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

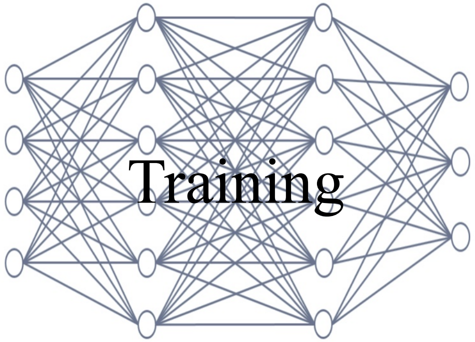
Qian Xie 谢倩 (Cornell ORIE)

Job Talk

Motivation: World of Optimization under Uncertainty

ML model training:

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



→ Accuracy

Motivation: World of Optimization under Uncertainty

ML model training:

≠ parameters
(weights, biases)

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

→

→ Accuracy

Motivation: World of Optimization under Uncertainty

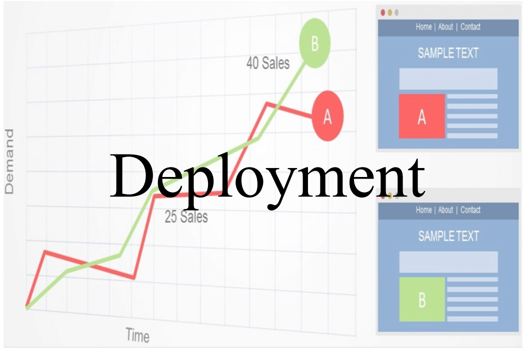
ML model training:

≠ parameters
(weights, biases)

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

Adaptive experimentation:

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



Motivation: World of Optimization under Uncertainty

non-analytical &
no gradient info

Design choices x $\longrightarrow$  $\longrightarrow$ Performance metric $f(x)$

ML model training:

≠ parameters
(weights, biases)

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

$\longrightarrow$ Accuracy

Adaptive experimentation:

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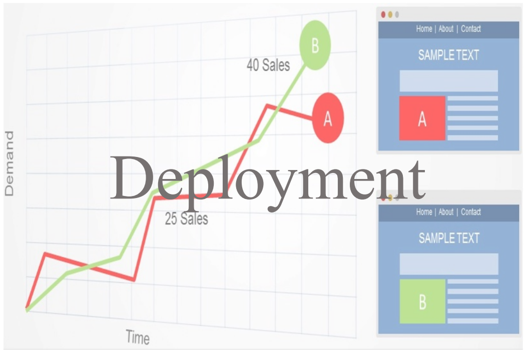
(e.g., layout, pricing level) $\longrightarrow$ 

$\longrightarrow$ 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

ML model training:

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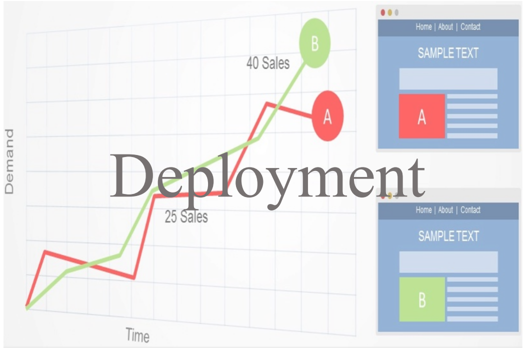
Training hyperparameters (e.g., learning rate, # layers) ⟶ 

⟶ Accuracy

Adaptive experimentation:

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

⟶ Revenue

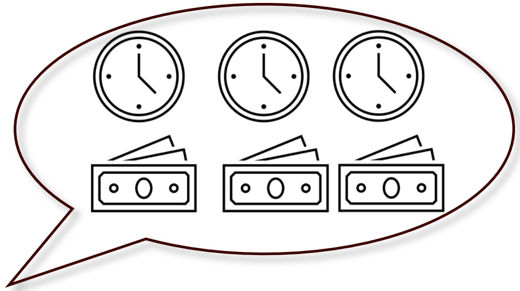
Background: Black-Box Optimization

Black-box optimization:

