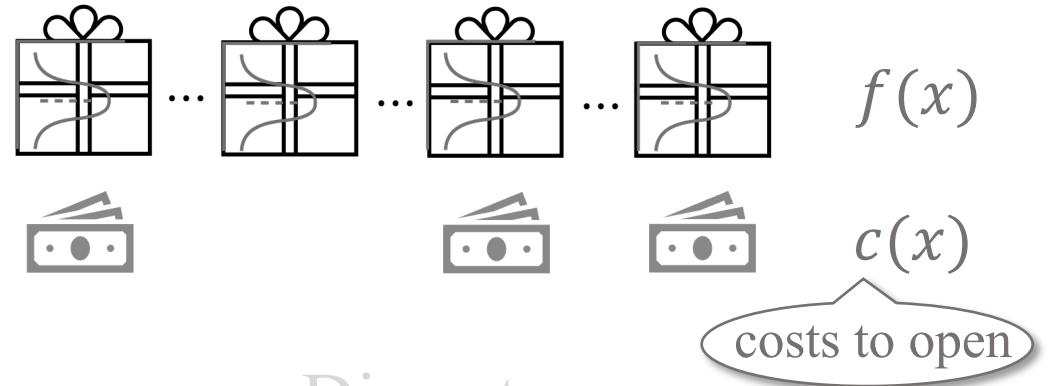
Continuous

Correlated

Our policy:  $\text{GI}_{f|D}(x; c(x))$   
How to compute?

# Pandora's Box

[Weitzman'79]

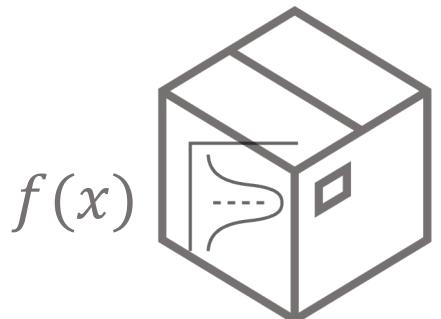


Discrete

Independent

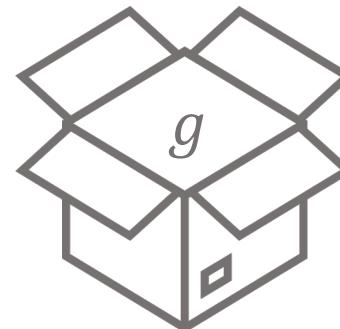
incorporate posterior  
take continuum limit  
Optimal policy:  $\text{GI}_f(x; c(x))$

# How to compute Gittins index?



↓ ?

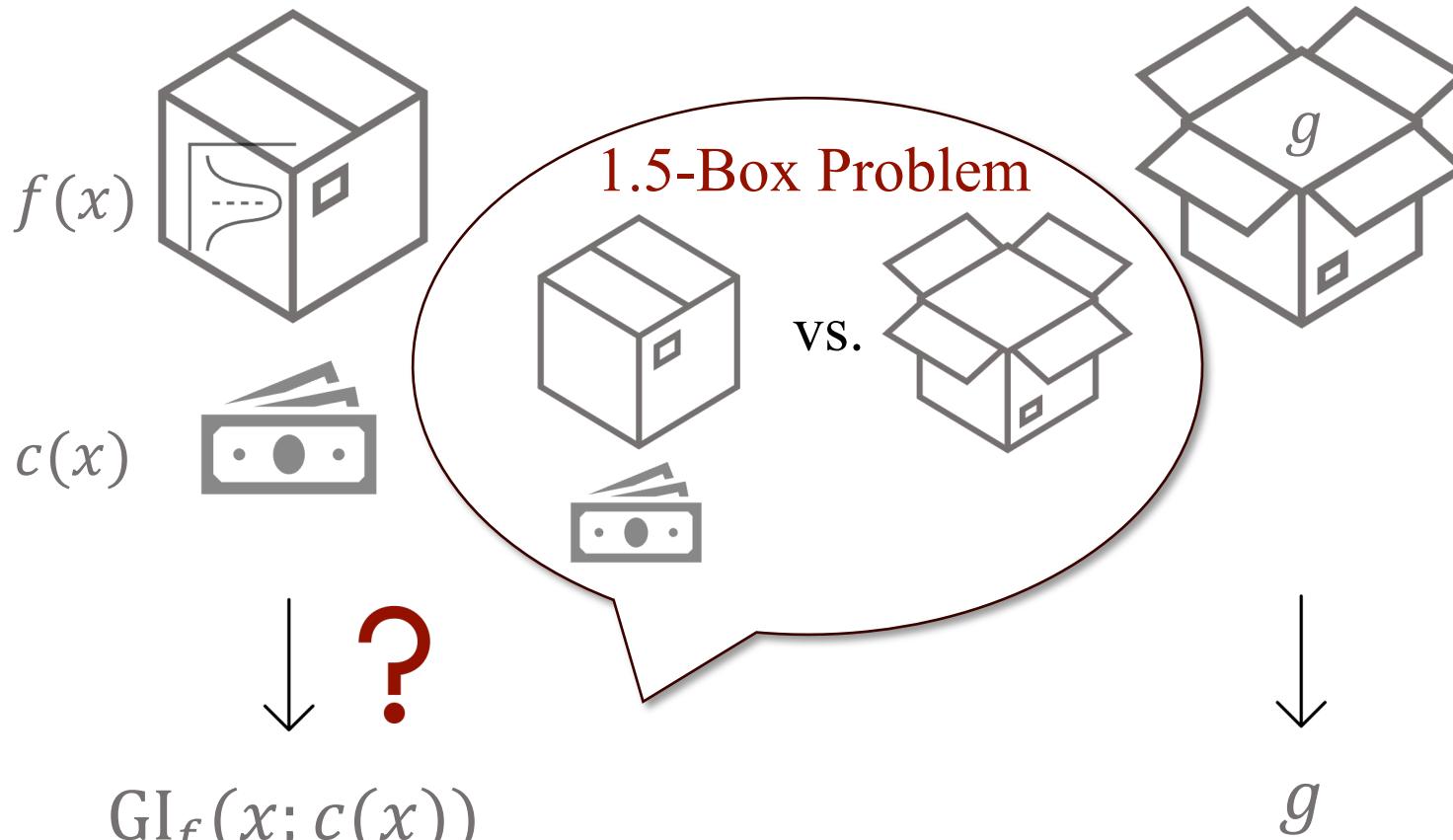
$$\text{GI}_f(x; c(x))$$



↓

$$g$$

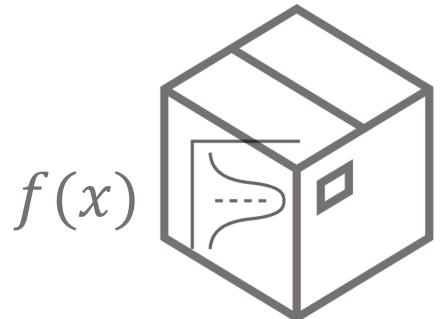
# How to compute Gittins index?



Whether to open a new box or take current best?

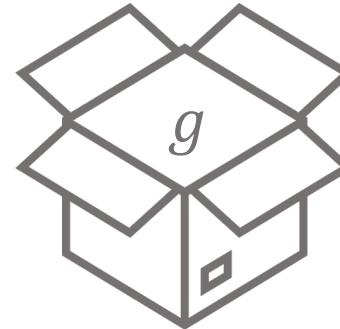
# Intuition of Gittins Computation: 1.5-Box Problem

Exploration



Open closed box

Exploitation

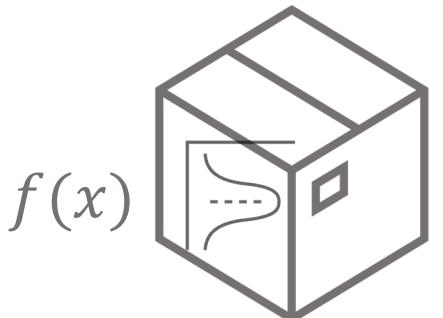


Take opened box

Whether to open a new box or take current best?

