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

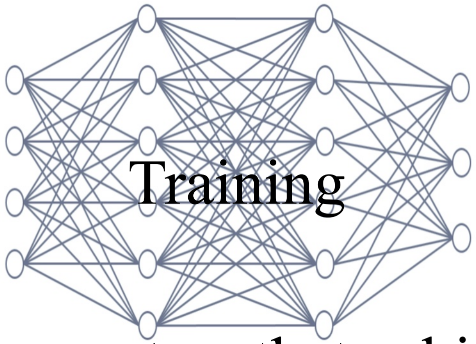
Qian Xie 谢倩 (Cornell ORIE)

Job Talk

# Motivation: World of Optimization under Uncertainty

## ML model training:

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




⟶ Accuracy

Goal: find hyperparameters that achieve high accuracy

# Motivation: World of Optimization under Uncertainty

## ML model training:

≠ parameters
(weights, biases)

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


⟶ Accuracy

Goal: find hyperparameters that achieve high accuracy

# Motivation: World of Optimization under Uncertainty

## ML model training:

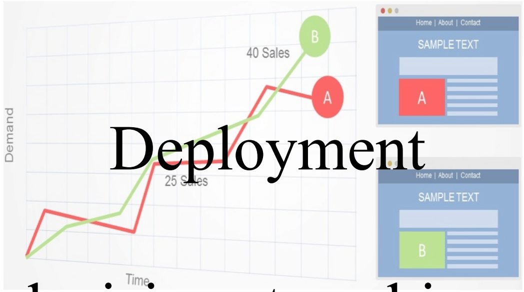
$\neq$ parameters
(weights, biases)

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

Goal: find hyperparameters that achieve high accuracy

## Adaptive experimentation:

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




Goal: make decisions to achieve high revenue

# Motivation: World of Optimization under Uncertainty

Design choices $x$ ⟶  ⟶ Performance metric $f(x)$

non-analytical & no gradient info

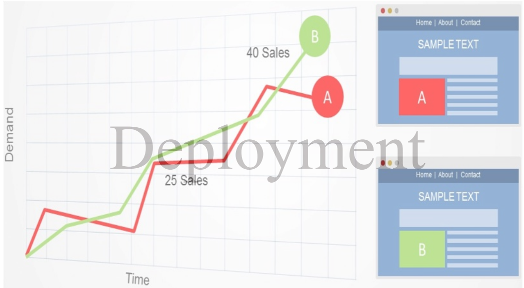
Goal: $\max_{x \in \mathcal{X}} f(x)$

## 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 methods not applicable)

Input $x$ ⟶  ⟶ Observed outcome $f(x)$

non-analytical &
no gradient info

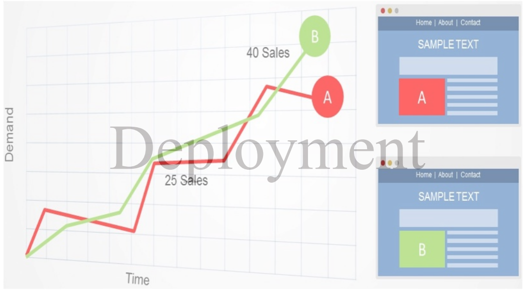
Goal: $\max_{x \in \mathcal{X}} f(x)$

## ML model training:

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

⟶ Accuracy

## Adaptive experimentation:

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

⟶ Revenue

# Background: Black-Box Optimization

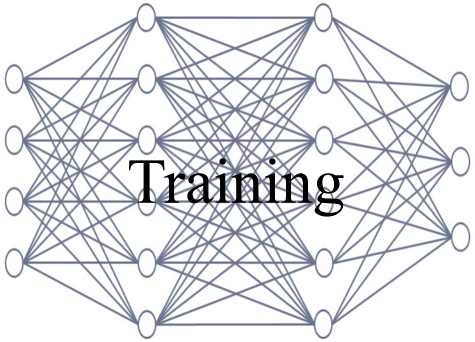
Black-box optimization:

Input $x$ →  → Observed outcome $f(x)$

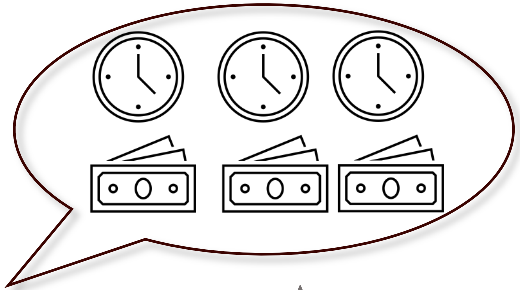
expensive-to-evaluate

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

ML model training:

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

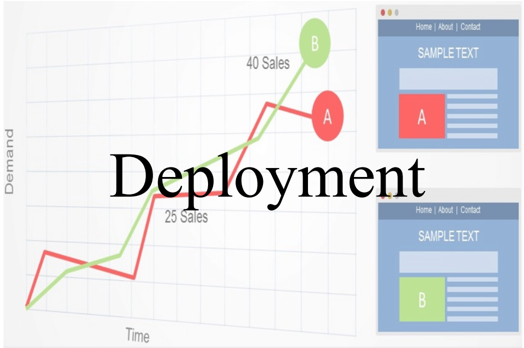
→ Accuracy



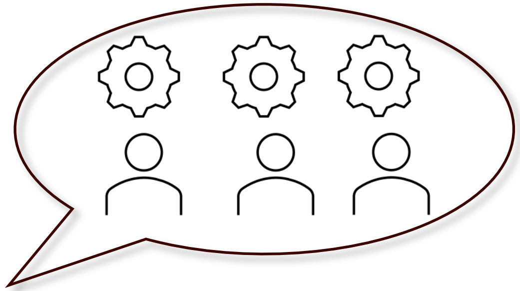
Training time

Compute credits

Adaptive experimentation:

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

→ Revenue



Operational cost

User experience

# Background: Black-Box Optimization

Black-box optimization:

Input $x$ ⟶  ⟶ Observed outcome $f(x)$

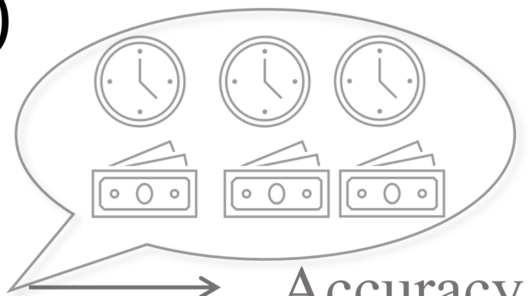
expensive-to-evaluate

limited #evaluations

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

ML model training:

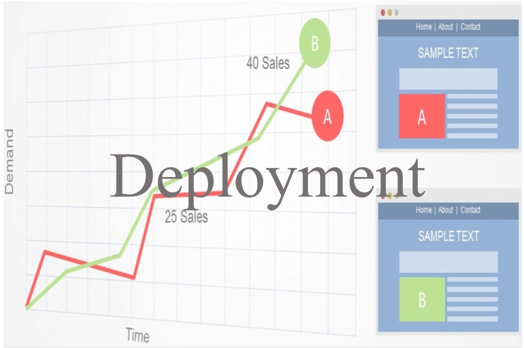
Training hyperparameters (e.g., learning rate, # layers) ⟶  Training ⟶ Accuracy



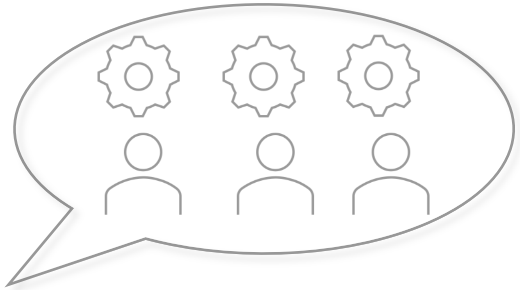
Training time

Compute credits

Adaptive experimentation:

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





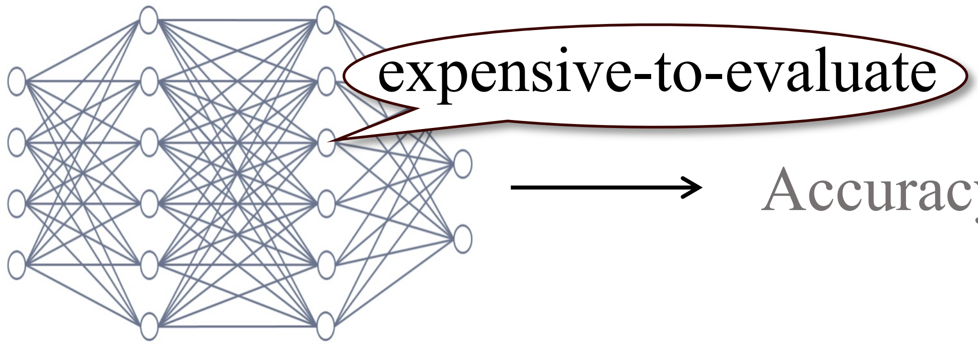
Operational cost

User experience

# Naïve Non-Adaptive Approach: Grid Search

ML model training:

Training hyperparameters ⟶



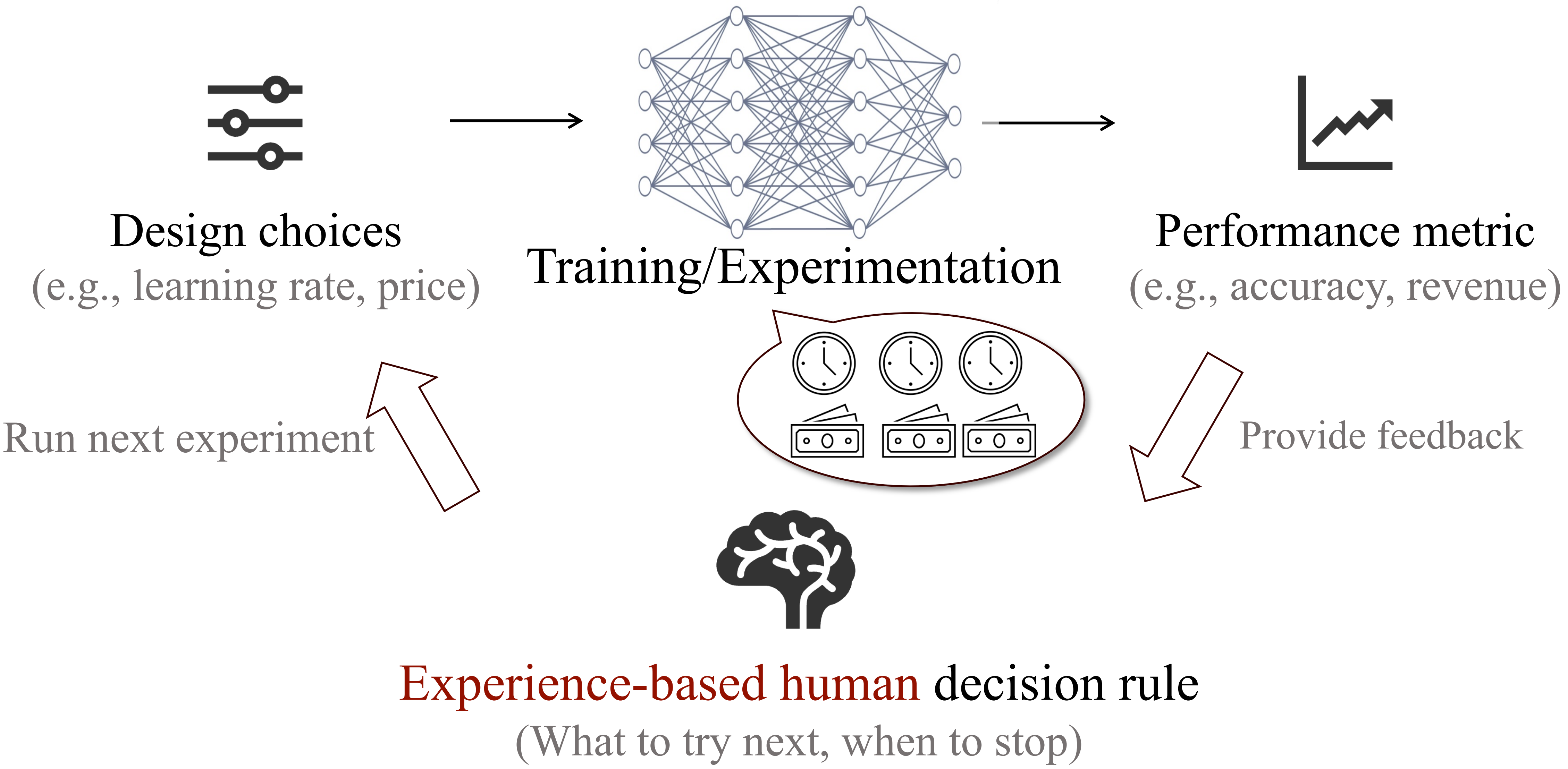

⟶ Accuracy

Goal: find hyperparameters that achieve high accuracy

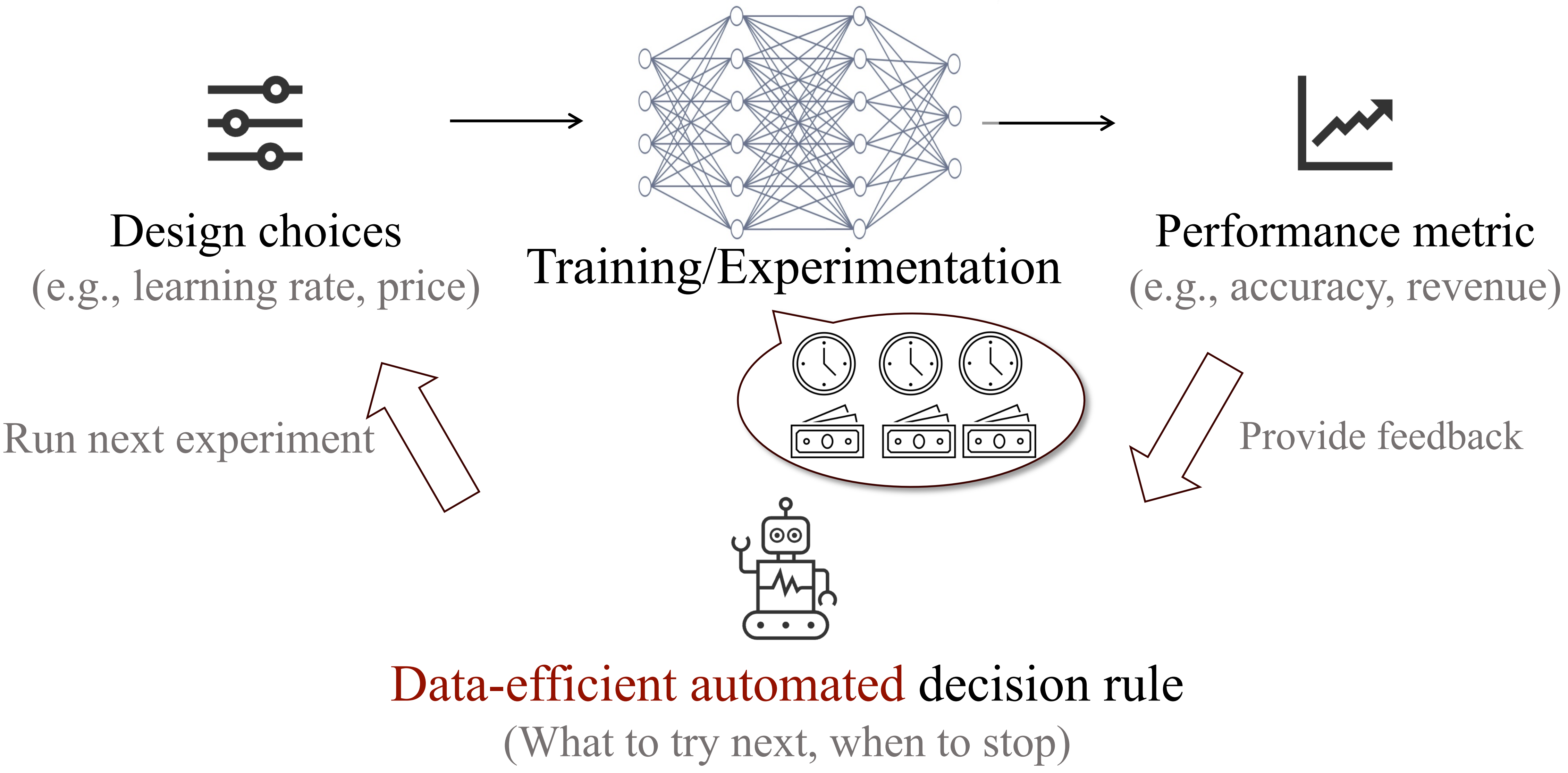
| Training hyperparameter | Range | Number of Options |
|---|---|---|
| Batch size | [16, 512] | 10 |
| Learning rate | [1e-4, 1e-1] | 10 |
| Momentum | [0.1, 0.99] | 10 |
| Weight decay | [1e-5, 1e-1] | 10 |
| Number of layers | {1, 2, 3, 4} | 4 |
| Max units per layer | [64, 1024] | 10 |
| Dropout | [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: | Data-driven approaches: |
|---|---|
| • Grid search | • Local search |
| • Random search | • Evolutionary algorithms |
| • Manual tuning | • Bayesian optimization |
| | • Reinforcement learning |
| | • LLM agent |