(gradient-based methods not applicable)

expensive-to-evaluate

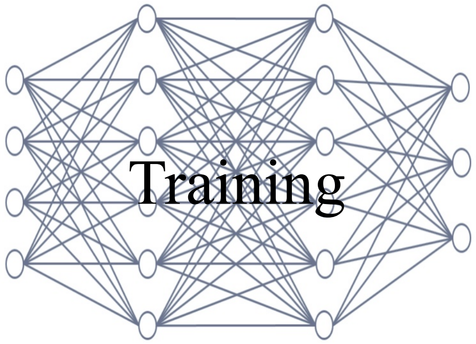
Input x → Observed outcome $f(x)$



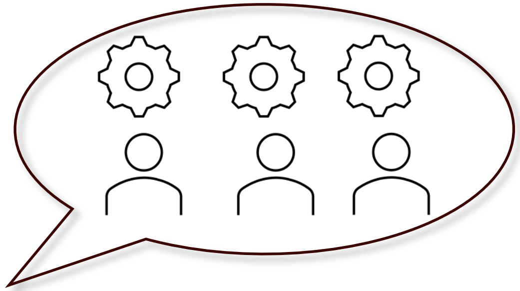
Training time

Compute credits

ML model training:



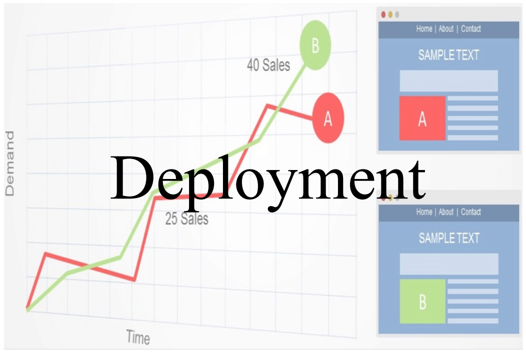
Training hyperparameters (e.g., learning rate, # layers) → Accuracy



Operational cost

User experience

Adaptive experimentation:



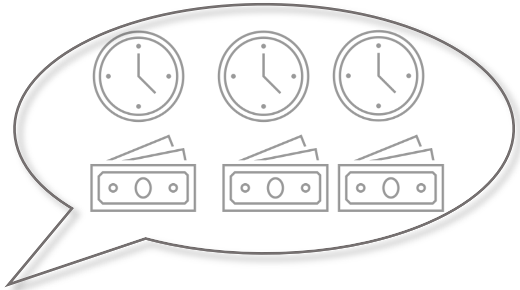
Decision/design variables (e.g., layout, pricing level) → Revenue

How to do black-box optimization efficiently?

Black-box optimization:
(gradient-based methods not applicable)

Input x →  → Observed outcome $f(x)$

expensive-to-evaluate



Training time

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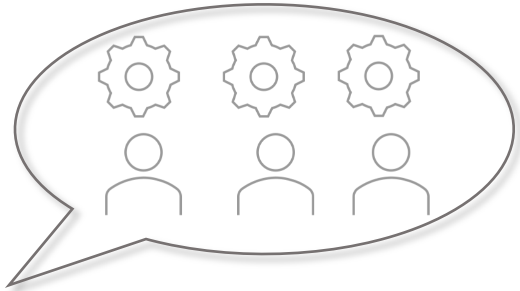
ML model training:

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

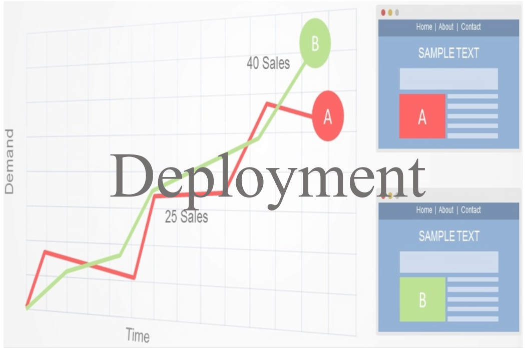
→ Accuracy



Operational cost

User experience

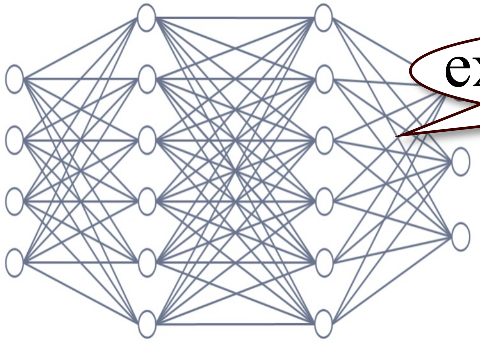
Adaptive experimentation:

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

→ Revenue

Naïve Non-Adaptive Approach: Grid Search

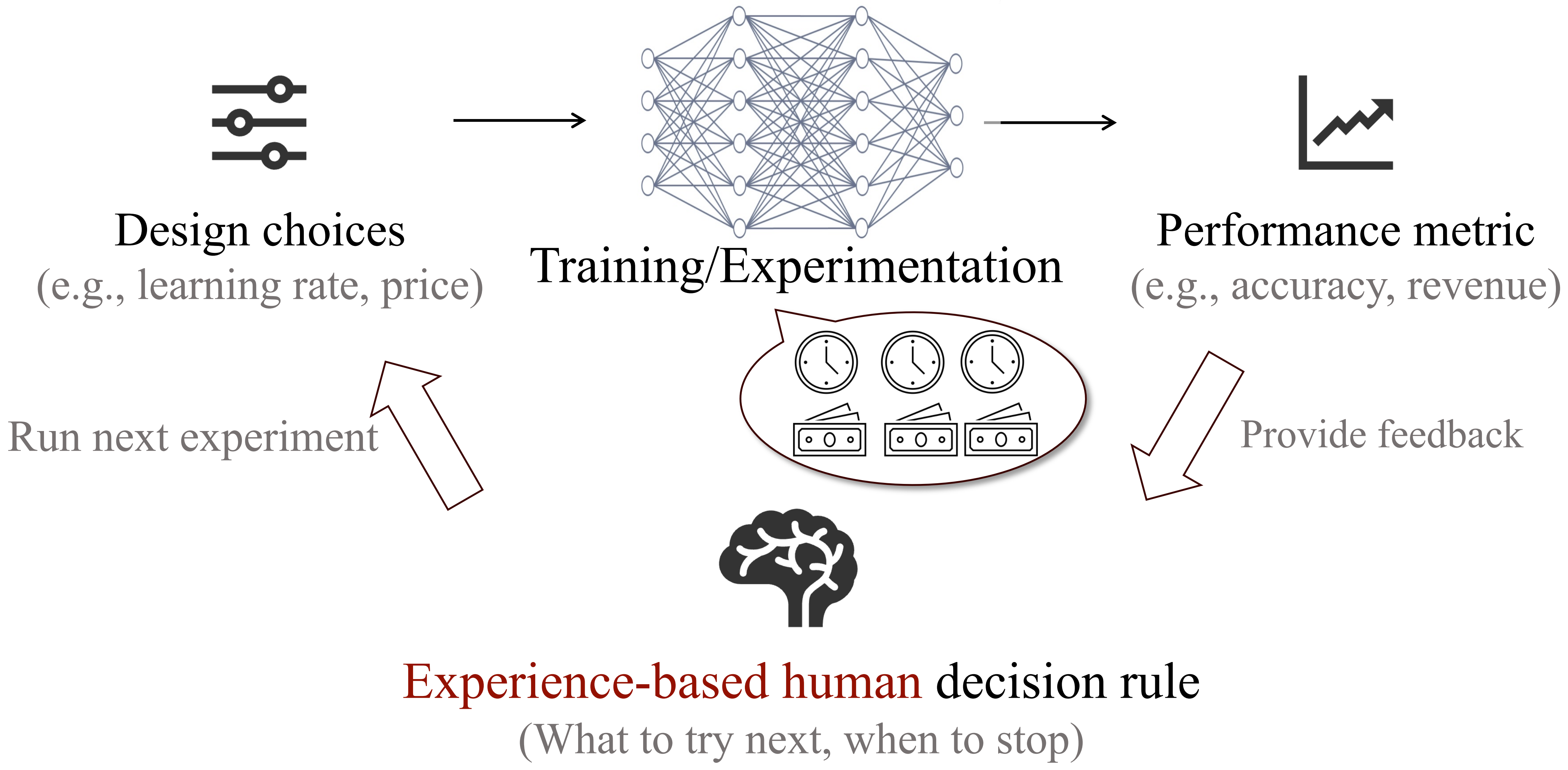
ML model training:

Training hyperparameters →  → Accuracy

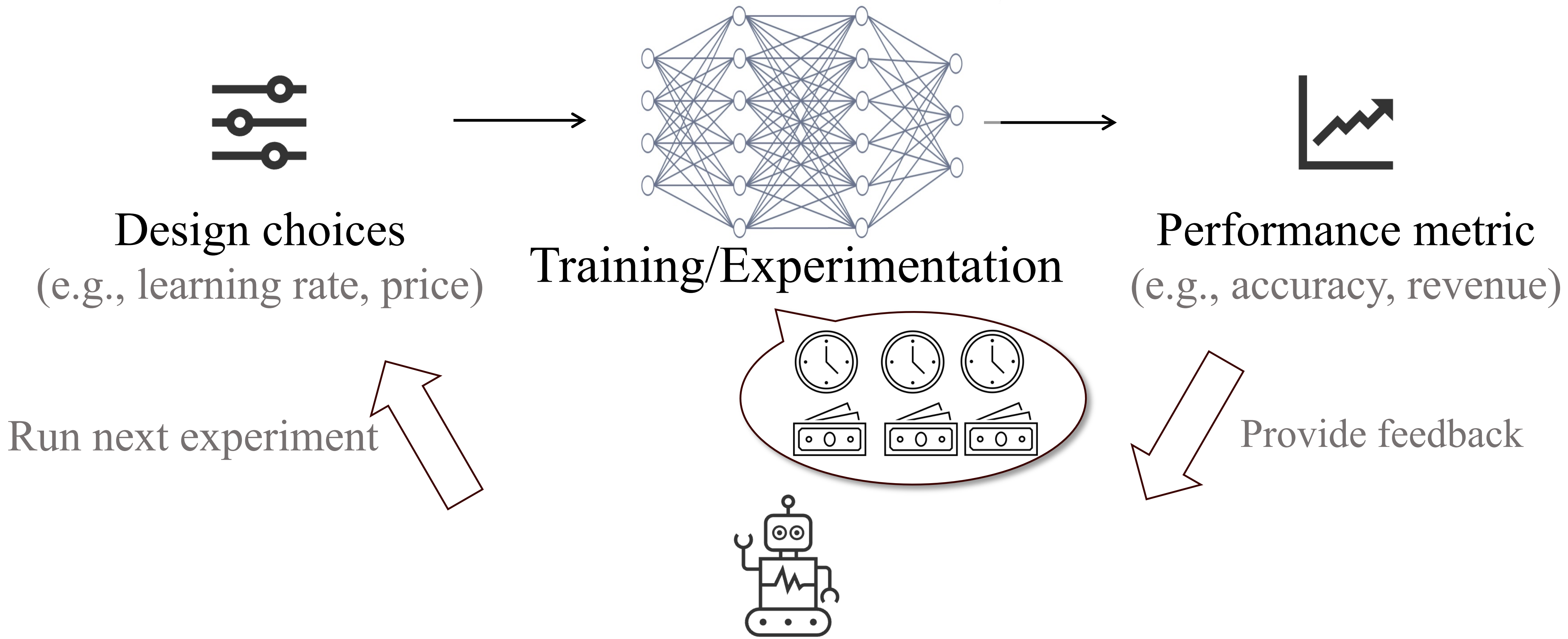
Training hyperparameter	Range	Number of Options
Batch size	[16, 512]	10
Learning rate	[1e-4, 1e-1]	10
Momentum	[0.1, 0.99]	10
Weight decay	[1e-5, 1e-1]	10
Number of layers	{1, 2, 3, 4}	4
Max units per layer	[64, 1024]	10
Dropout	[0.0, 1.0]	10

40,000,000 combinations!