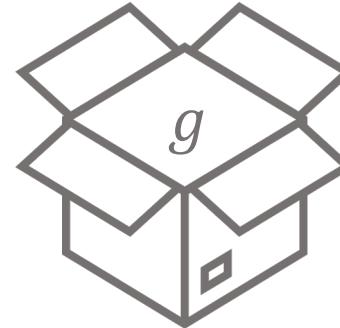
# Intuition of Gittins Computation: 1.5-Box Problem

Exploration



vs.

Exploitation



Open closed box



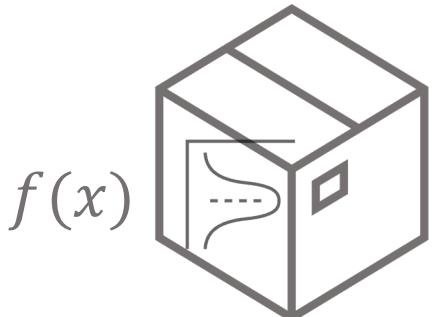
Profit:

Profit:

$$\begin{cases} \text{take inside value, } f(x) > g \\ \text{take outside option, } f(x) \leq g \end{cases}$$

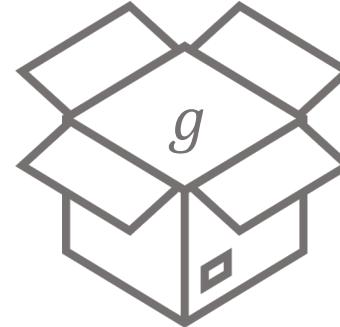
# Intuition of Gittins Computation: 1.5-Box Problem

Exploration



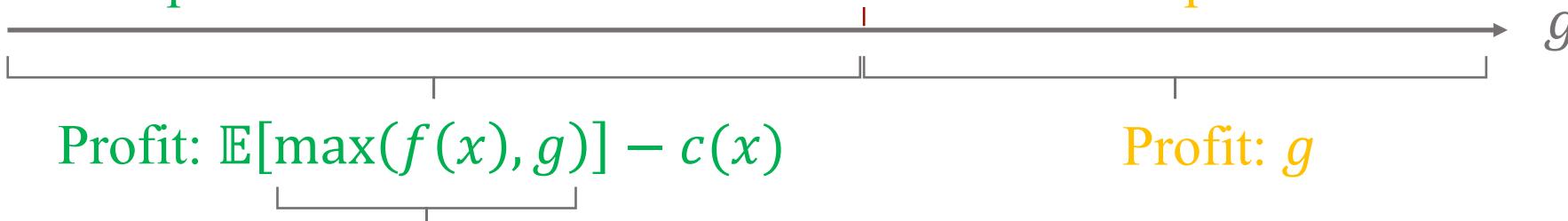
vs.

Exploitation



Open closed box

Take opened box



Profit:  $\mathbb{E}[\max(f(x), g)] - c(x)$

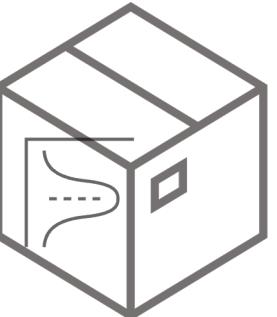
Profit:  $g$

$$\begin{cases} \text{take inside value, } f(x) > g \\ \text{take outside option, } f(x) \leq g \end{cases}$$

# Intuition of Gittins Computation: 1.5-Box Problem

Exploration

$$f(x)$$



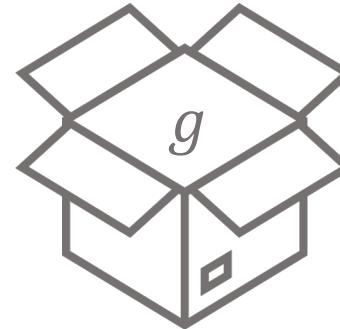
$$c(x)$$



Open closed box

Exploitation

$$g$$



vs.

Gittins index

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

$$g$$

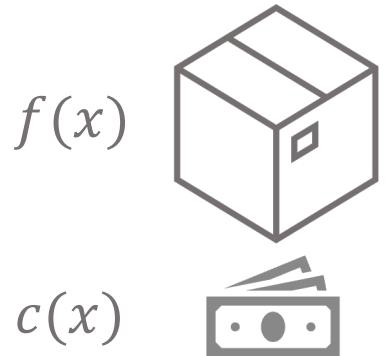
Profit:  $\mathbb{E}[\max(f(x), g)] - c(x)$

Profit:  $g$

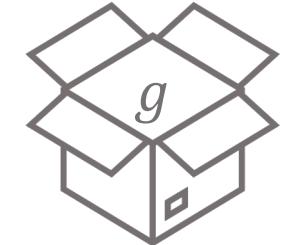
$\text{GI}_f(x; c(x))$ : solution  $g$  to  $\mathbb{E}[\max(f(x), g)] - c(x) = g$

# Intuition

Exploration



Exploitation



vs.

Open closed box

Take opened box

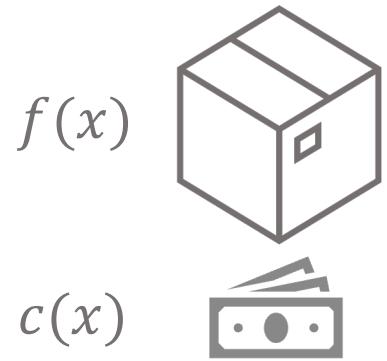
$$\mathbb{E}[\max(f(x), g)] - c(x) \quad g$$

$\text{GI}_f(x; c)$ : = solution  $g$  s.t.

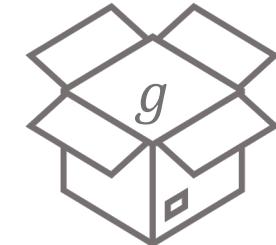
$$\mathbb{E}[\max(f(x), g)] - c(x) = g$$

# Intuition

Exploration



Exploitation



vs.

Open closed box

$$\mathbb{E}[\max(f(x), g)] - c(x)$$

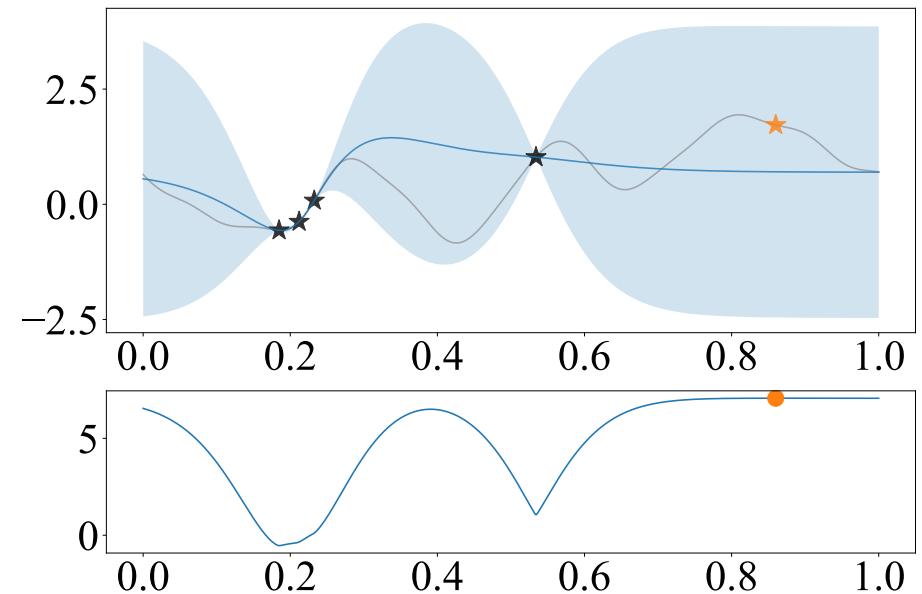
Take opened box

$$g$$

$\text{GI}_f(x; c)$ := solution  $g$  s.t.

$$\mathbb{E}[\max(f(x), g)] - c(x) = g$$

# Gittins Index

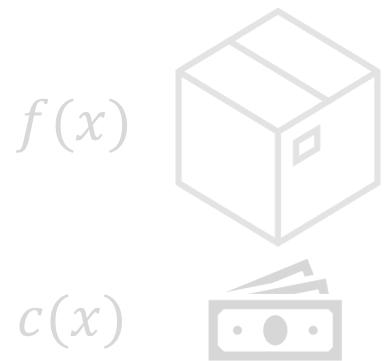


$\text{GI}_{f|D}(x; c)$ := solution  $g$  s.t.

$$\mathbb{E}[\max(f(x), g) | D] - c(x) = g$$

# Intuition

Exploration



Exploitation



vs.