# New Methods for Black-Box Optimization

| Naïve approaches: | Data-driven approaches: |
|---|---|
| • Grid search | • Local search |
| • Random search | • Evolutionary algorithms |
| • Manual tuning | • 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

| Naïve approaches: | Data-driven approaches: |
|---|---|
| • Grid search | • Local search |
| • Random search | • Evolutionary algorithms |
| • Manual tuning | • Bayesian optimization ★ |
| | • Reinforcement learning ★ |
| | • LLM agent ★ |

This talk's focus

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

# Bayesian Optimization

$f \sim$ Stochastic Process

$x \longrightarrow$  $\longrightarrow f(x)$

Black-box function

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

# Bayesian Optimization

Time 0

$f \sim$Stochastic Process

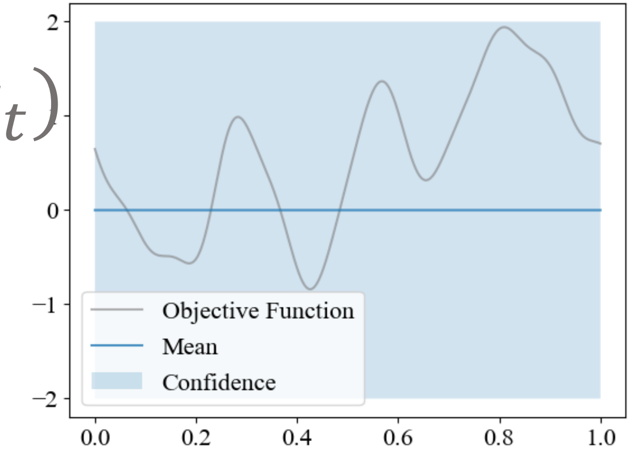
$x \longrightarrow$

$\longrightarrow f(x)$

Model belief

Black-box function

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




Probabilistic model

(e.g., Gaussian process)

# Bayesian Optimization

Time $t$

$x_1, \ldots, x_t$ $\longrightarrow$

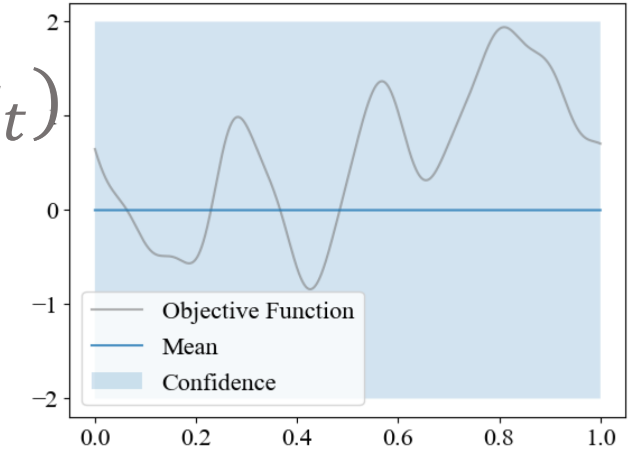
Black-box function

$\longrightarrow$ $f(x_1), \ldots, f(x_t)$

$f \sim$Stochastic Process

Model belief

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




Probabilistic model

(e.g., Gaussian process)

# Bayesian Optimization

Time $t$

$x_1, \ldots, x_t \longrightarrow$

$\longrightarrow f(x_1), \ldots, f(x_t)$

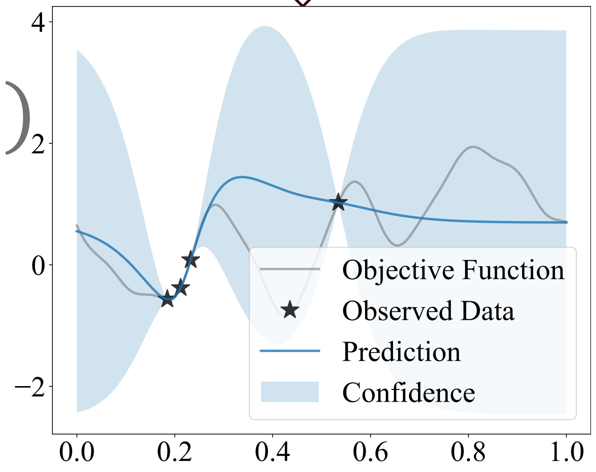
$f \sim$Stochastic Process

Black-box function

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

Update belief

(Bayes' rule)




Probabilistic model

(e.g., Gaussian process)

# Bayesian Optimization

Time $t$

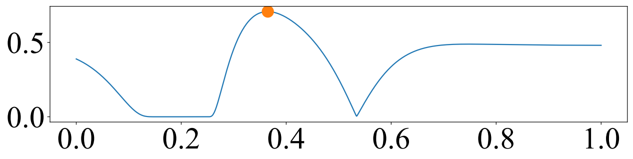
$x_1, \dots, x_t$

Black-box function

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

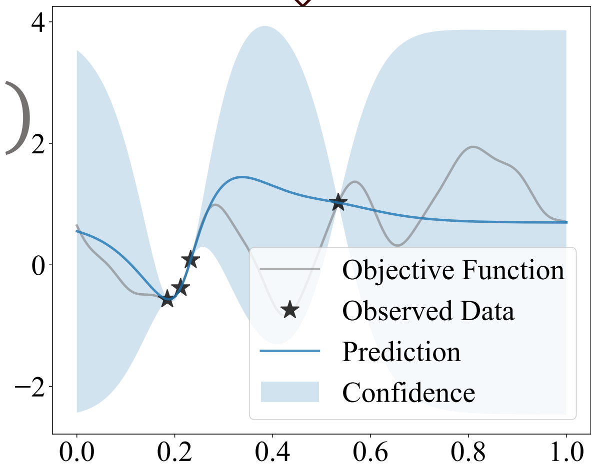
Update belief
(Bayes' rule)

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)

# Bayesian Optimization

Time $t$

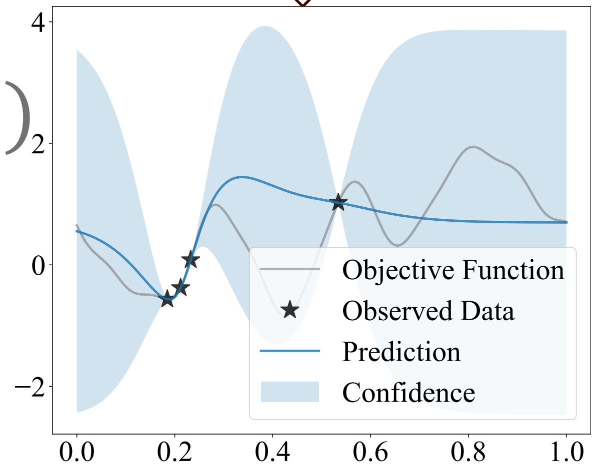
$x_1, \dots, x_t \longrightarrow$  $\longrightarrow f(x_1), \dots, f(x_t)$

Black-box function

Decide next input
(gradient-based optimization)

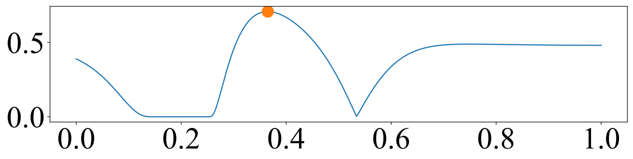
Update belief
(Bayes' rule)

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




Probabilistic model
(e.g., Gaussian process)

scoring (worth of each point




Decision rule
(What to evaluate next)

# Bayesian Optimization

Time $t + 1$

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

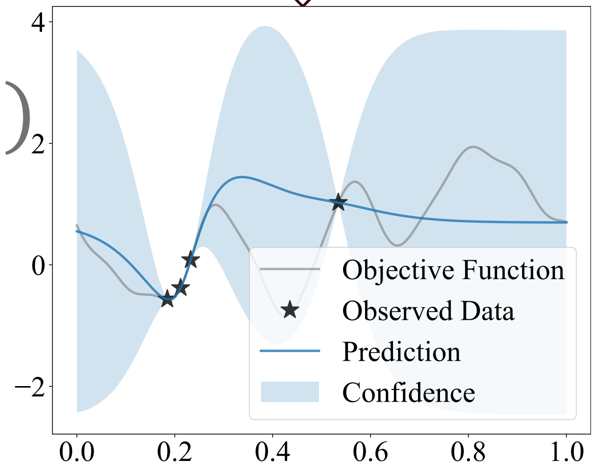
$\longrightarrow$ $f(x_1), \dots, f(x_{t+1})$

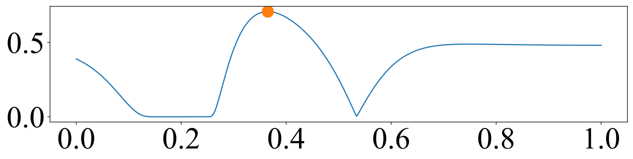
Decide next input
(gradient-based optimization)

Black-box function

Update belief
(Bayes' rule)

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)

# Bayesian Optimization

Time $t + 1$

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

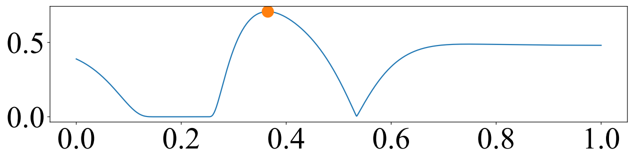
Black-box function

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

Update belief
(Bayes' rule)




Probabilistic model
(e.g., Gaussian process)



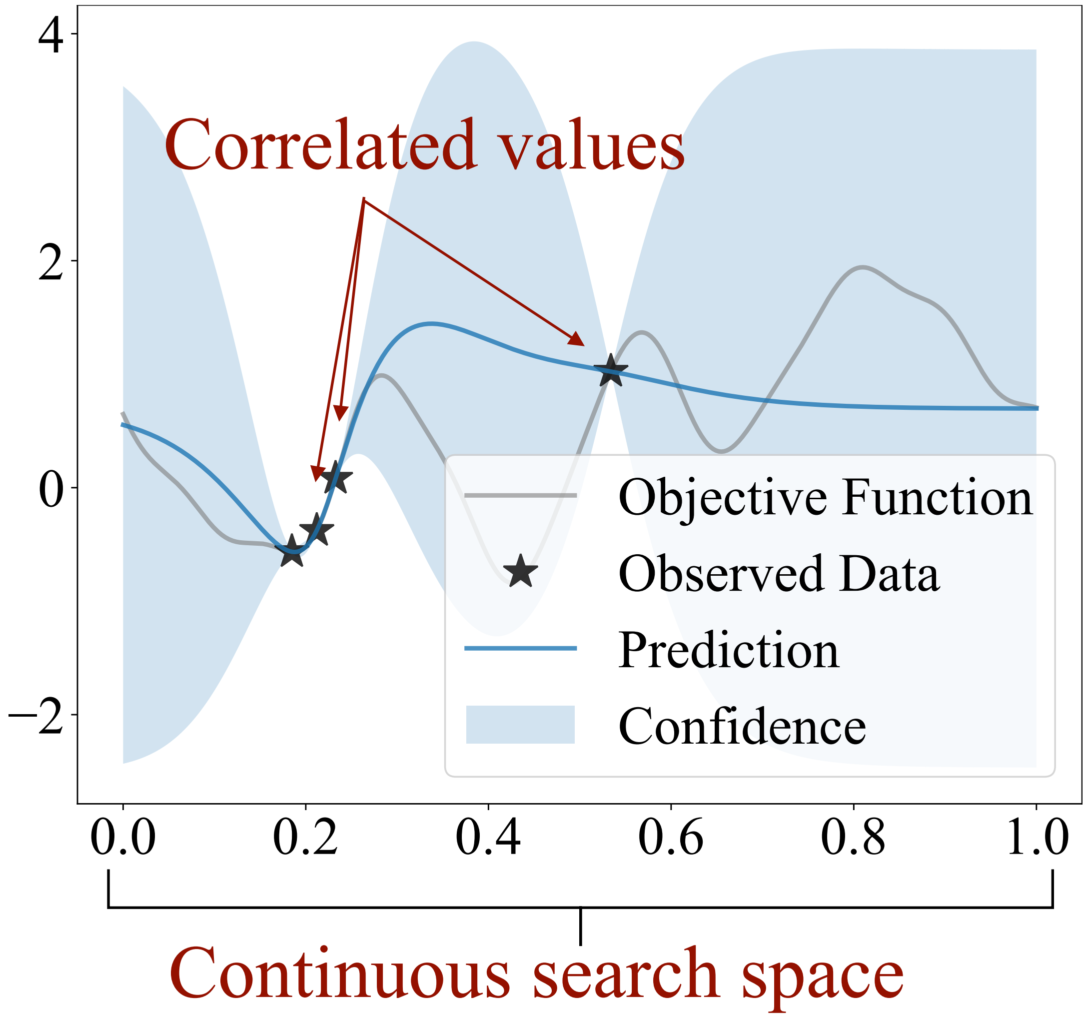

My focus

scoring (worth of each point

Decision rule
(What to evaluate next)

Decide next input
(gradient-based
optimization)