Naïve Adaptive Approach: Manual Tuning



Data-Driven Adaptive Approaches



Data-efficient automated decision rule

(What to try next, when to stop)

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

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• Grid search	• Local search
• Random search	• Evolutionary algorithms
• Manual tuning	• Bayesian optimization ★
	• Reinforcement learning ★
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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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This talk's focus

Contributions of new methods proposed in my work:

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2. Principled decision rules

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★ New methods under this umbrella

Bayesian Optimization

$f \sim$Stochastic Process

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

Black-box function

Bayesian Optimization

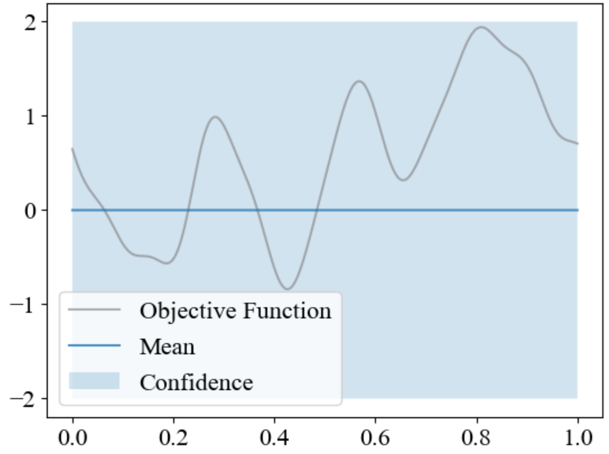
Time 0

f ~Stochastic Process

x →  → $f(x)$

Black-box function

Model belief



Probabilistic model

(e.g., Gaussian process)

Bayesian Optimization

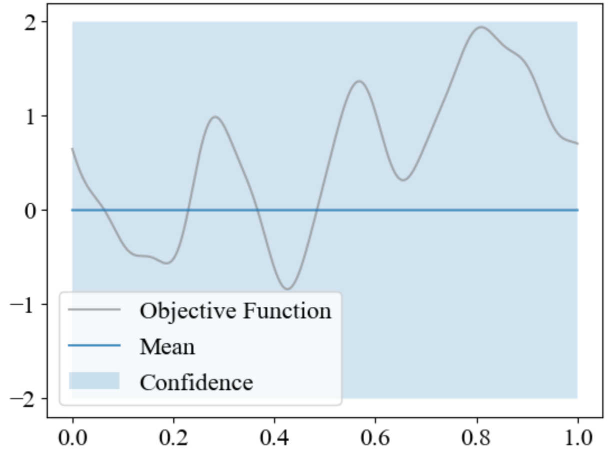
Time t

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

Black-box function

$f \sim$ Stochastic Process

Model belief



Probabilistic model
(e.g., Gaussian process)

Bayesian Optimization

Time t

$f \sim$ Stochastic Process

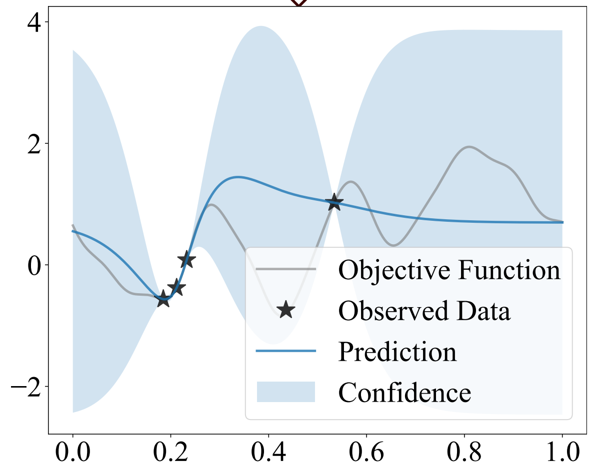
$x_1, \ldots, x_t \longrightarrow$

Black-box function

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

Update belief

(Bayes' rule)