Open closed box

Take opened box

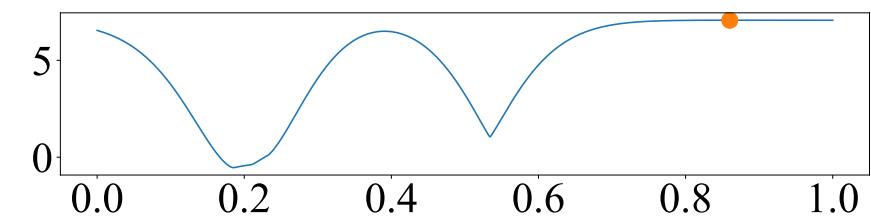
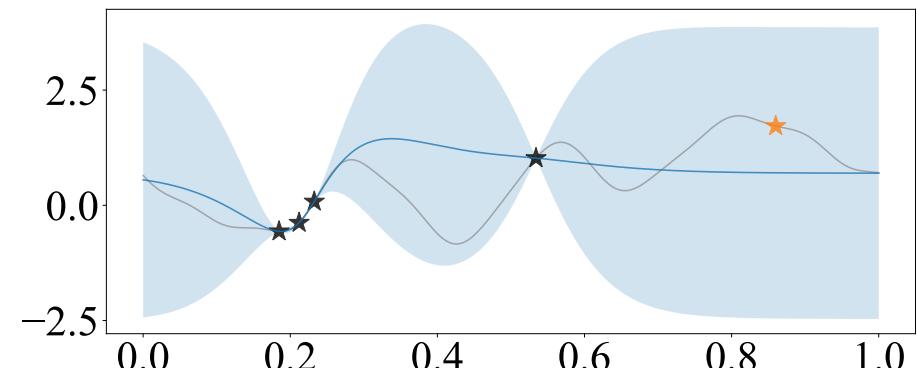
$$\mathbb{E}[\max(f(x), g)] - c(x)$$

$$g$$

$\text{GI}_f(x; c) :=$  solution  $g$  s.t.

$$\mathbb{E}[\max(f(x), g)] - c(x) = g$$

# Gittins Index



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

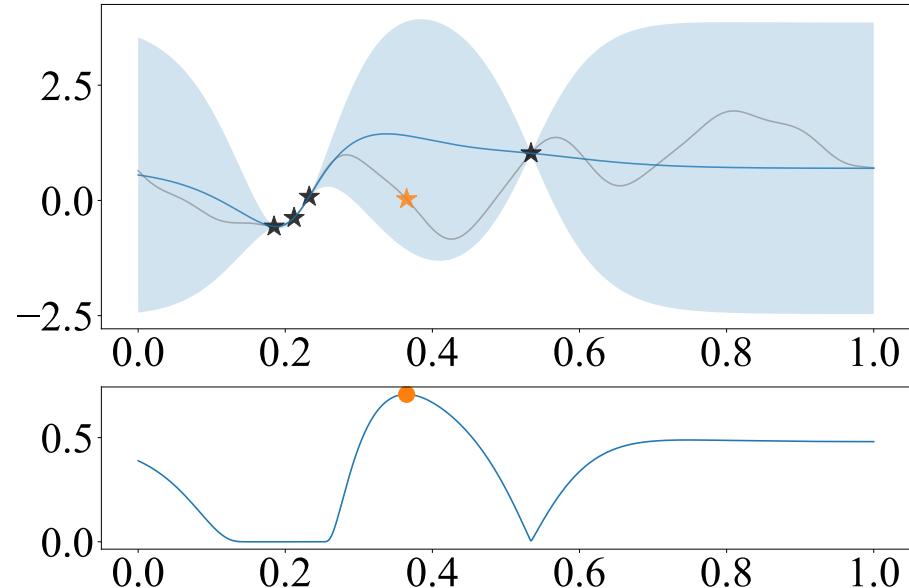
$$\mathbb{E}[\max(f(x), g) | D] - c(x) = g$$