# Challenges in Decision Rule Design




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

# Popular Decision Rule: Expected Improvement

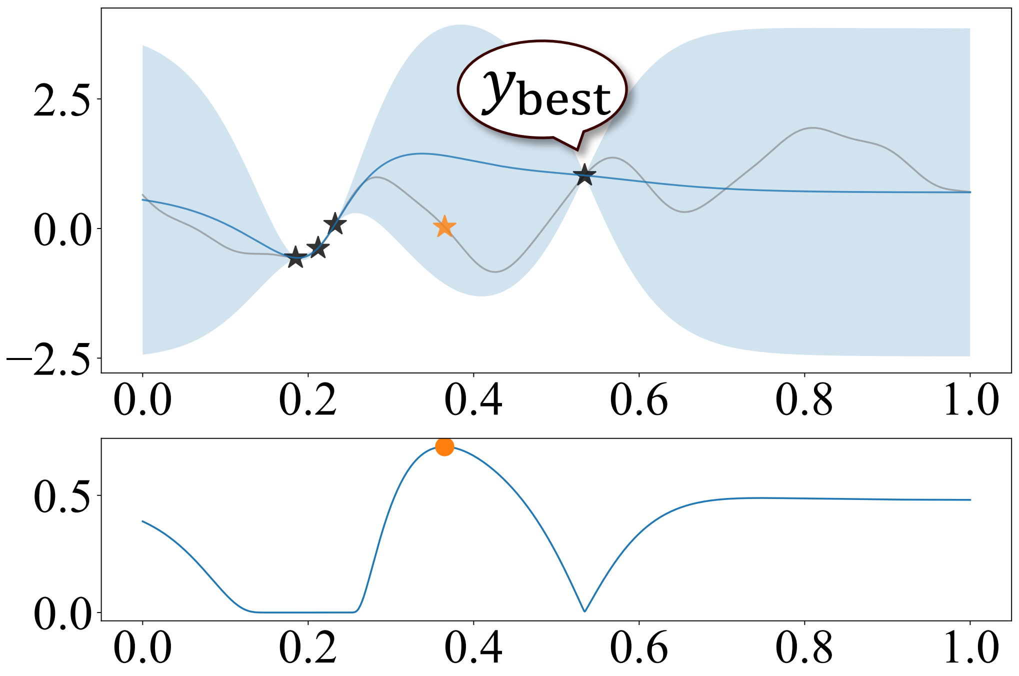
current best observed

data $D$

$$\mathrm{EI}(x) = \mathbb{E}[\underbrace{\max(f(x) - y_{\text{best}}, 0)}_{\text{“improvement”}} \mid x_1, \ldots, x_t]$$

$$x_{t+1} = \operatorname{argmax}_x \mathrm{EI}_{f|D}(x)$$

posterior distribution




One-step approximation to MDP

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

# Popular Decision Rule: Expected Improvement

current best observed

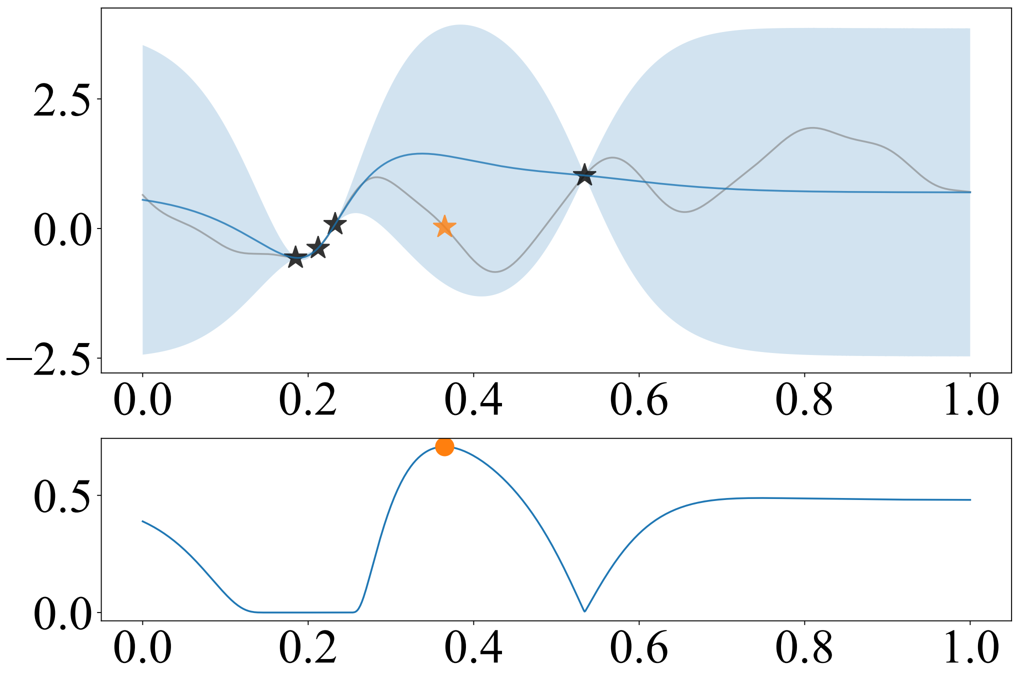
data $D$

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

$$x_{t+1} = \max_x \mathrm{EI}_{f|D}(x; y_{\mathrm{best}})$$

posterior distribution

One-step approximation to MDP

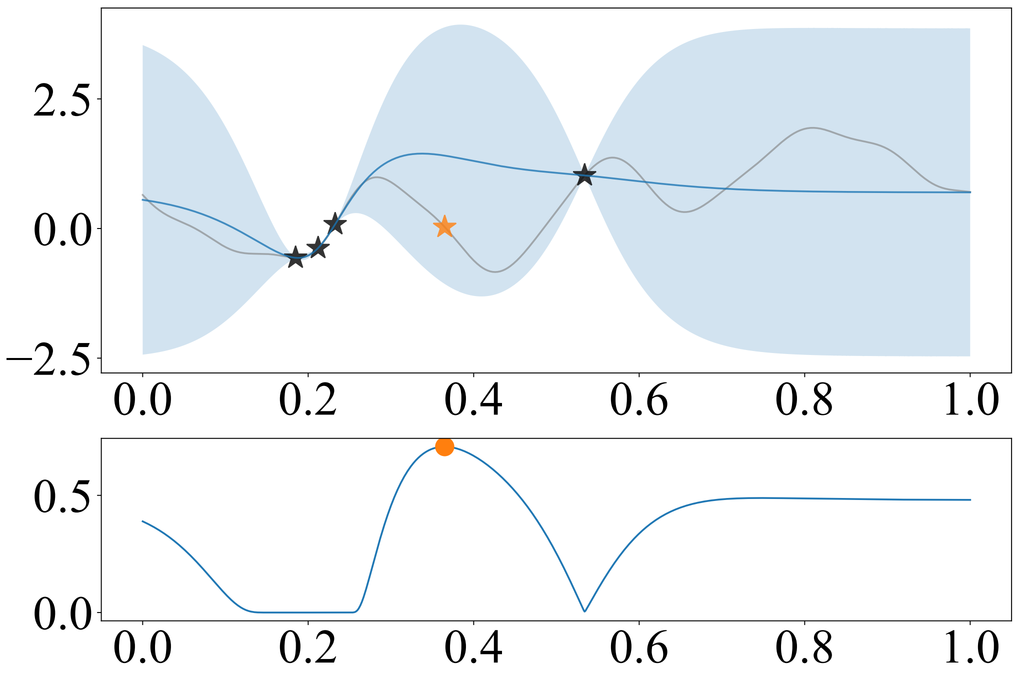



Expected improvement $\mathrm{EI}(x)$

Improvement-based design principle

# Existing Design Principles

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

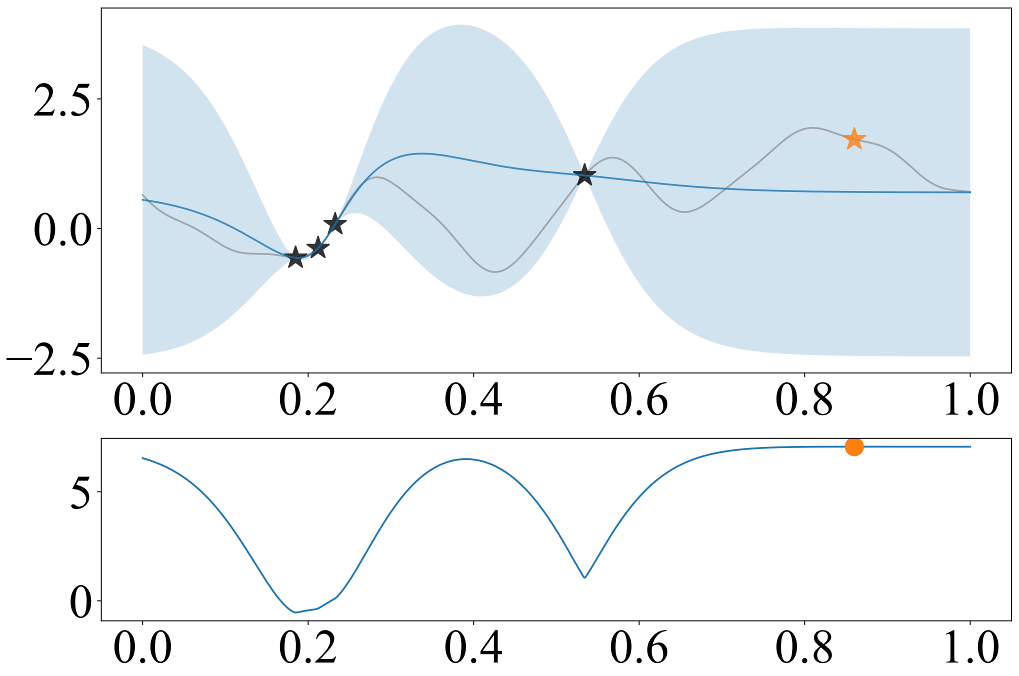



Expected improvement $\mathrm{EI}(x)$

Improvement-based design principle

# New Design Principle: Gittins Index

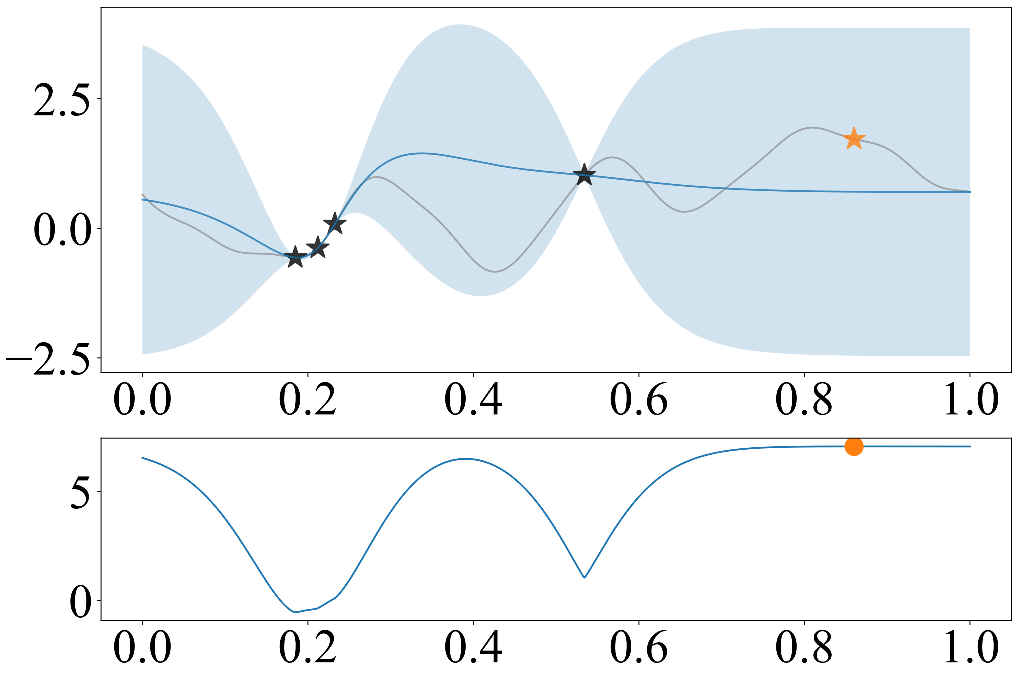
- Improvement-based (e.g., EI)
- Entropy-based
- Confidence bounds (UCB/LCB)
- Thompson sampling (TS)
- Gittins Index




Gittins index $\mathrm{GI}(x)$

# New Design Principle: Gittins Index

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

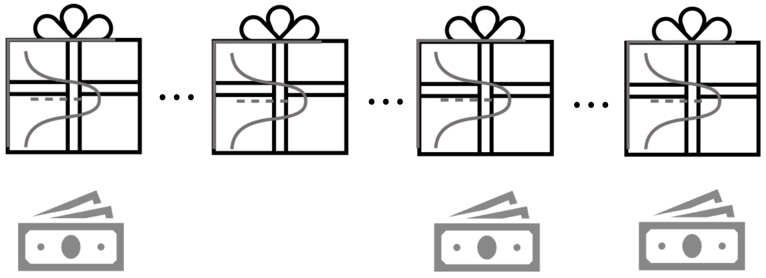



Gittins index $\mathrm{GI}(x)$

? Why another principle?

# Our Contribution: Gittins Index Principle

## Novel connection



Link to Pandora's Box problem
& Gittins index theory

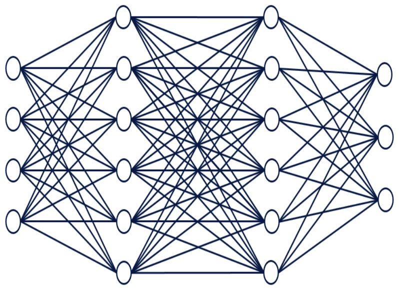
## Principled decision rules

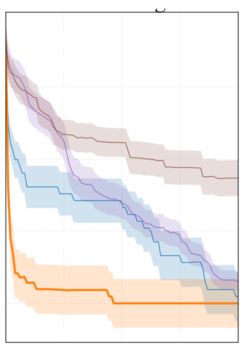
Varying evaluation costs

Adaptive stopping time

Unified framework for
selection and stopping

## Competitive empirical performance





Interests from practitioners (e.g., Meta)

## Future potential

Best-prompt identification

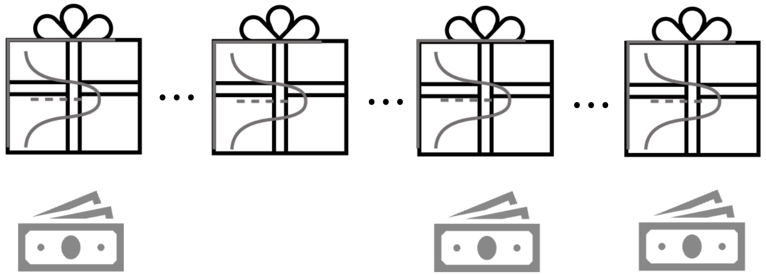
Adaptive response sampling

Chain-of-thought selection

Application to efficient LLM

# Our Contribution: Gittins Index Principle

## Novel connection



Link to Pandora's Box problem
& Gittins index theory

## Principled decision rules

Varying evaluation costs

Adaptive stopping time

Unified framework for cost-aware selection and stopping

## Competitive empirical performance





Interests from practitioners (e.g., Meta)

## Future potential

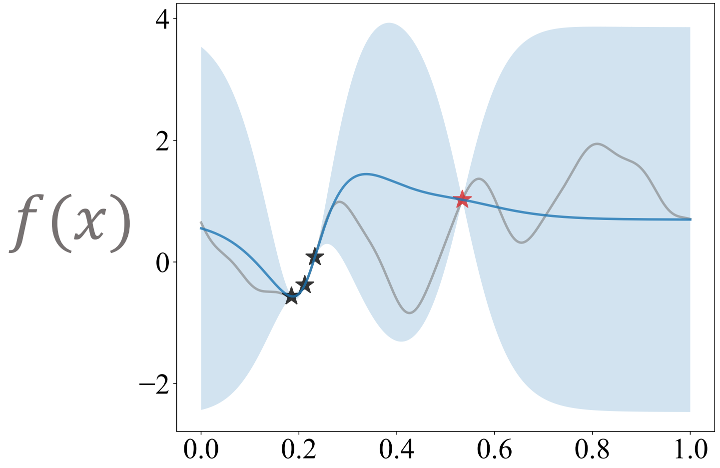
Best-prompt identification

Adaptive response sampling

Chain-of-thought selection

Application to efficient LLM

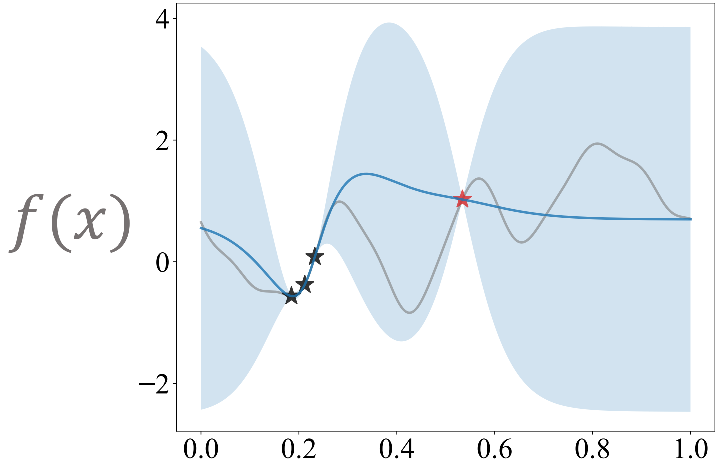
# Bayesian Optimization




**Continuous** search space

**Correlated** function values

# Bayesian Optimization

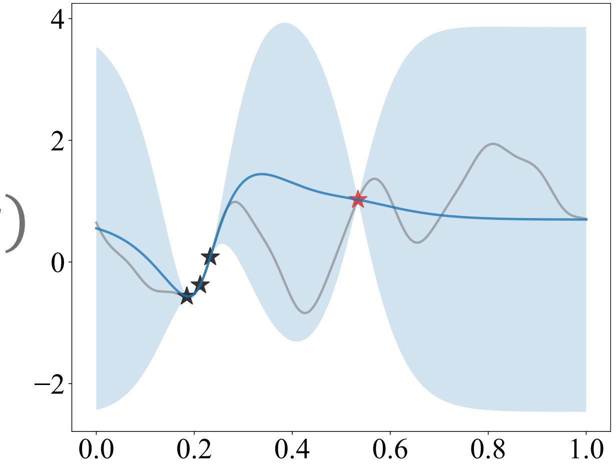



Continuous search space $\Longrightarrow$ Discrete

Correlated function values $\Longrightarrow$ Independent

# Bayesian Optimization

$f(x)$

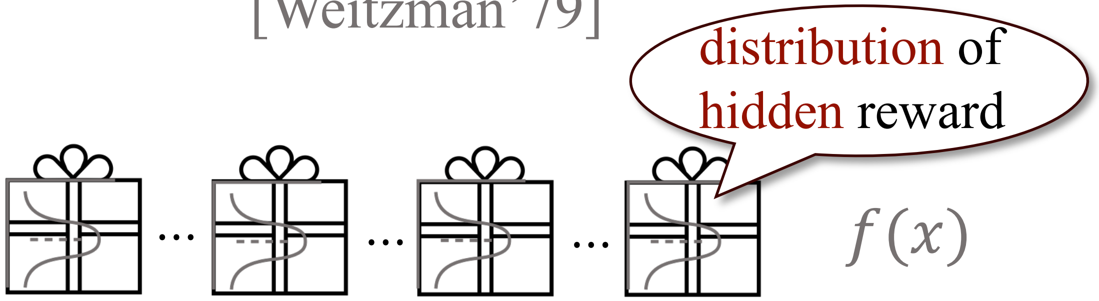



Continuous search space

Correlated function values

# Pandora's Box

[Weitzman'79]