$$\Leftrightarrow \mathbb{E}[\max(f(x) - g, g - g) | D] - c(x) = 0$$

$$\Leftrightarrow \mathbb{E}[\max(f(x) - g, 0) | D] = c(x)$$

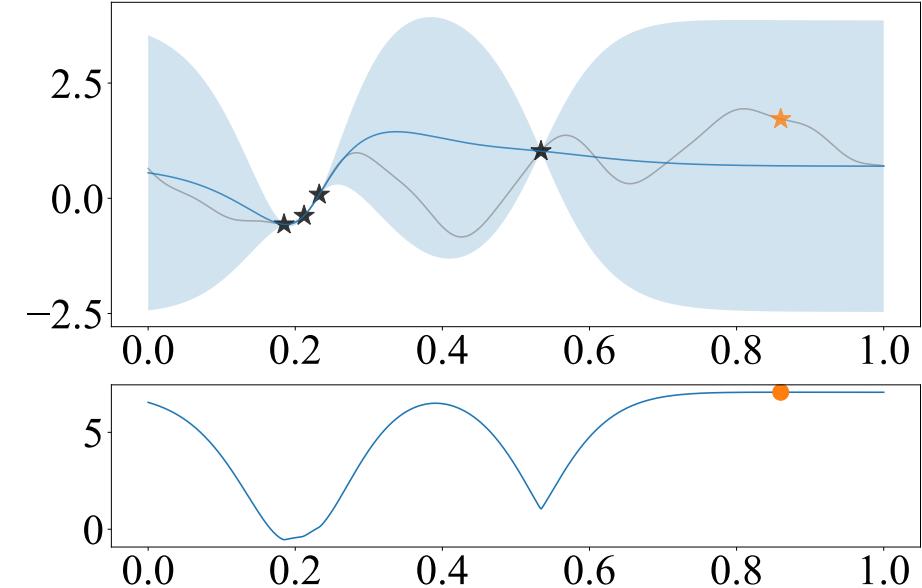
$$\text{EI}_{f|D}(x; g)$$

# Expected Improvement

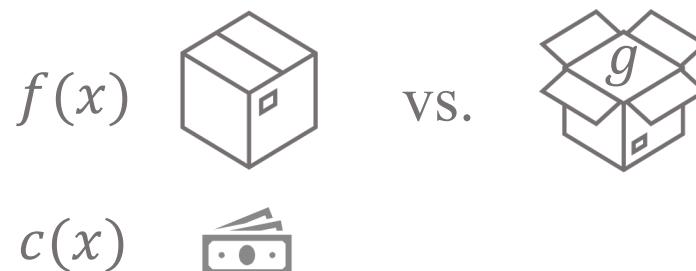


$$\text{EI}_{f|D}(x) := \mathbb{E}[\max(f(x) - y_{\text{best}}, 0) \mid D]$$

# Gittins Index

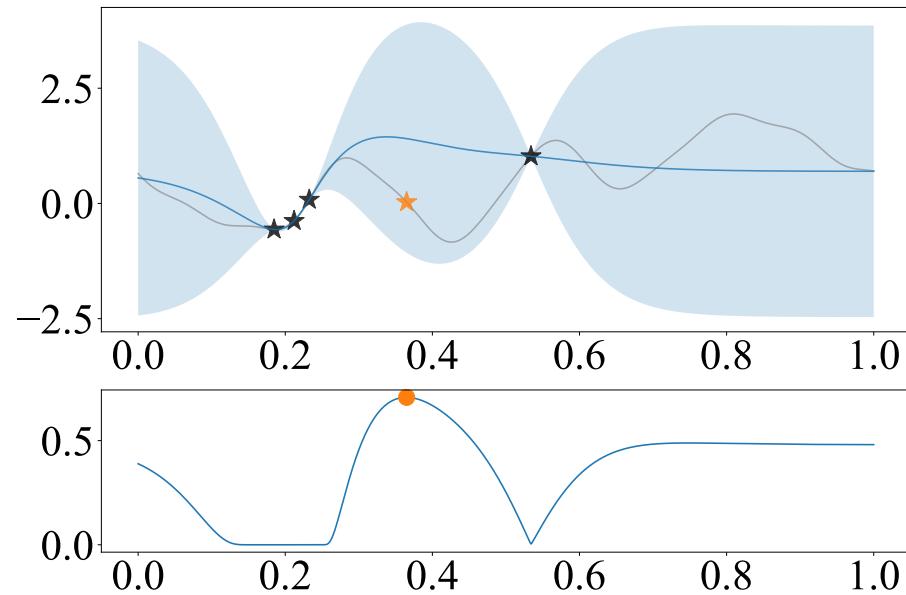


$$\begin{aligned} \text{GI}_{f|D}(x; c) &:= \text{solution } g \text{ s.t. } \text{EI}_{f|D}(x; g) = c(x) \\ \text{where } \text{EI}_{f|D}(x; g) &:= \mathbb{E}[\max(f(x) - g, 0) \mid D] \end{aligned}$$



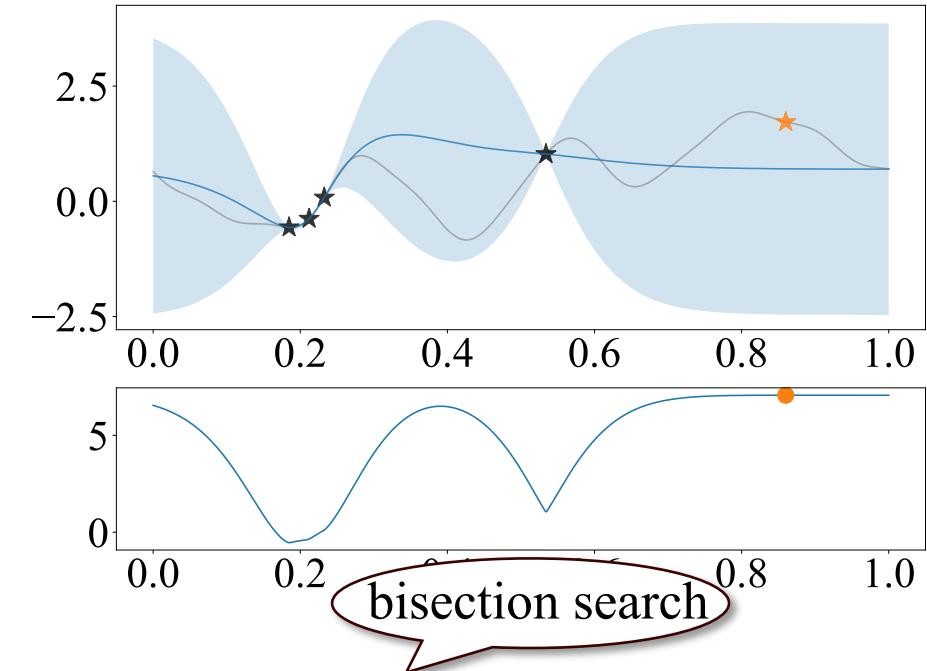
Exploration      Exploitation

# Expected Improvement



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

# Gittins Index



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

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

analytical expression



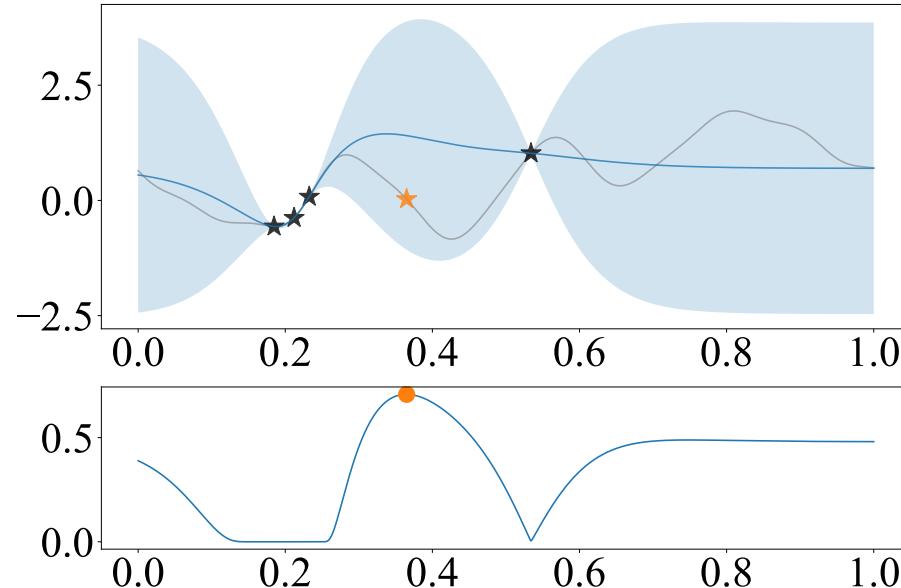
Easy-to-compute decision rule!



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

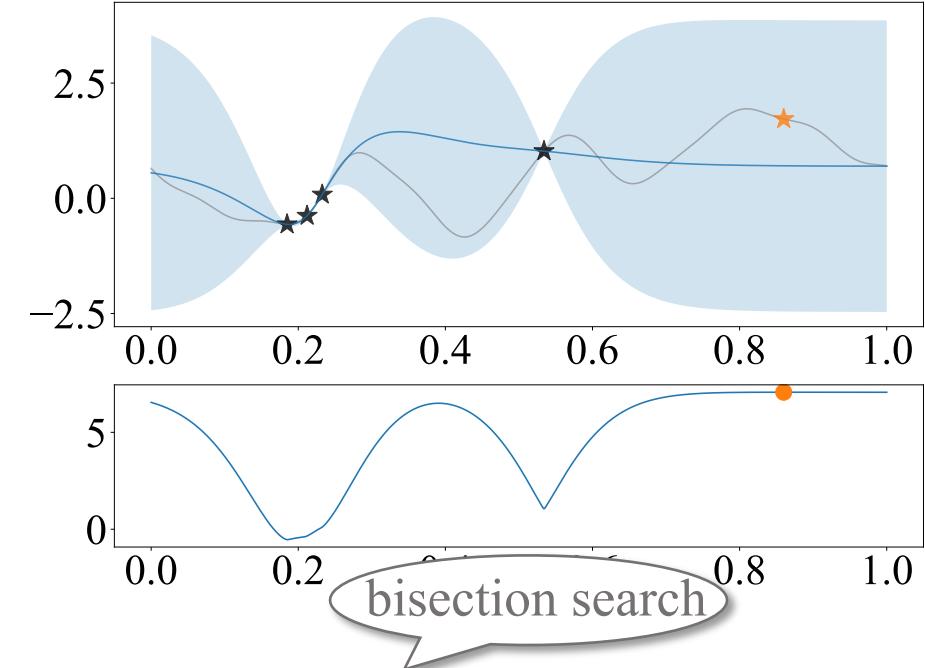


# Expected Improvement



$$EI_{f|D}(x) := \mathbb{E}[\max(f(x) - y_{\text{best}}, 0) \mid D]$$

# Gittins Index



$$GI_{f|D}(x; c) := \text{solution } g \text{ s.t. } EI_{f|D}(x; g) = c(x)$$

where  $EI_{f|D}(x; g) := \mathbb{E}[\max(f(x) - g, 0) \mid D]$

Google DeepMind

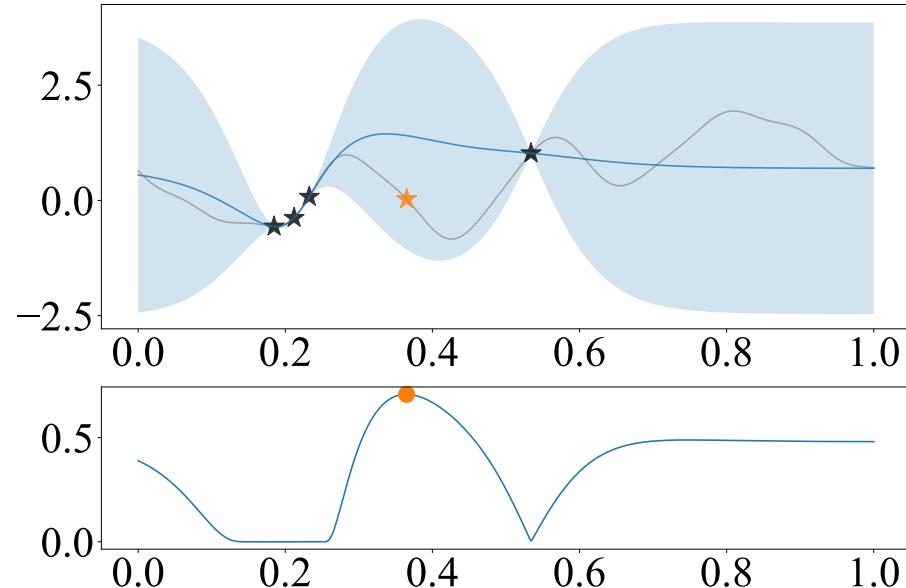
FunBO: Discovering new acquisition functions for  
Bayesian Optimization with FunSearch



GI is not easy to discover!

LLM-driven evolutionary  
search method

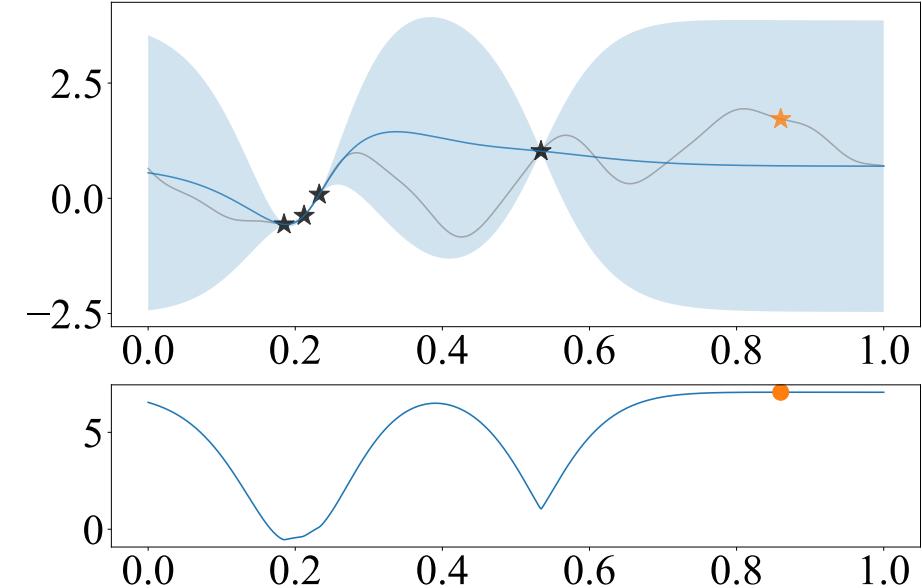
# Expected Improvement



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

Temporal simplification to MDP  
(One-step)

# Gittins Index



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

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

Spatial simplification to MDP



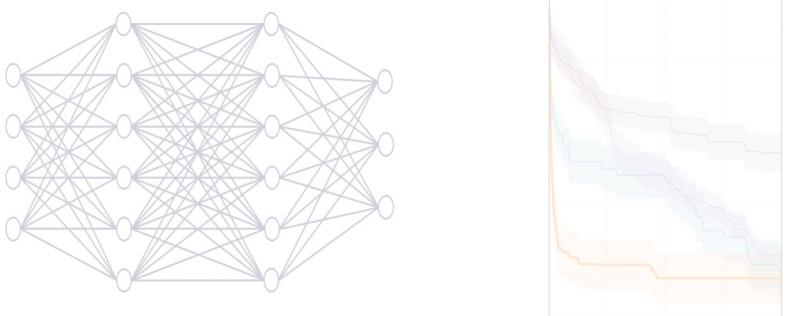
# Our Contribution: Gittins Index Principle

Novel connection



Link to Pandora's Box problem  
& Gittins index theory

Competitive empirical performance



Interests from practitioners (e.g., Meta)

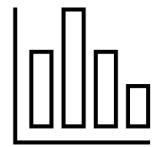
Principled decision rules

- Varying evaluation costs
- Adaptive stopping time

Unified framework for  
selection and stopping

- Future potential
- Best-prompt identification
- Adaptive response sampling
- Chain-of-thought selection
- Application to efficient LLM

# Under-explored Factors for Better Decisions



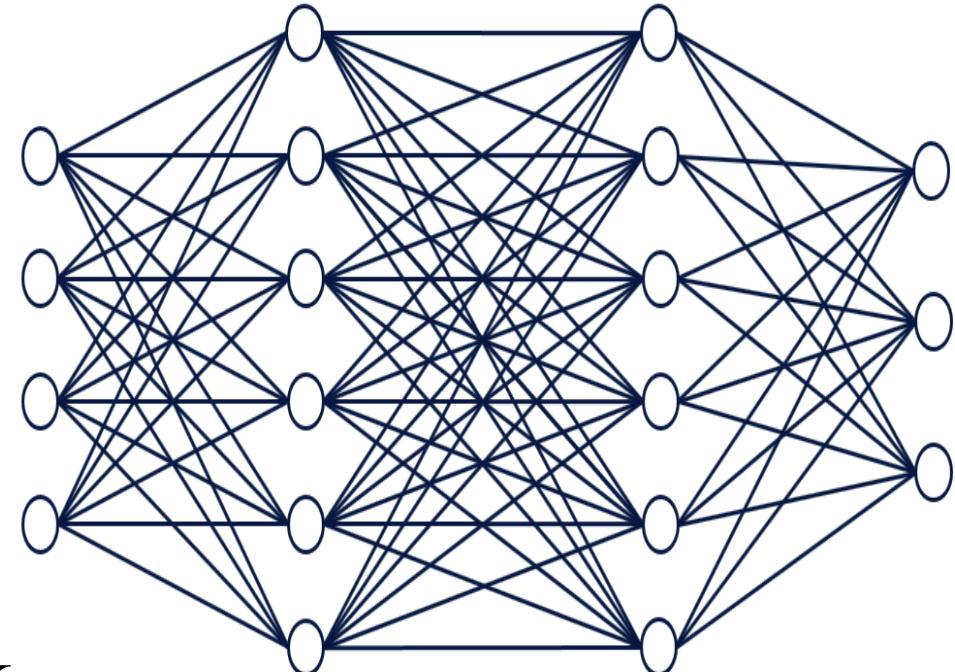
Varying evaluation costs



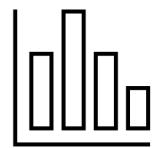
Smart stopping time



Observable multi-stage feedback



# How does existing principle incorporate them?



Varying evaluation costs

$$\text{EIPC}(x; c) = \text{EI}(x) / c(x)$$

[Snoek et al.'12]

Arbitrarily bad

[Astudillo et al.'21]