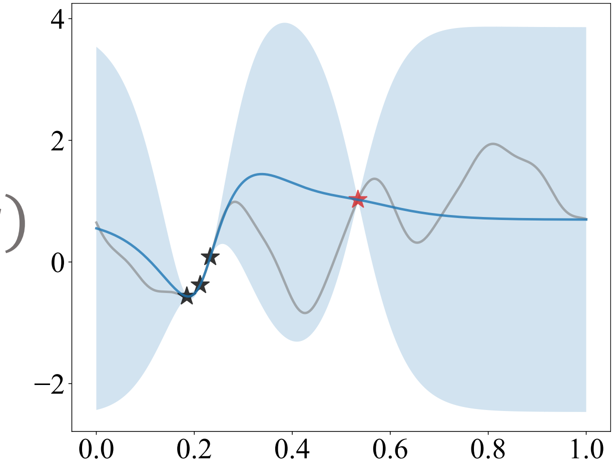

$f(x)$

Discrete

Independent

# Bayesian Optimization

$f(x)$



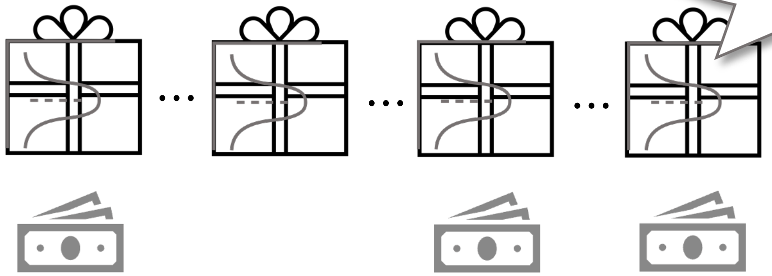

Continuous search space

Correlated function values

# Pandora's Box

[Weitzman'79]

distribution of hidden reward



$f(x)$

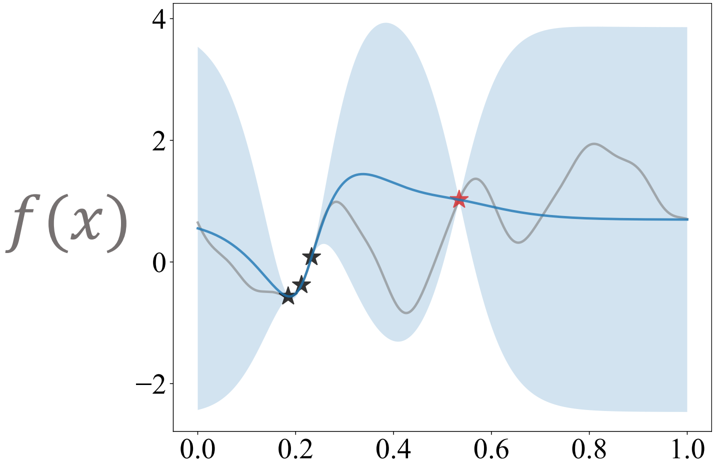
$c(x)$

costs to open

Discrete

Independent

# Bayesian Optimization

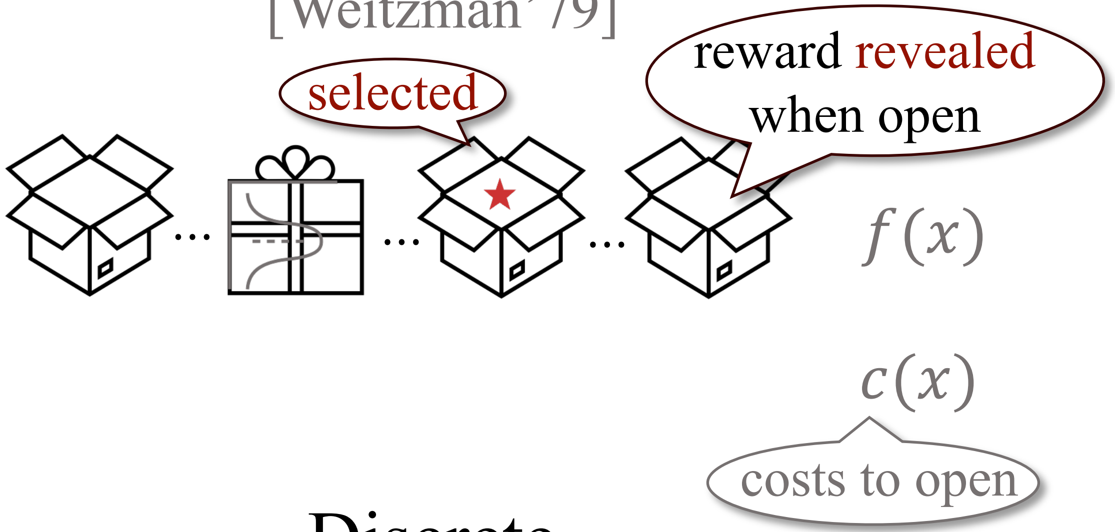



Continuous search space

Correlated function values

# Pandora's Box

[Weitzman'79]

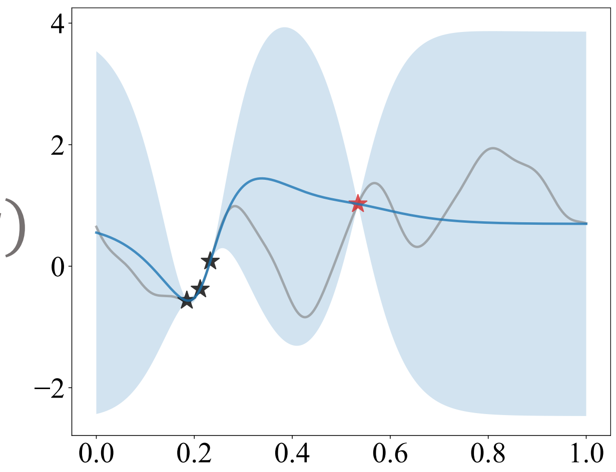



Discrete

Independent

# Bayesian Optimization

$f(x)$



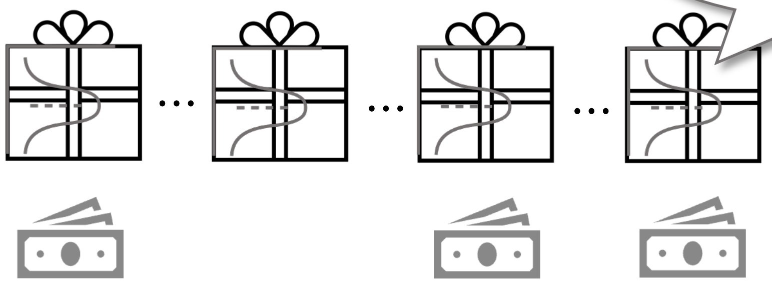

Continuous search space

Correlated function values

# Pandora's Box

[Weitzman'79]

distribution of hidden reward



$f(x)$

$c(x)$

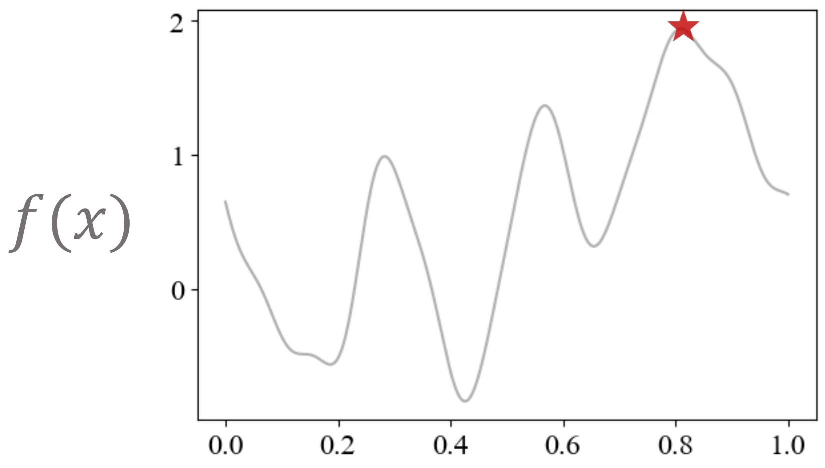
costs to open

Discrete

Independent

Optimal policy: Gittins index

# Bayesian Optimization




Continuous

Correlated

# Pandora's Box

[Weitzman'79]

$\mathrm{GI}_f(x; c(x))$ $g$

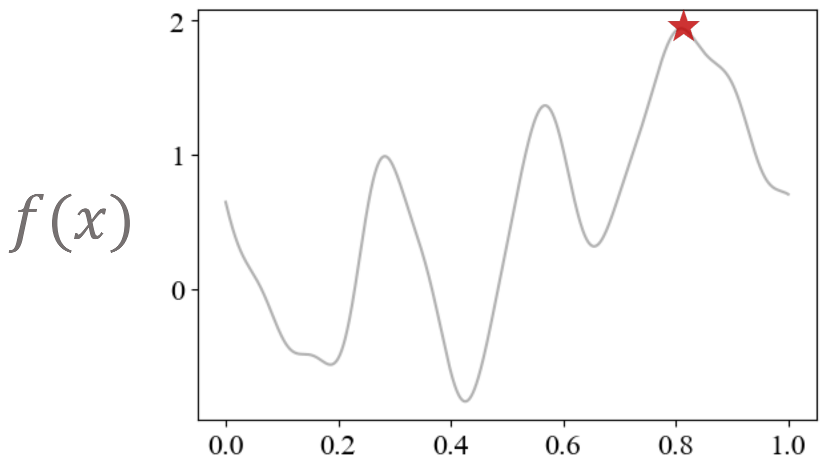

Step 1: Assign each box a Gittins index

Discrete

Independent

Optimal policy: Gittins index

## Bayesian Optimization

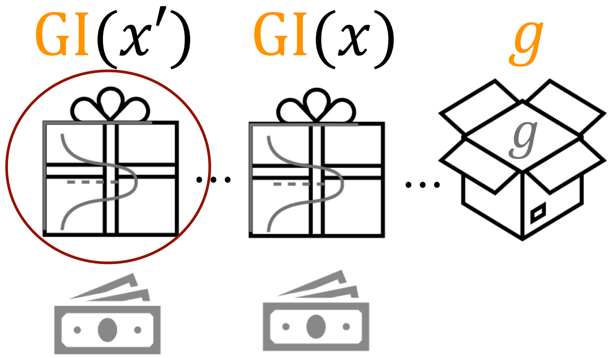



Continuous

Correlated

## Pandora's Box

[Weitzman'79]




Step 2: Act on the box with the highest index

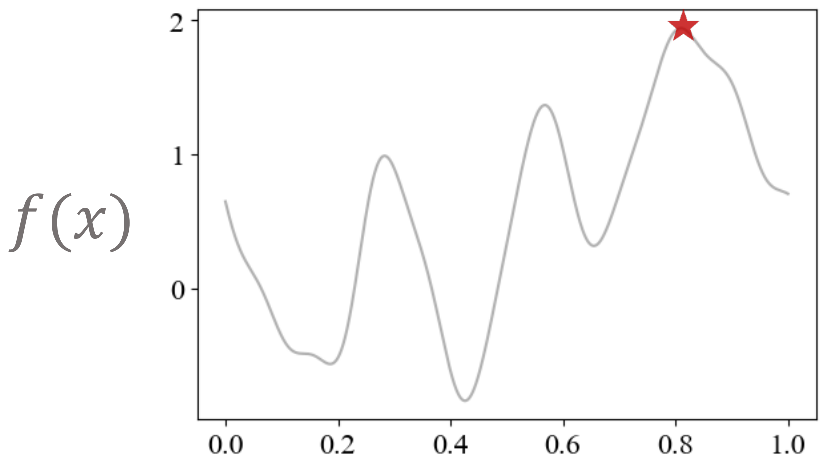
- *Closed*: open it
- *Opened*: select & stop

Discrete

Independent

Optimal policy: Gittins index

## Bayesian Optimization

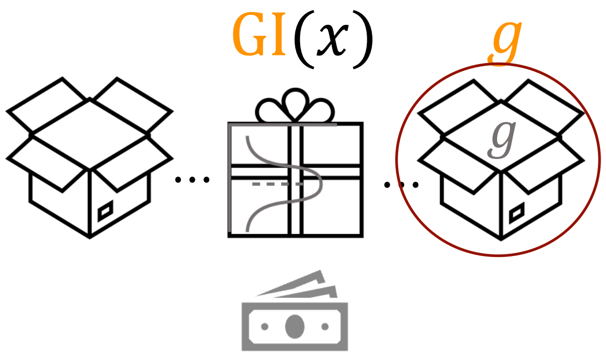



Continuous

Correlated

## Pandora's Box

[Weitzman'79]




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

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

Discrete

Independent

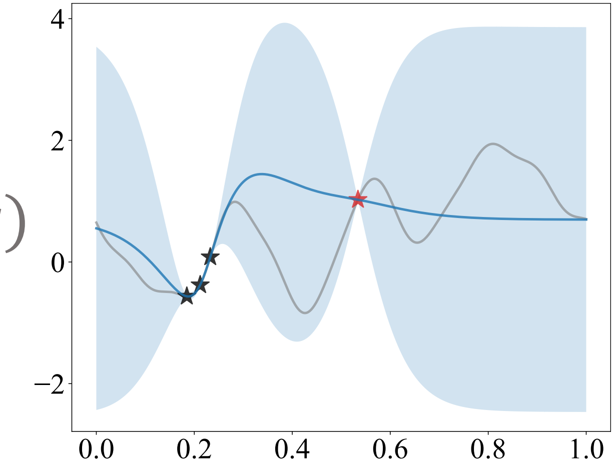
Optimal policy: Gittins index

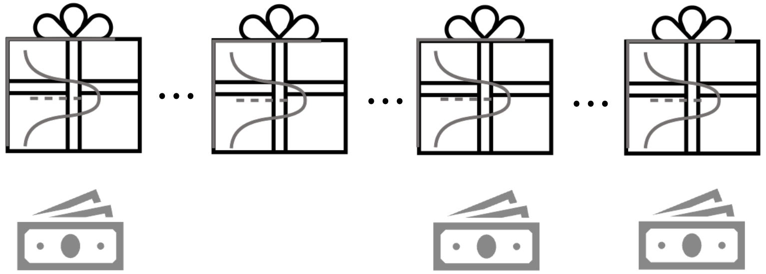
# Bayesian Optimization

# Pandora's Box

[Weitzman'79]

$f(x)$



$f(x)$

$c(x)$

costs to open

Continuous search space | Discrete

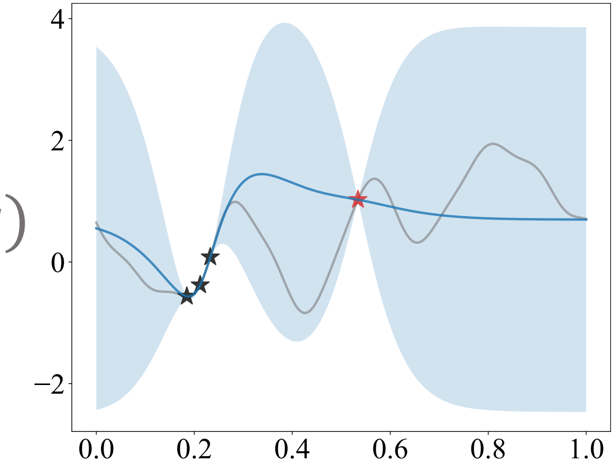
Correlated function values | Independent

How to translate?

$\Leftarrow$ Optimal policy: Gittins index

# Bayesian Optimization

$f(x)$

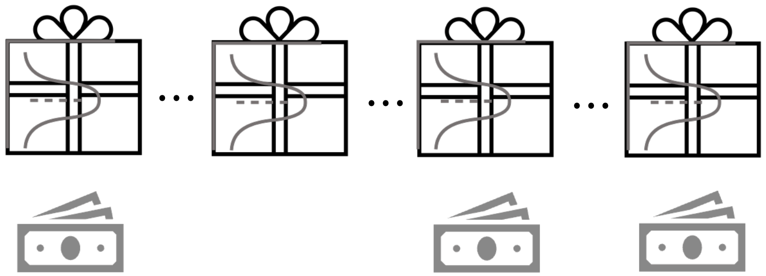



Continuous search space

Correlated function values

# Pandora's Box

[Weitzman'79]



$f(x)$

$c(x)$

costs to open

Discrete

Independent

New!

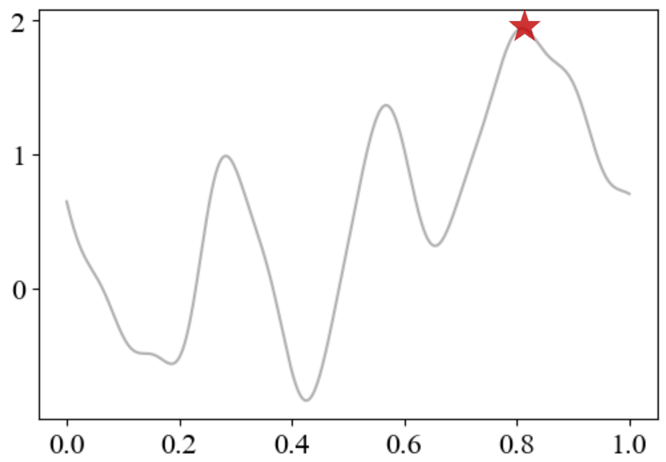
incorporate posterior

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

take continuum limit

# Bayesian Optimization

$f(x)$

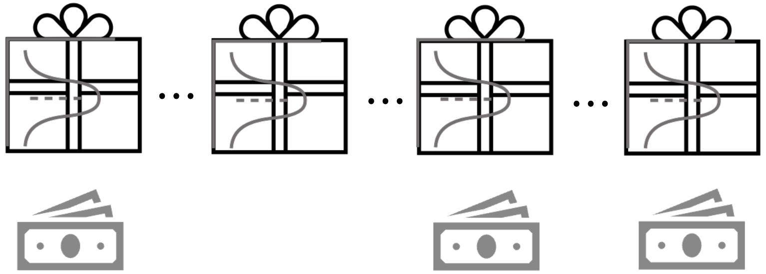



Continuous

Correlated

# Pandora's Box

[Weitzman'79]



$f(x)$

$c(x)$

costs to open

Discrete

Independent

incorporate posterior

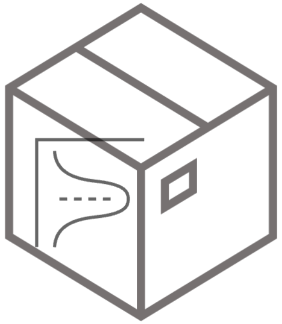
Our policy: $\mathrm{GI}_{f|D}(x; c(x))$ $\Leftarrow$ Optimal policy: $\mathrm{GI}_{f}(x; c(x))$

take continuum limit

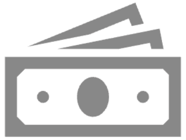
How to compute?

# How to compute Gittins index?

$f(x)$

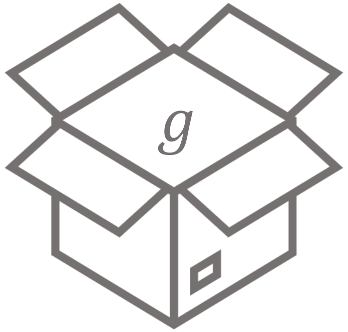


$c(x)$



$\downarrow$ ?

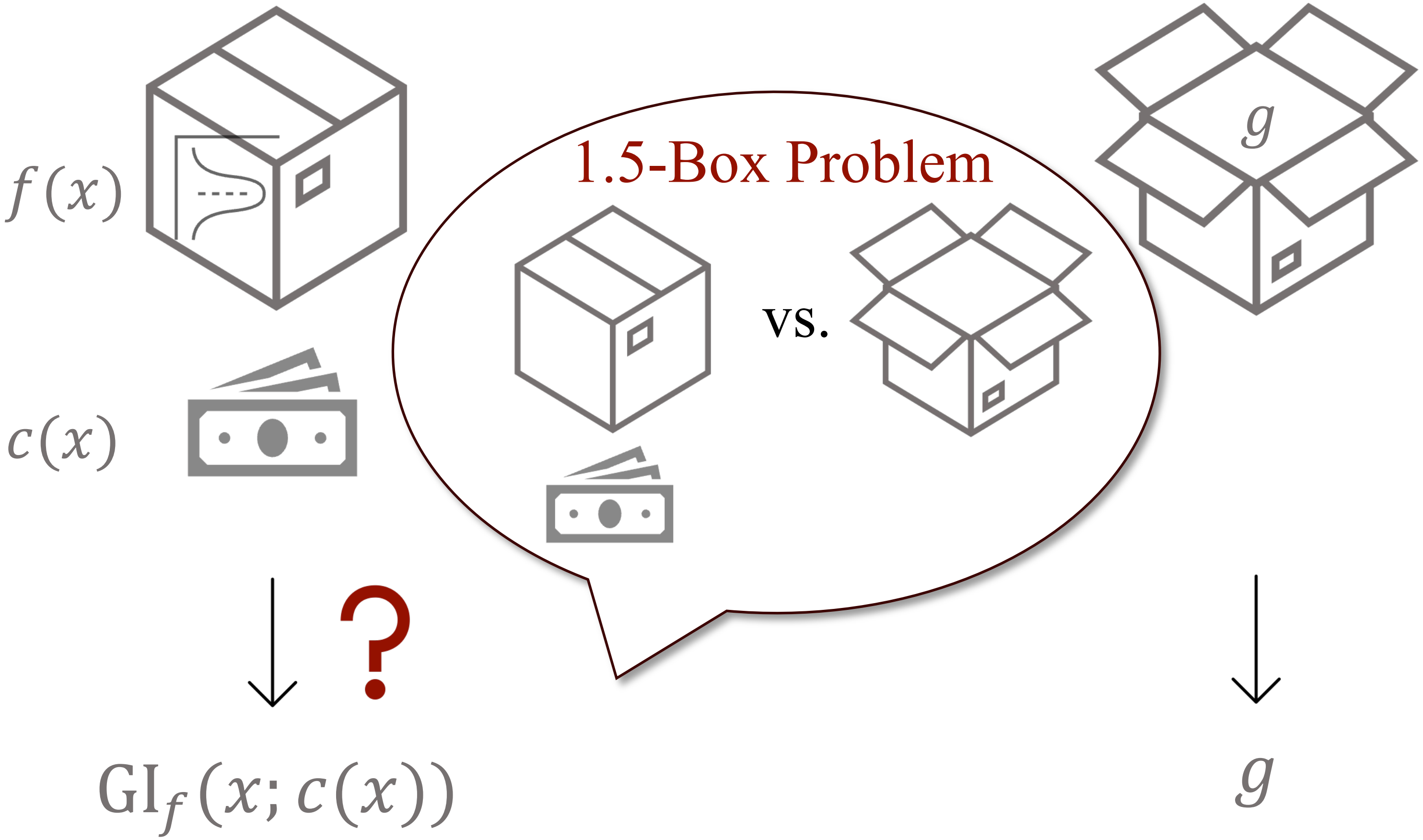
$\mathrm{GI}_f(x; c(x))$




$\downarrow$

$g$

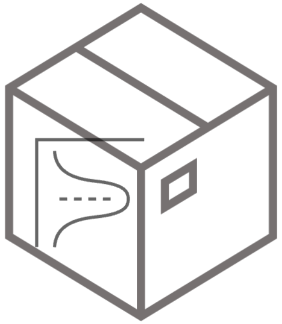
# How to compute Gittins index?

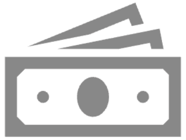



Whether to open a new box or take current best?

# Intuition of Gittins Computation: 1.5-Box Problem

Exploration

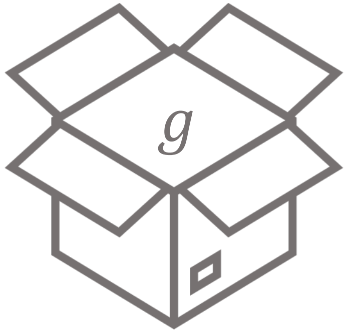
$f(x)$ 

$c(x)$ 

Open closed box

vs.

Exploitation



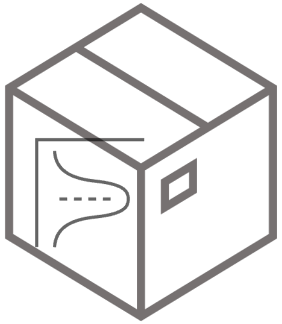

Take opened box

Whether to open a new box or take current best?

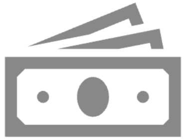
# Intuition of Gittins Computation: 1.5-Box Problem

Exploration

$f(x)$

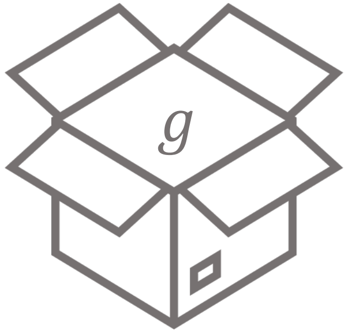


$c(x)$



vs.

Exploitation




Open closed box

Take opened box

$g$

Profit:

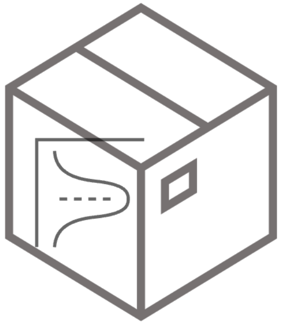
Profit:

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

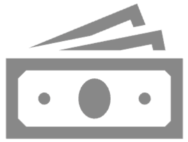
# Intuition of Gittins Computation: 1.5-Box Problem

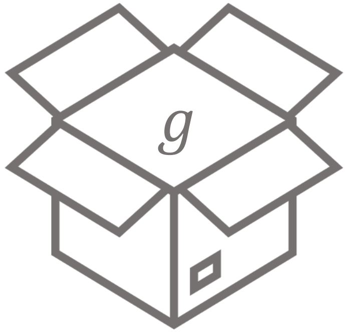
**Exploration** vs. **Exploitation**

$f(x)$



$c(x)$



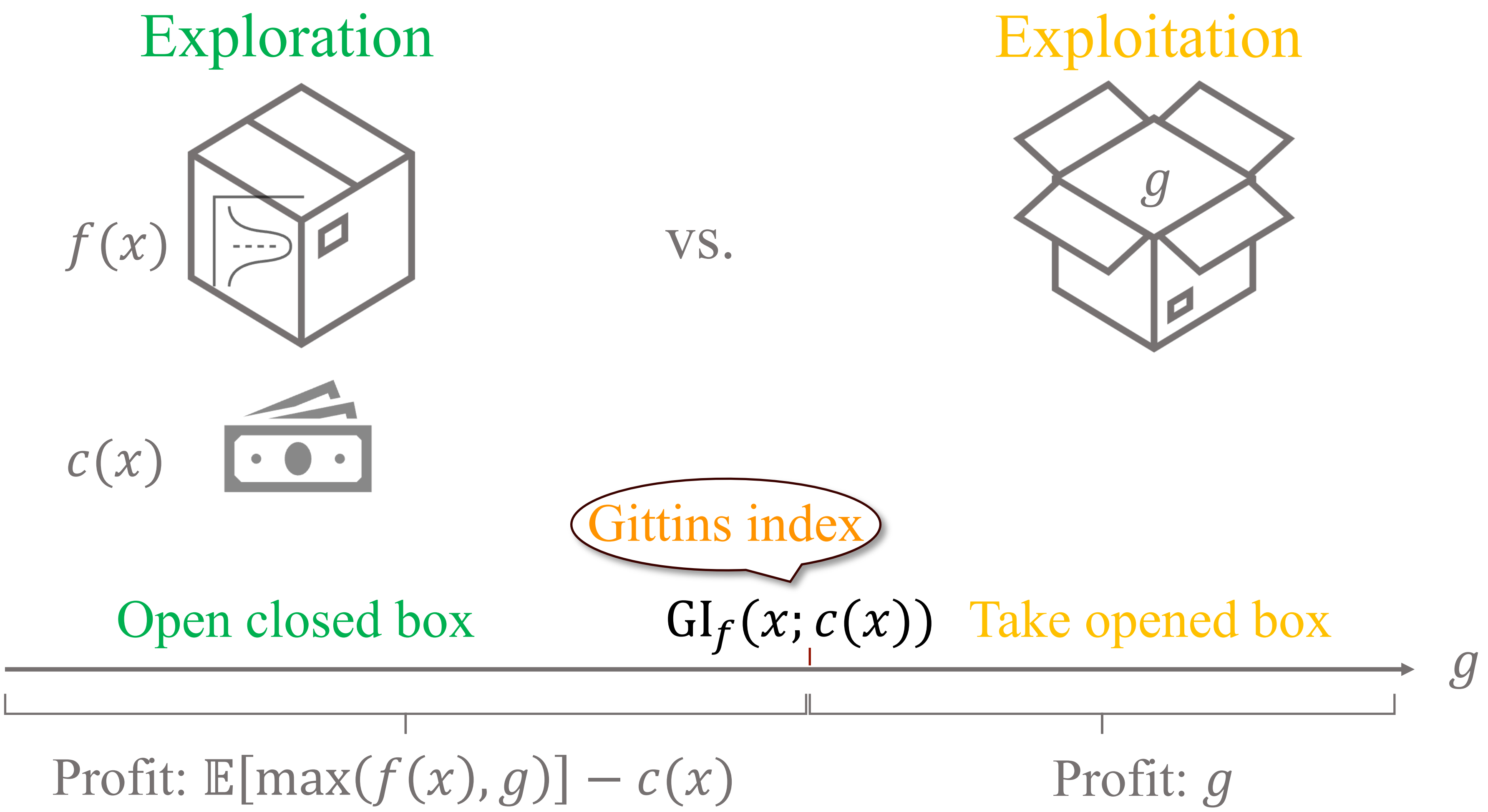



Open closed box | Take opened box → $g$

Profit: $\mathbb{E}[\underbrace{\max(f(x), g)}_{\begin{cases} \text{take inside value}, & f(x) > g \\ \text{take outside option}, & f(x) \le g \end{cases}}] - c(x)$

Profit: $g$

# Intuition of Gittins Computation: 1.5-Box Problem



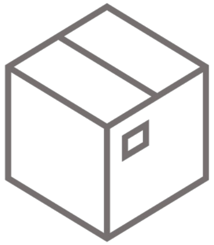

$\mathrm{GI}_f(x; c(x))$: solution $g$ to $\mathbb{E}[\max(f(x), g)] - c(x) = g$

# Intuition

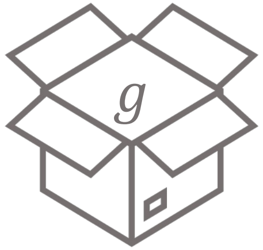
Exploration

Exploitation

$f(x)$



vs.