Smart stopping time

$$\tau: \text{EI}(x_\tau) \leq \theta$$

[Locatelli'97,

Nguyen et al.'17,

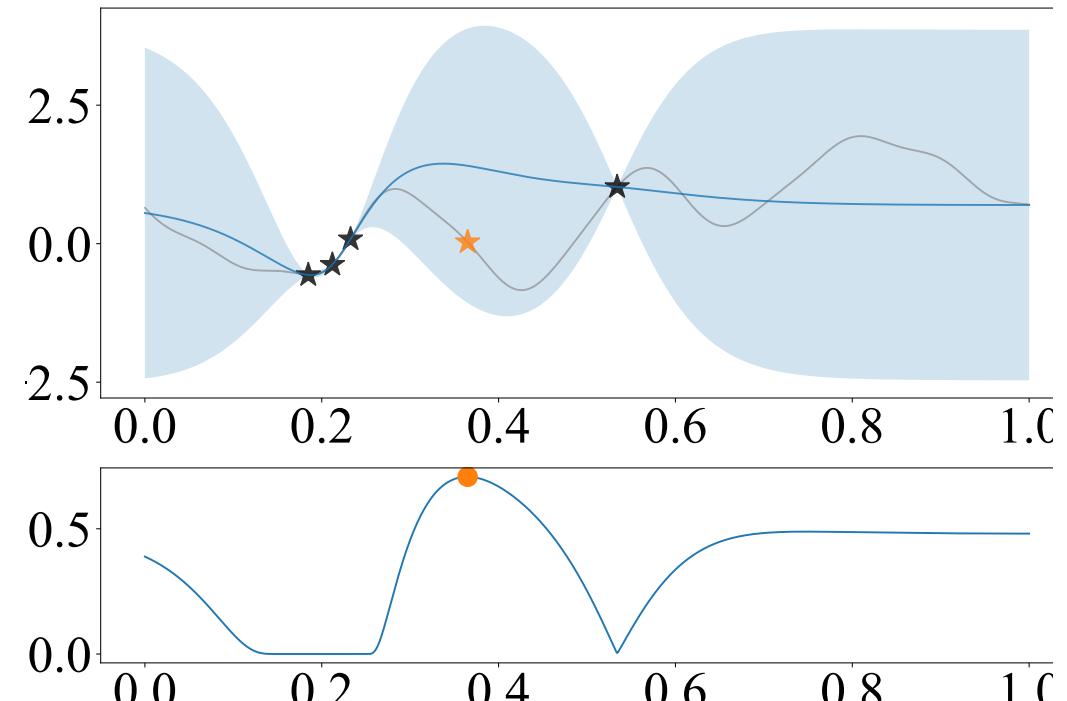
Ishibashi et al.'23]

Which threshold?



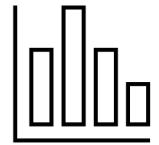
Observable multi-stage feedback

?

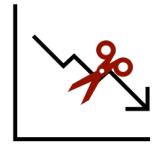


Expected improvement  $\text{EI}(x)$

# Under-explored Factors for Better Decisions



Varying evaluation costs



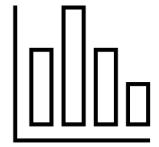
Smart stopping time



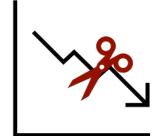
Observable multi-stage feedback

New design principle:  
**Gittins index**

# Why Gittins index?



Varying evaluation costs



Smart stopping time

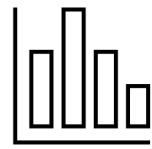


Observable multi-stage feedback

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

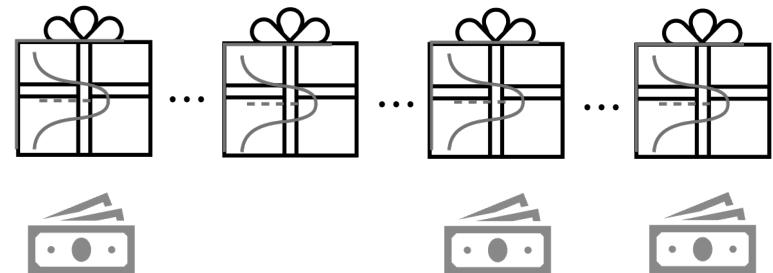
Features in **Pandora's box**



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

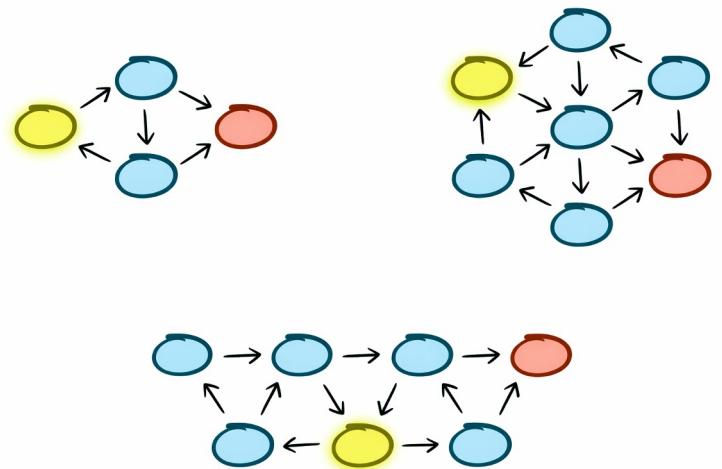


Observable multi-stage feedback

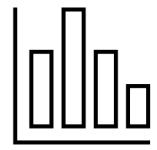
Features in **Markov chain selection**

New design principle:  
Gittins index

Optimal in related sequential  
decision problems

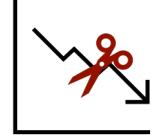


# Why Gittins index?



Varying evaluation costs

Features in **Pandora's box**



Smart stopping time

Features in **Pandora's box**



Observable multi-stage feedback

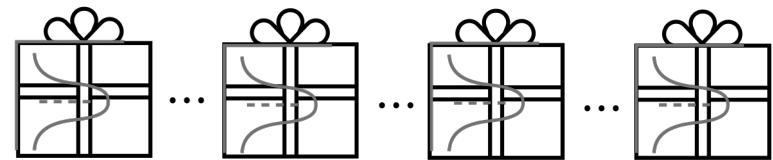
Features in Markov chain selection



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

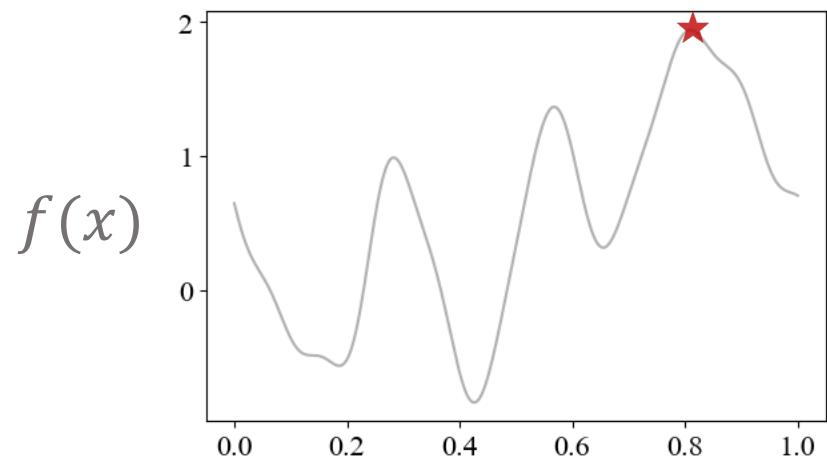
New design principle:  
Gittins index

Optimal in related sequential  
decision problems



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

# Bayesian Optimization



Continuous

Correlated

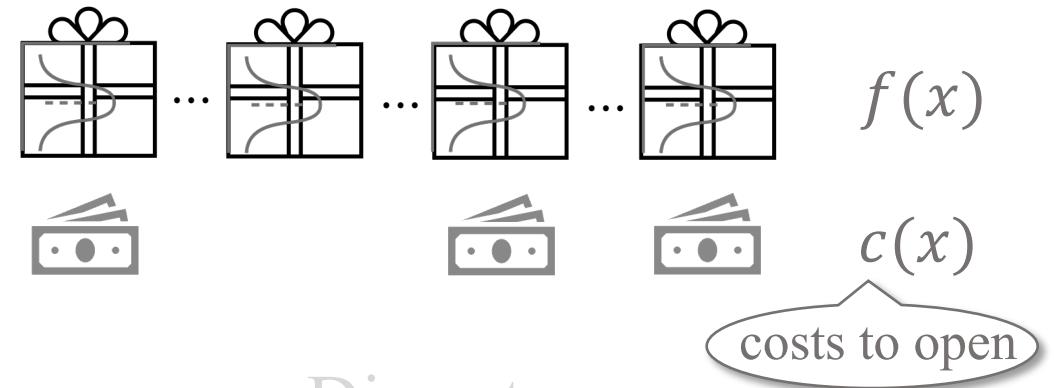
Cost-unaware

Fixed-iteration

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

# Pandora's Box

[Weitzman'79]