$c(x)$

Open closed box

Take opened box

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

$g$

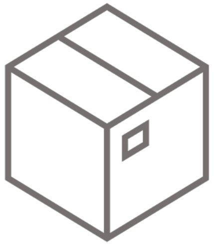
$\mathrm{GI}_f(x; c) := $ solution $g$ s.t.

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

# Intuition

Exploration | Exploitation

$f(x)$



vs.


$c(x)$

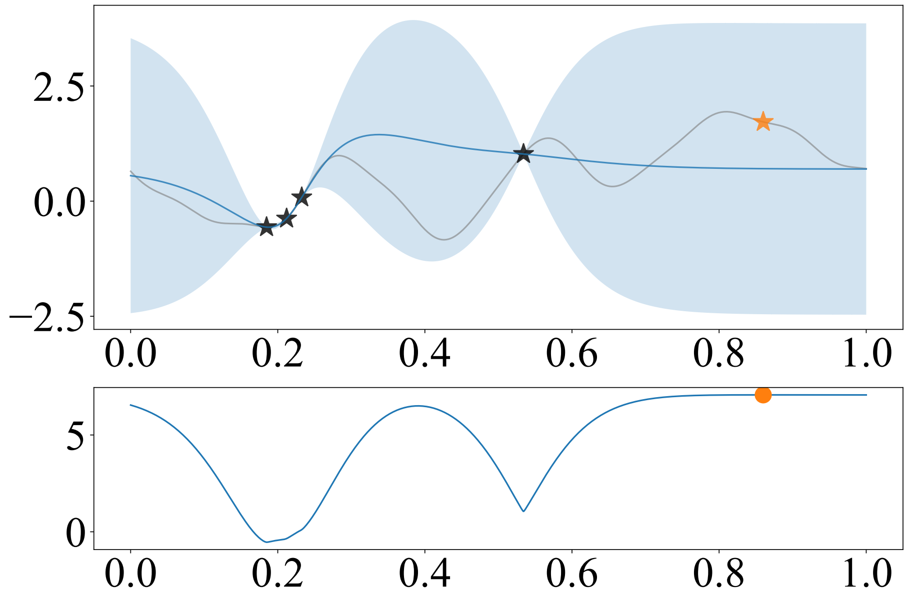
Open closed box | Take opened box

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

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

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

# Gittins Index




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

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

# Intuition

Exploration | Exploitation

$f(x)$  vs. 


$c(x)$ 

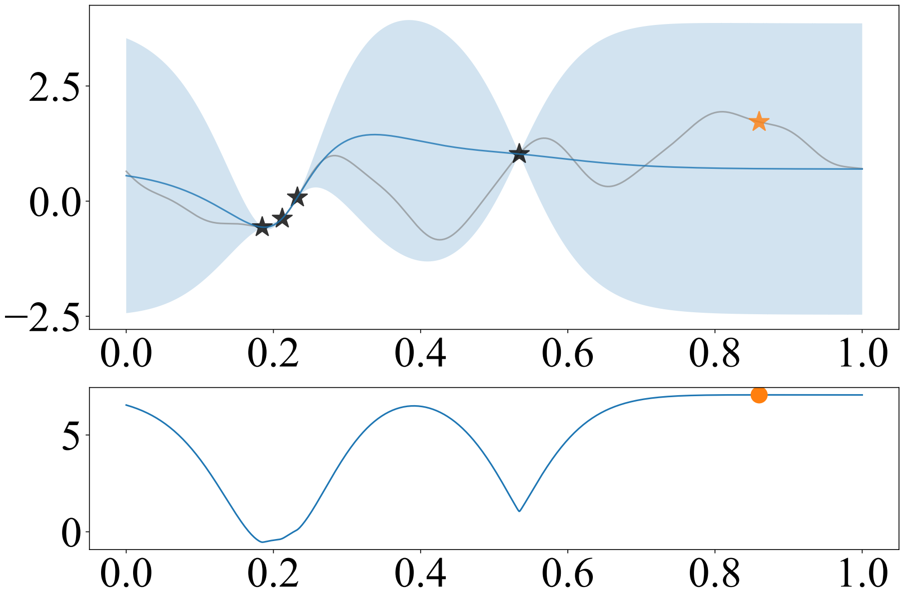
Open closed box: $\mathbb{E}[\max(f(x), g)] - c(x)$

Take opened box: $g$

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

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

# Gittins Index



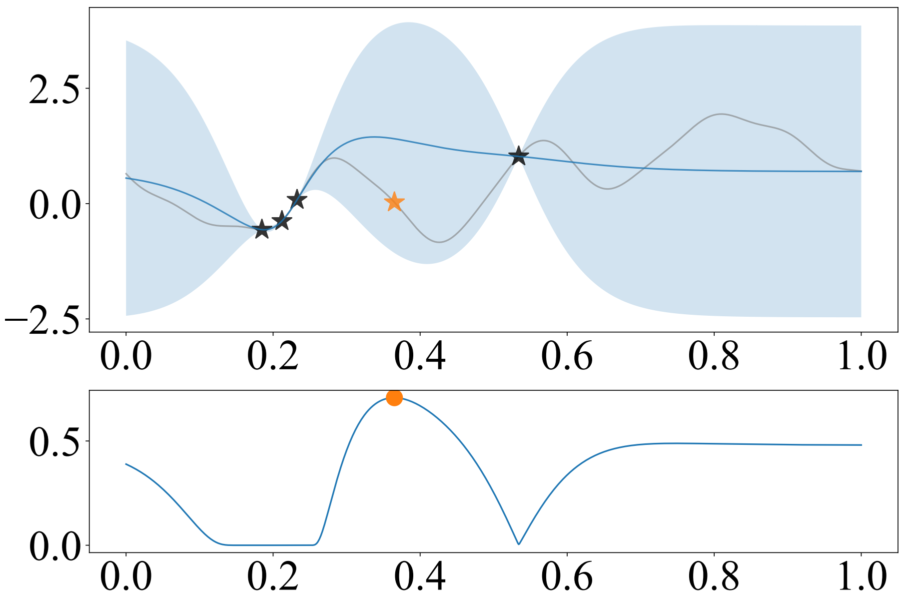

$\mathrm{GI}_{f|D}(x; c) :=$ solution $g$ s.t.

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

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

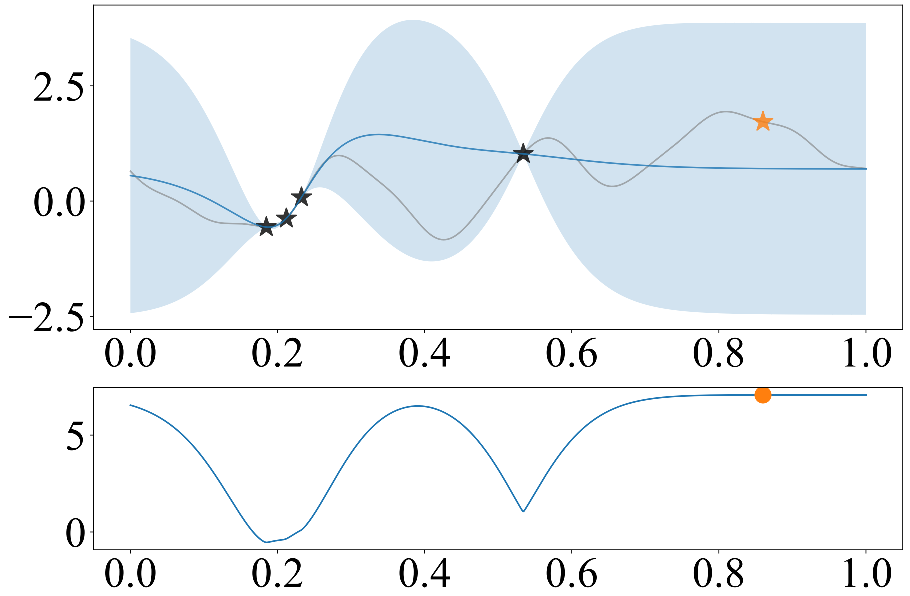
$$\Leftrightarrow \underbrace{\mathbb{E}[\max(f(x) - g, 0) \mid D]}_{\mathrm{EI}_{f|D}(x;\, g)} = c(x)$$

# Expected Improvement

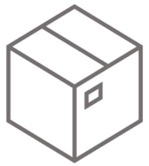



$$\mathrm{EI}_{f|D}(x) := \mathbb{E}[\max(f(x) - y_{\mathrm{best}}, 0) \mid D]$$

# Gittins Index



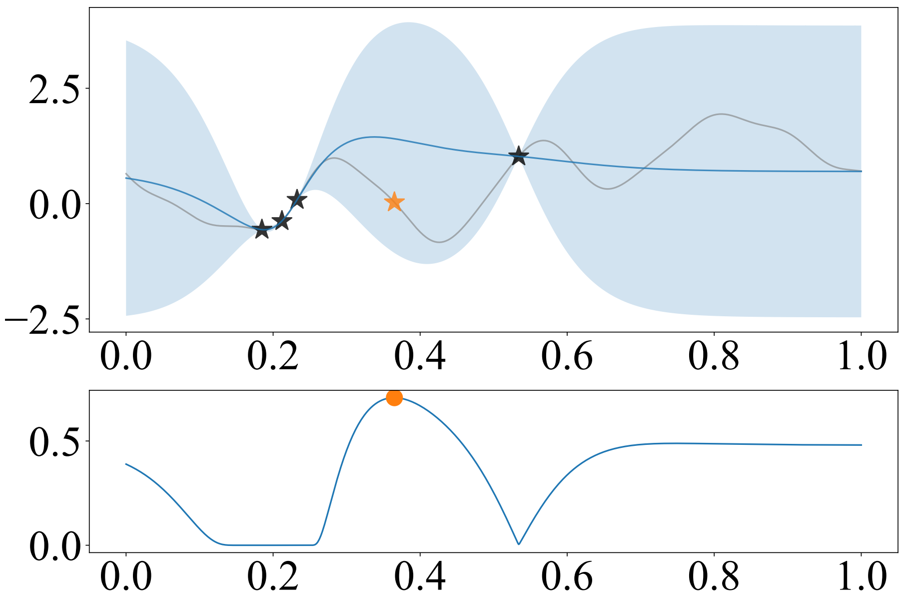

$$\mathrm{GI}_{f|D}(x; c) := \text{solution } g \text{ s.t. } \mathrm{EI}_{f|D}(x; g) = c(x)$$
$$\text{where } \mathrm{EI}_{f|D}(x; g) := \mathbb{E}[\max(f(x) - g, 0) \mid D]$$

$f(x)$  vs. 

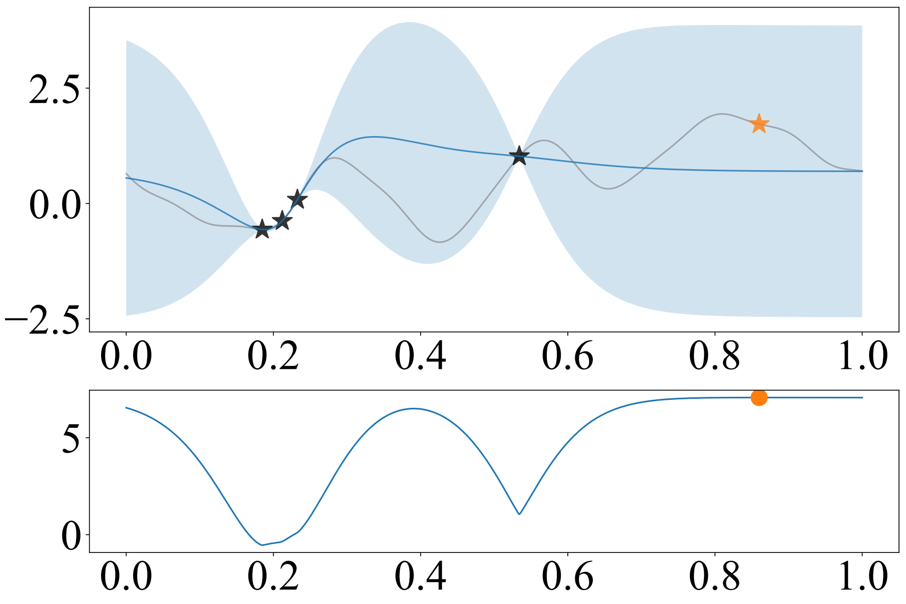

$c(x)$ 

Exploration Exploitation

# Expected Improvement




# Gittins Index




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

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

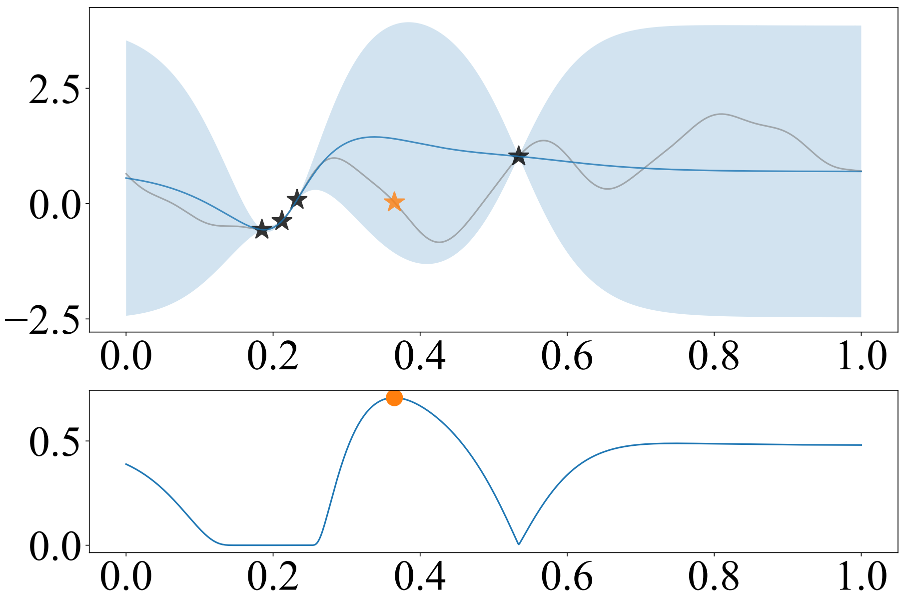
where $\mathrm{EI}_{f|D}(x; g) := \mathbb{E}[\max(f(x) - g, 0) \mid D]$

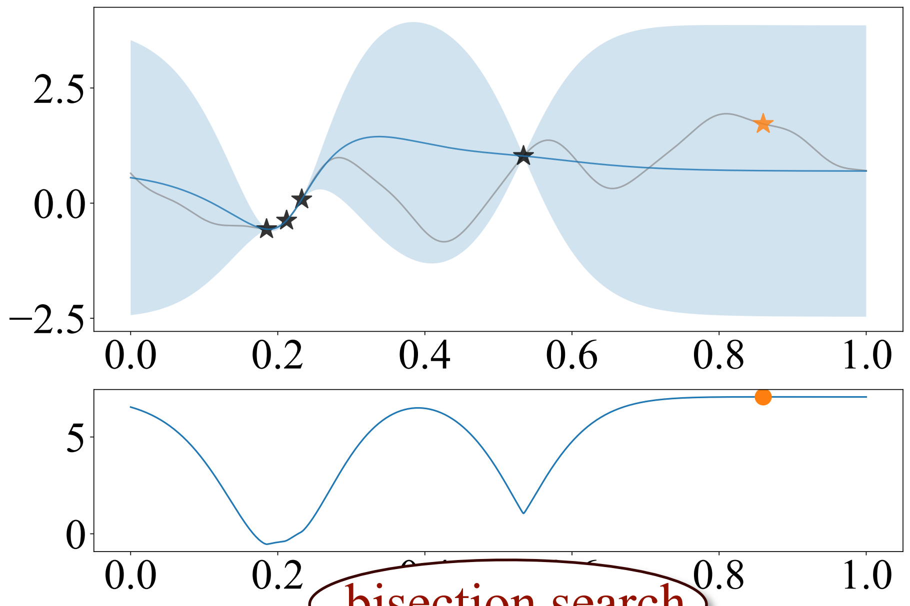
Selection rule: $\max_x \mathrm{EI}_{f|D}(x; y_{\text{best}})$ $\max_x \mathrm{GI}_{f|D}(x; c(x))$