Discrete

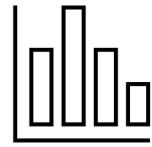
Independent

Cost-aware

Flexible-stopping

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

# Expected Improvement vs Gittins Index



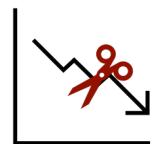
Varying evaluation costs

$$\text{EIPC}(x; c) = \text{EI}(x)/c(x)$$

$\text{GI}(x; c)$ : = solution  $g$  s.t.  $\text{EI}(x; g) = c(x)$

Arbitrarily bad

naturally incorporates costs



Smart stopping time

$$\tau: \text{EI}(x_\tau) \leq \theta$$

Which threshold?

$$\tau: \text{GI}(x_\tau; c) \leq y_{\text{best}}$$

$$\Leftrightarrow \tau: \text{EIPC}(x_\tau; c) \leq 1$$

derived shared stopping rule



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



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

# 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:

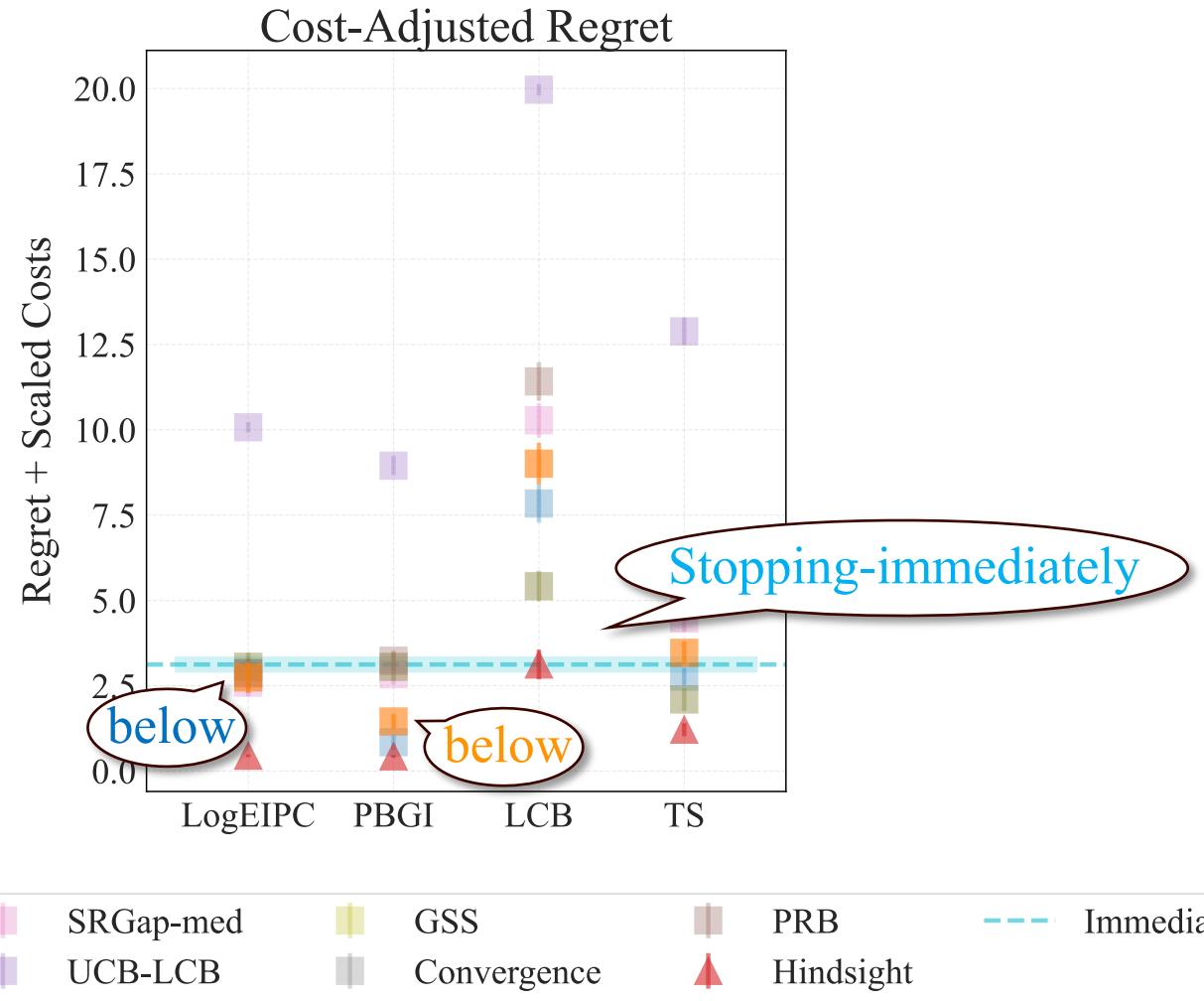
- Matches the **best achievable performance in the worst case** (evaluations are all very costly).
- Avoids **over-spending** — a property many cost-unaware stopping rules lack.

New

**Proof idea:** For all  $t < \tau$ ,  $\text{EI}(x_{t+1}) \geq c(x_{t+1})$ .

stopping time

PBGI/LogEIPC  
LogEIPC-med



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

# Our Contribution: Gittins Index Principle

Novel connection



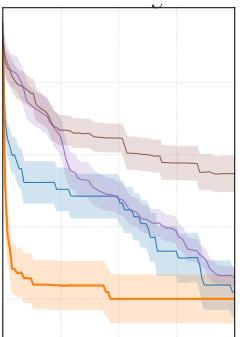
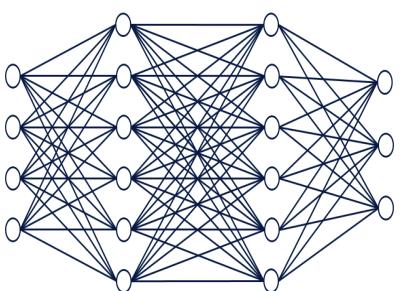
Link to Pandora's Box problem  
& Gittins index theory