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

# Expected Improvement

# Gittins Index




bisection search

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

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

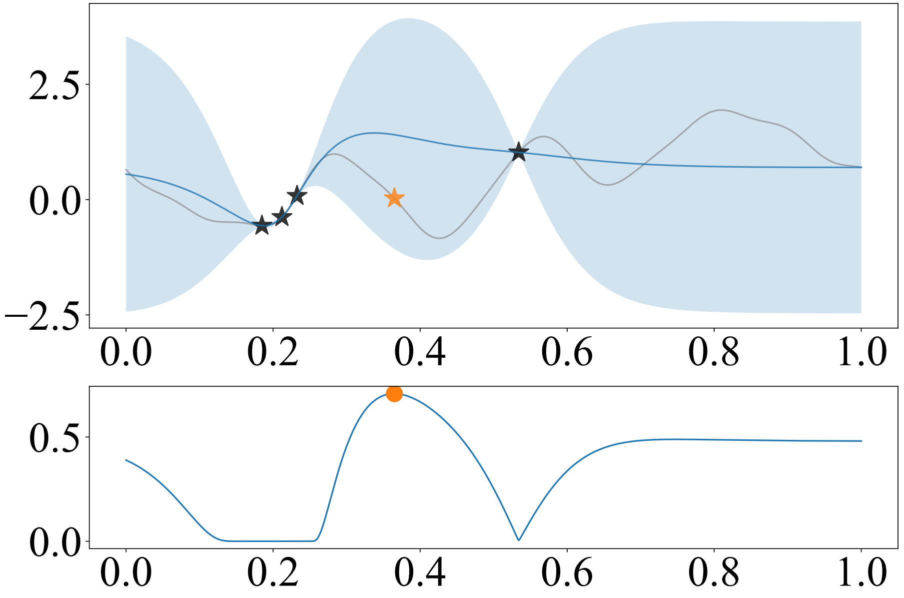
where $\mathrm{EI}_{f|D}(x; g) := \mathbb{E}[\max(f(x) - g, 0) \mid D]$

analytical expression

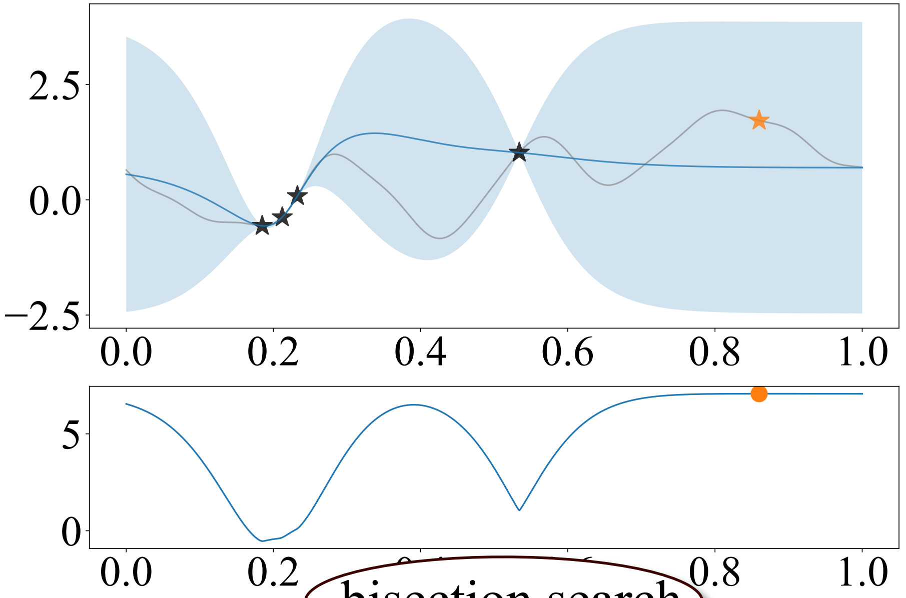
Selection rule: $\max_x \mathrm{EI}_{f|D}(x; y_{\text{best}})$ $\max_x \mathrm{GI}_{f|D}(x; c(x))$

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

# Expected Improvement




# Gittins Index




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

bisection search

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

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

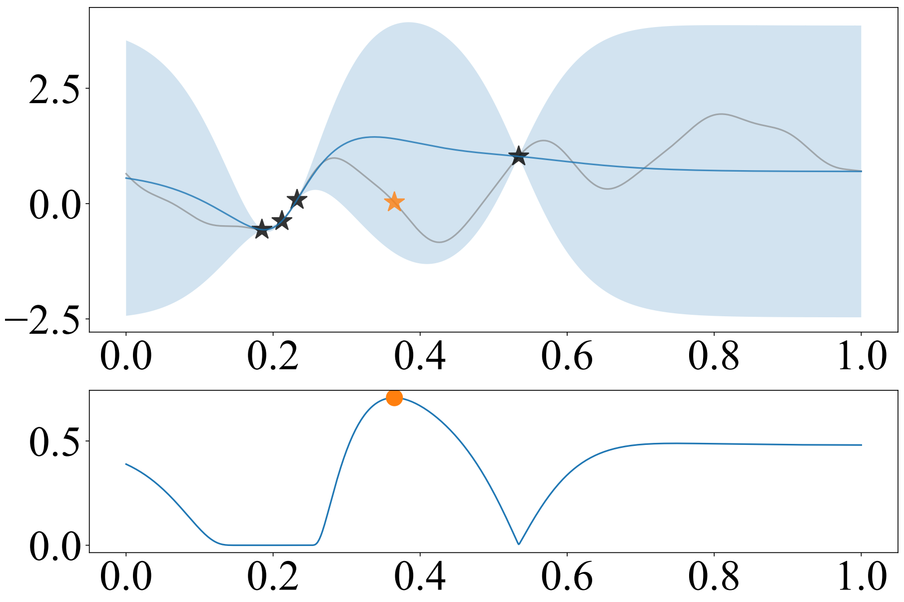
analytical expression

Selection rule: $\max_x \mathrm{EI}_{f|D}(x; y_{\mathrm{best}})$ $\max_x \mathrm{GI}_{f|D}(x; c(x))$

Easy-to-compute decision rules!

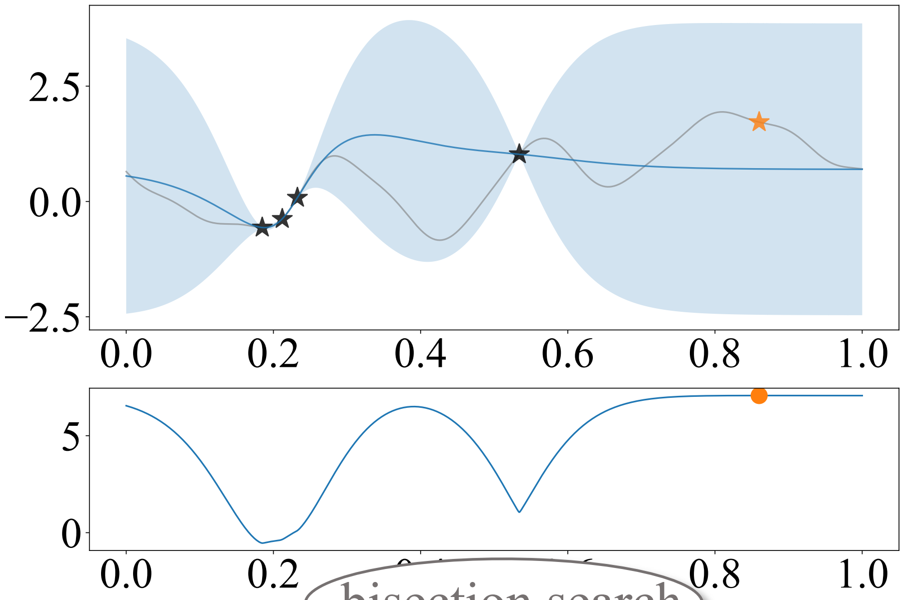
"Cost-aware Bayesian Optimization via the Pandora's Box Gittins Index." NeurIPS'24.

# Expected Improvement




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

# Gittins Index




bisection search

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

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

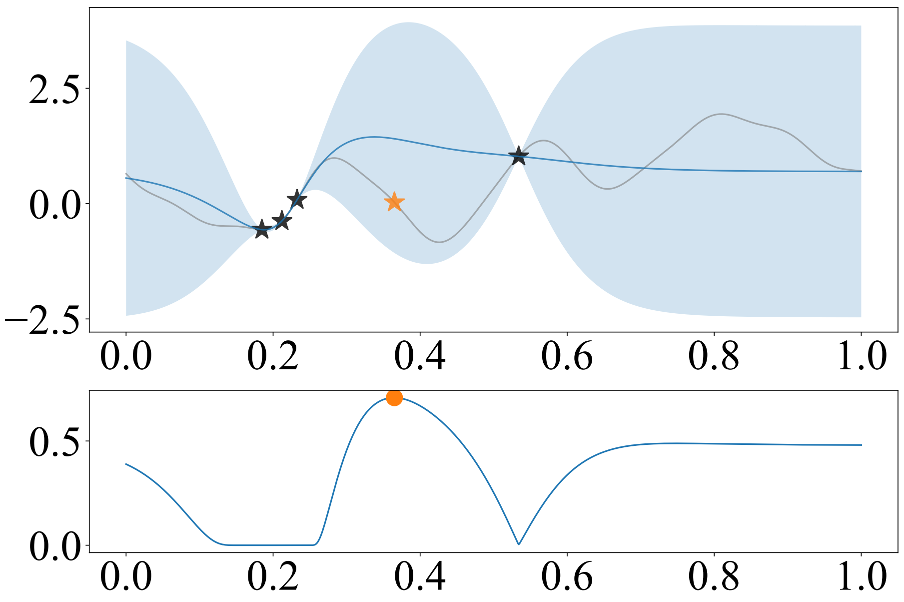
Google DeepMind

**FunBO: Discovering new acquisition functions for Bayesian Optimization with FunSearch**

LLM-driven evolutionary search method

GI is not easy to discover!

# Expected Improvement

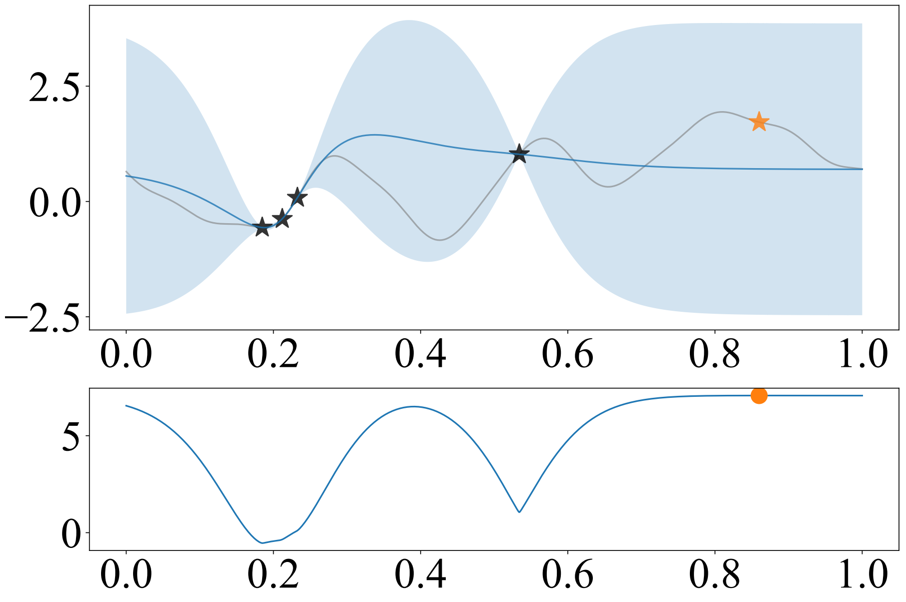



$\mathrm{EI}_{f|D}(x) := \mathbb{E}[\max(f(x) - y_{\text{best}}, 0) \mid D]$

Temporal simplification to MDP

(One-step)

# Gittins Index




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

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

Spatial simplification to MDP

# Our Contribution: Gittins Index Principle

## Novel connection

Link to Pandora's Box problem
& Gittins index theory

## Principled decision rules

- Varying evaluation costs
- Adaptive stopping time

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

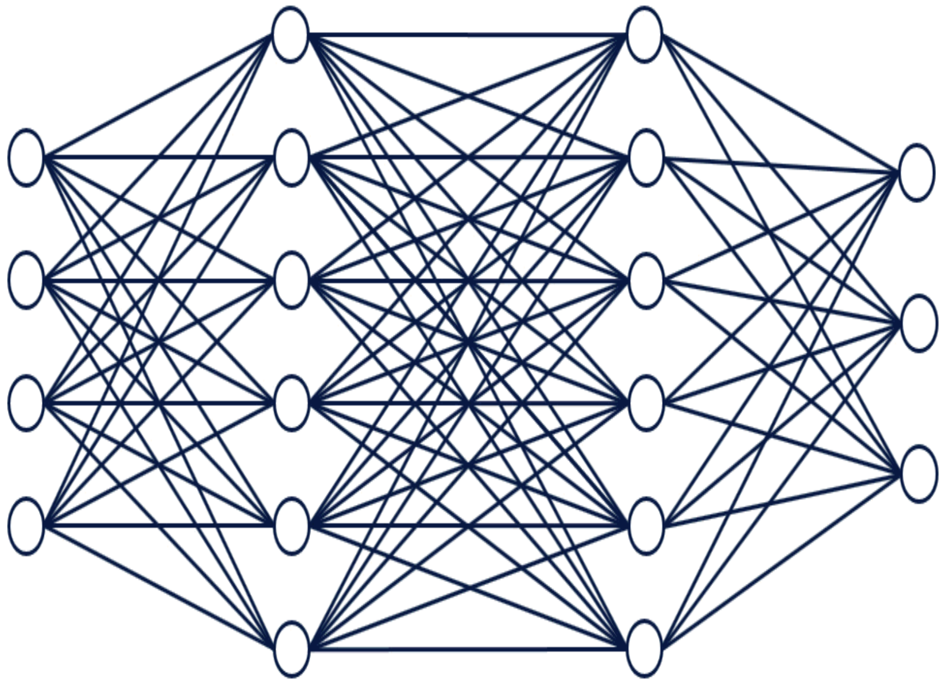
Application to efficient LLM

# 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

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

[Snoek et al.'12]

Arbitrarily bad

[Astudillo et al.'21]

## Smart stopping time

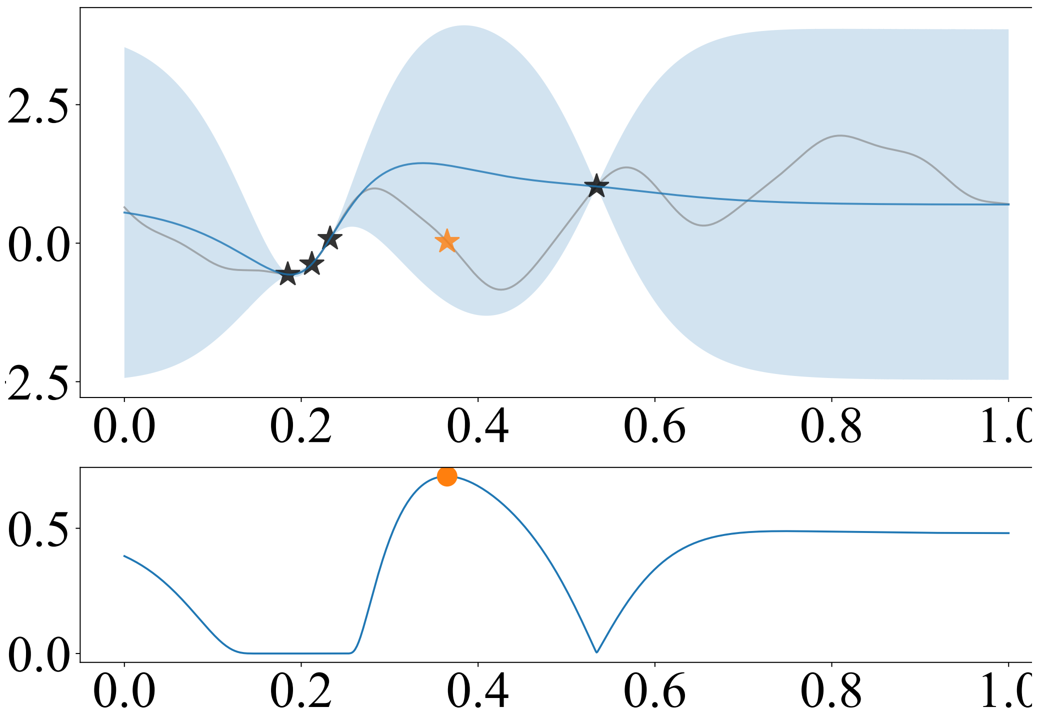
$$\tau:\ \mathrm{EI}(x_\tau) \le \theta$$

[Locatelli'97,
Nguyen et al.'17,
Ishibashi et al.'23]

Which threshold?

## Observable multi-stage feedback

?




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

# 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

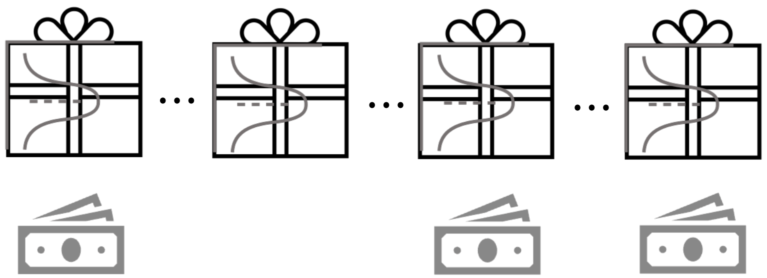
Smart stopping time

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

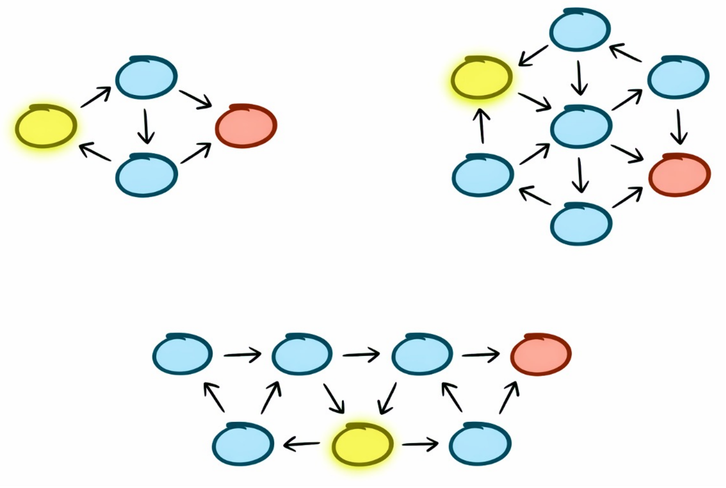
Features in Pandora's box

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

This talk's focus

Smart stopping time

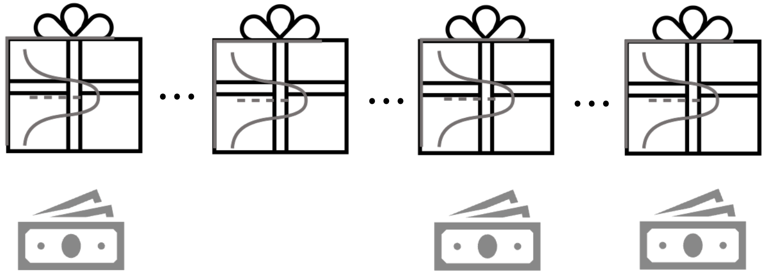
Features in Pandora's box

Observable multi-stage feedback

Features in Markov chain selection

New design principle: Gittins index

Optimal in related sequential decision problems

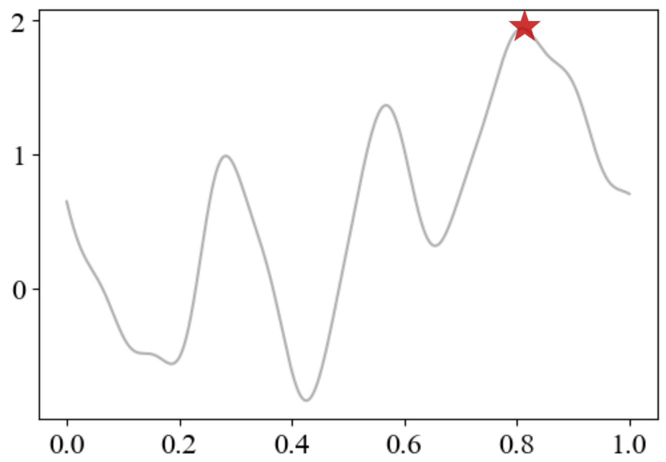


"Cost-aware Bayesian Optimization via the Pandora's Box Gittins Index." NeurIPS'24.

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

# Bayesian Optimization

$f(x)$




Continuous

Correlated

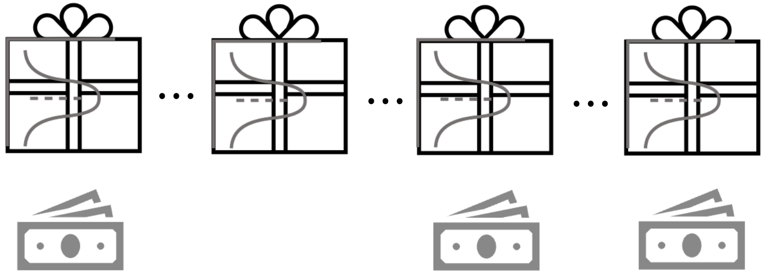
Cost-unaware

Fixed-iteration

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

# Pandora's Box

[Weitzman'79]



$f(x)$

$c(x)$

costs to open

Discrete

Independent

Cost-aware

Flexible-stopping

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

# Expected Improvement vs Gittins Index

## Varying evaluation costs

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

Arbitrarily bad

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

naturally incorporates costs

## Smart stopping time

$\tau\colon\ \mathrm{EI}(x_\tau) \leq \theta$

Which threshold?

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

$\Longleftrightarrow\ \tau\colon \mathrm{EIPC}(x_\tau;c) \leq 1$

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)**

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

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


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

# Our Contribution: Gittins Index Principle

## Novel connection

Link to Pandora's Box problem
& Gittins index theory

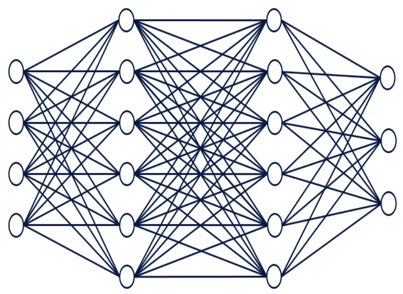
## Principled decision rules

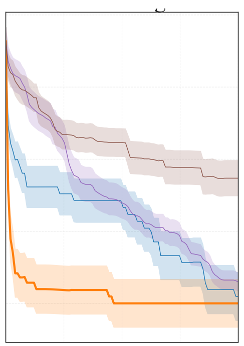
Varying evaluation costs

Adaptive stopping time

Unified framework for
selection and stopping

## Competitive empirical performance





Interests from practitioners (e.g., Meta)

## Future potential

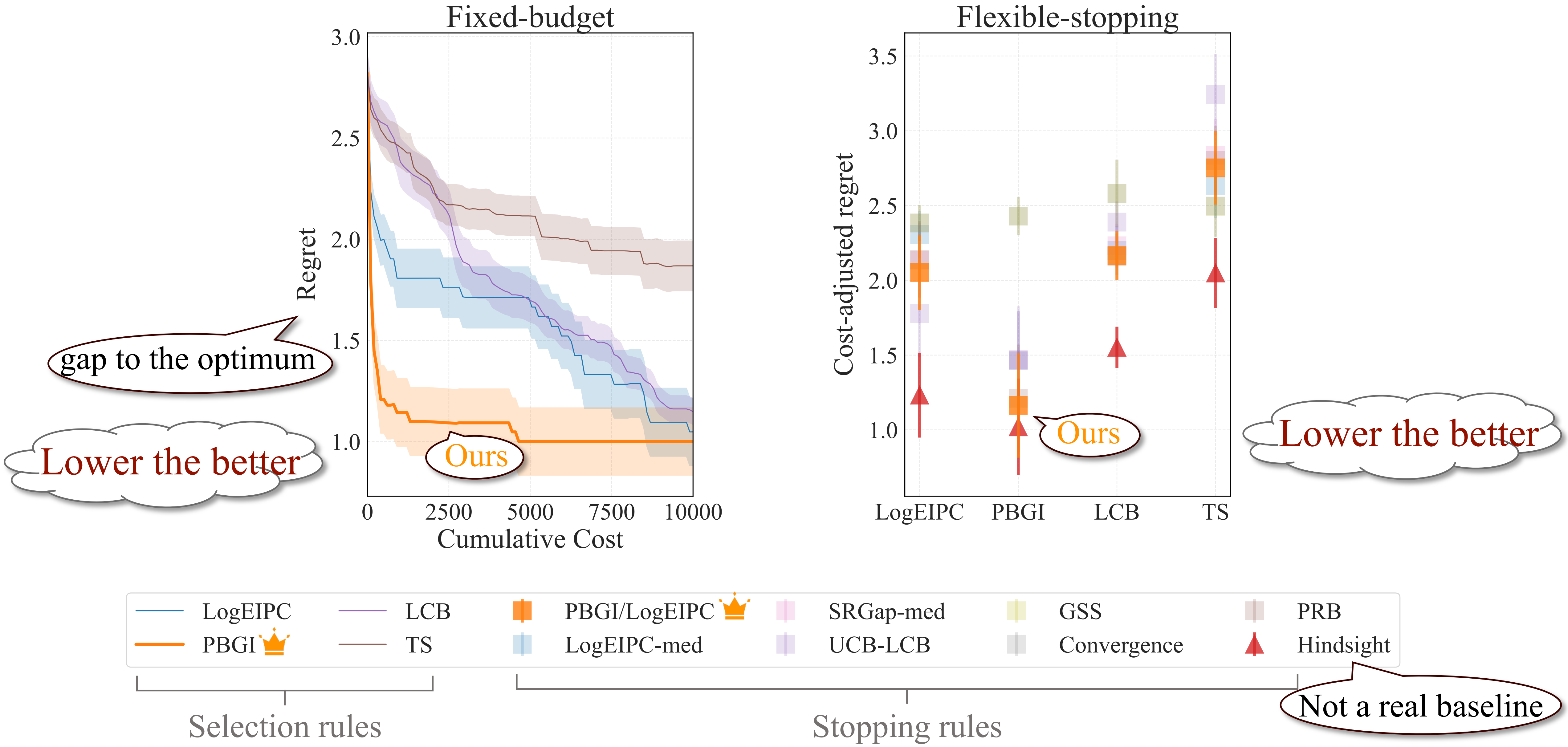
Best-prompt identification

Adaptive response sampling

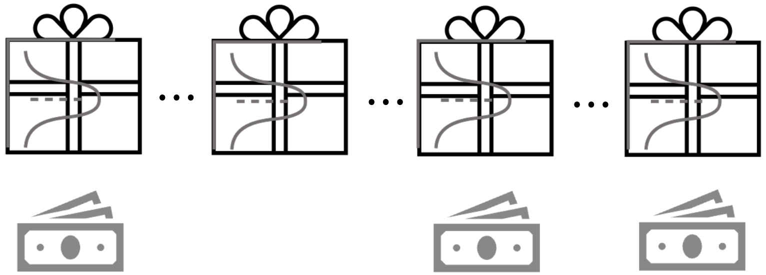
Chain-of-thought selection

Application to efficient LLM

# Gittins Index vs Baselines on AutoML Benchmark



## Novel connection



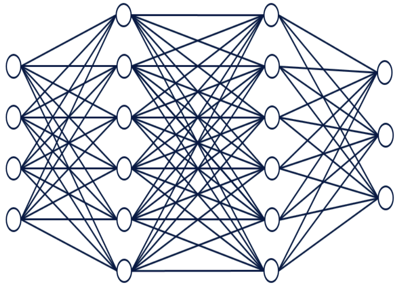
Link to Pandora's Box problem & Gittins index theory

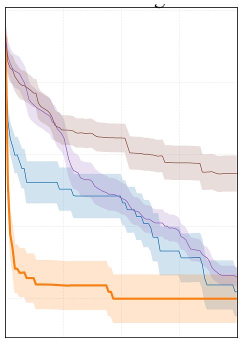
## Principled decision rules

- Varying evaluation costs
- Adaptive stopping time

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

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

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

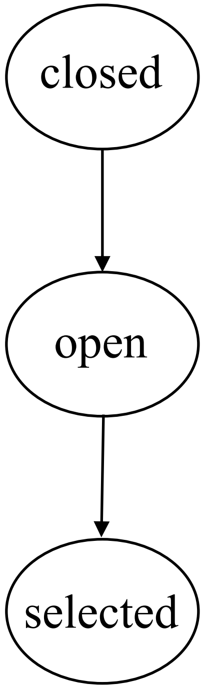
# Find my papers on arXiv!

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

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

# Markovian Bandits

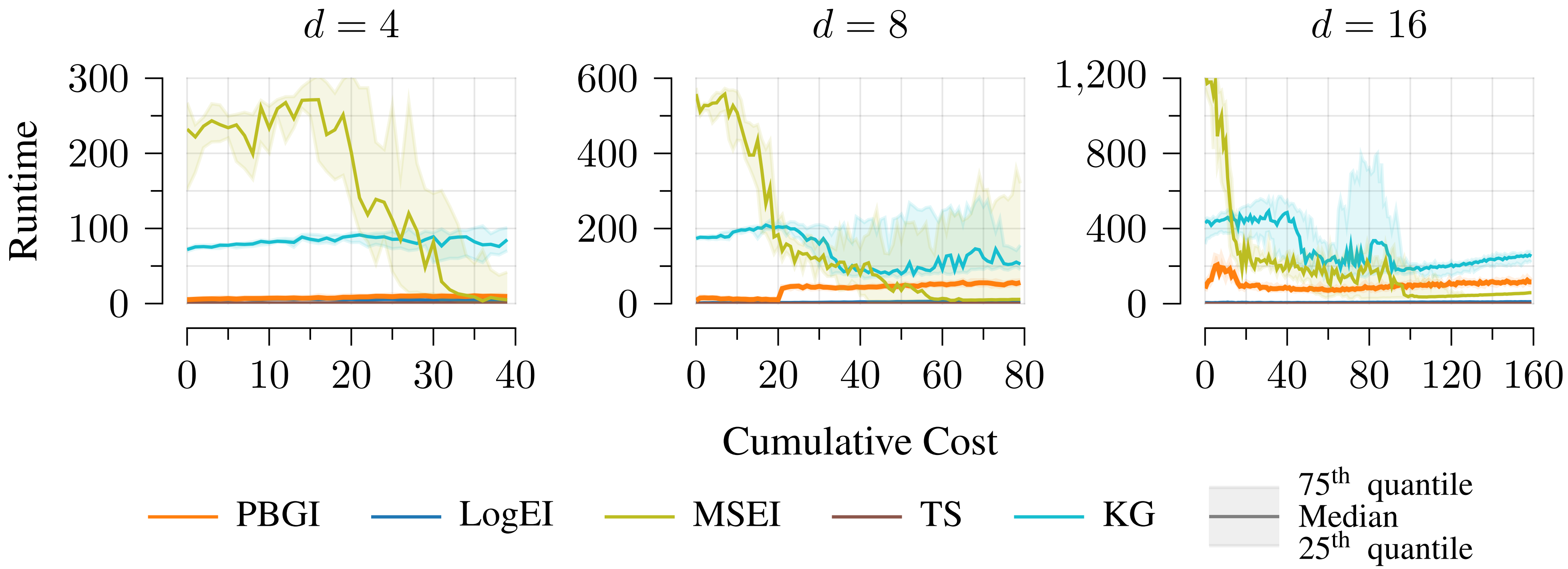
[Gittins'79]




# Pandora's Box

[Weitzman'79]

# Timing Experiment: Gittins Index vs Baselines




PBGI is computationally-efficient!

# EI vs PBGI vs UCB