Principled decision rules



Unified framework for  
selection and stopping

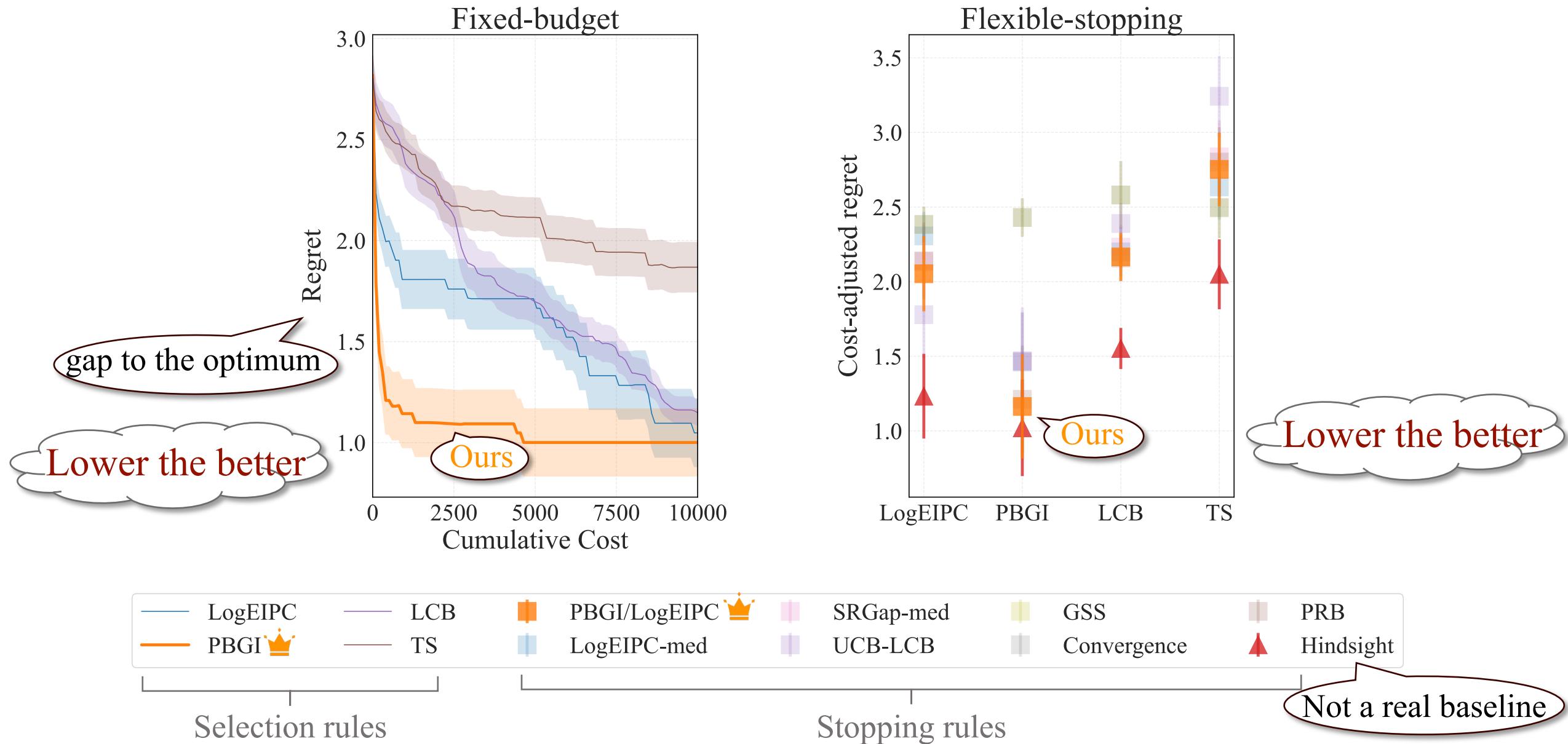
## Competitive empirical performance



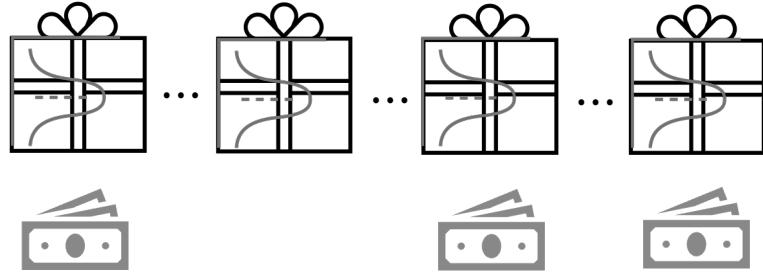
Interests from practitioners (e.g., Meta)

- Future potential
- Best-prompt identification
- Adaptive response sampling
- Chain-of-thought selection
- Application to efficient LLM

# Gittins Index vs Baselines on AutoML Benchmark

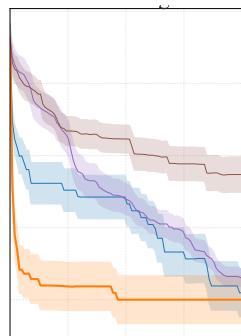
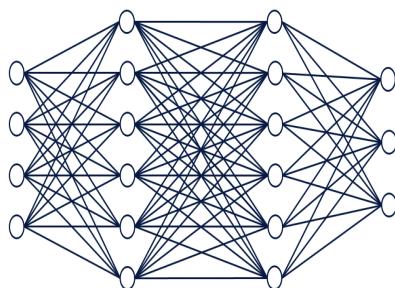


## Novel connection



Link to **Pandora's Box** problem  
& **Gittins index** theory

## Competitive empirical performance



Interests from practitioners (e.g., Meta)

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

## Principled decision rules



Varying evaluation costs



Adaptive stopping time

Unified framework for selection and stopping

## Future potential



Best-prompt identification



Adaptive response sampling



Chain-of-thought selection



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

# Find my papers on arXiv!



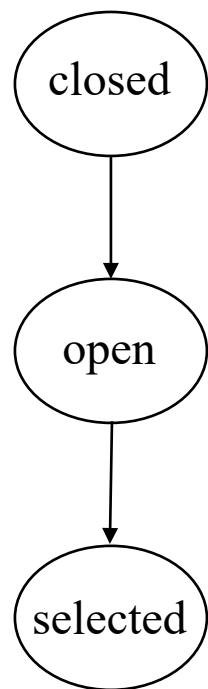
"Cost-aware Bayesian Optimization via the Pandora's Box Gittins Index." NeurIPS'24.



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

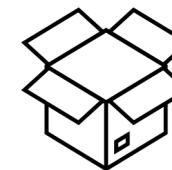
# Markovian Bandits

[Gittins'79]

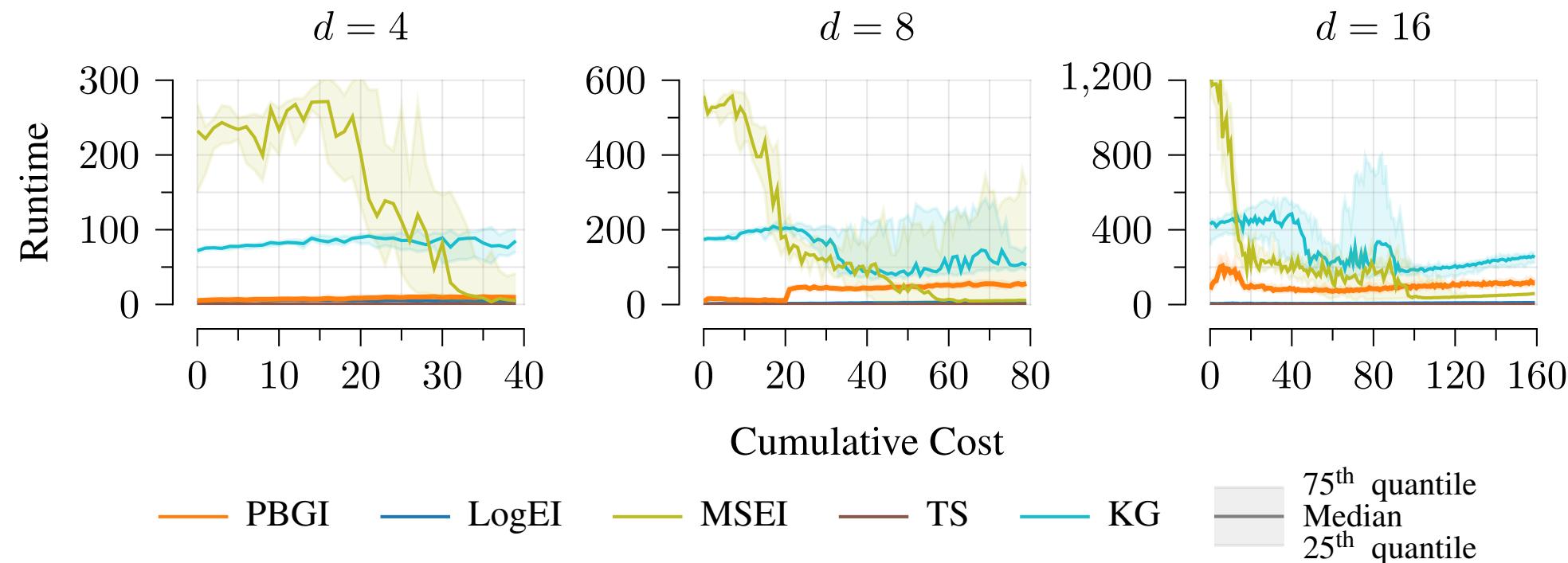


# Pandora's Box

[Weitzman'79]



# Timing Experiment: Gittins Index vs Baselines



PBGI is computationally-efficient!



# EI vs PBGI vs UCB