Probabilistic model

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Time t

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Update belief
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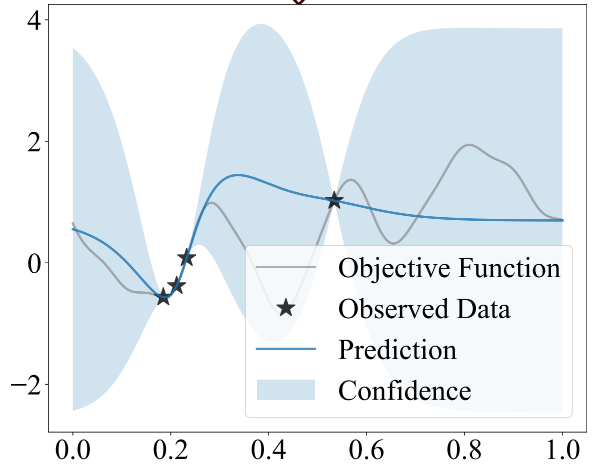
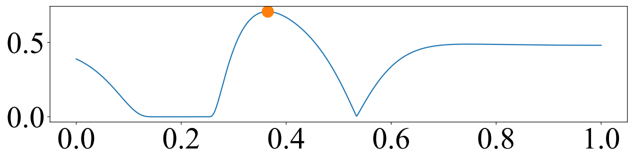


Probabilistic model
(e.g., Gaussian process)

scoring (worth of each point



Decision rule
(e.g., EI, UCB, TS)

Bayesian Optimization

Time t

$x_1, \ldots, x_t$

Black-box function

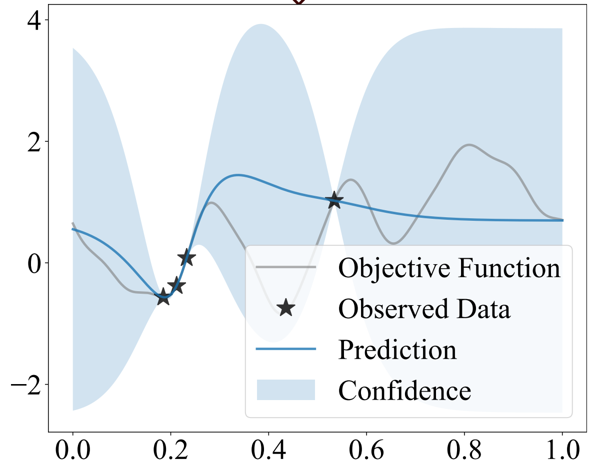
$f(x_1), \ldots, f(x_t)$

Decide next input

(gradient-based optimization)

Update belief

(Bayes' rule)



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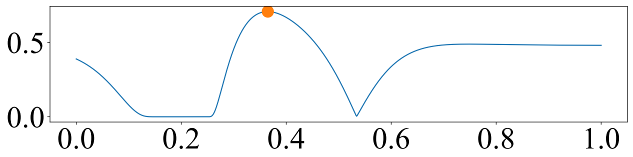


Decision rule

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

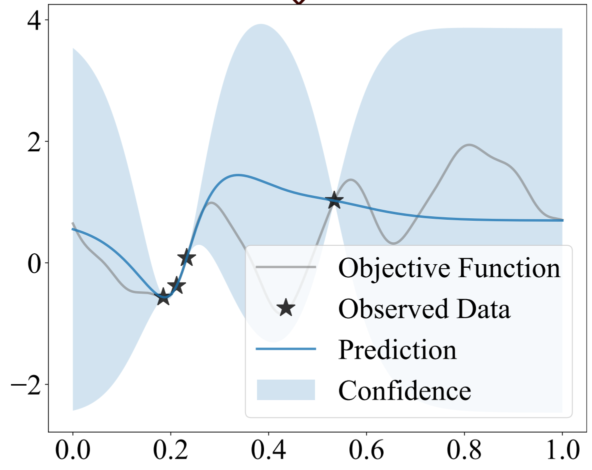
Bayesian Optimization

Time $t+1$

$x_1, \ldots, x_{t+1}$ → Black-box function → $f(x_1), \ldots, f(x_{t+1})$

Black-box function

Update belief
(Bayes' rule)



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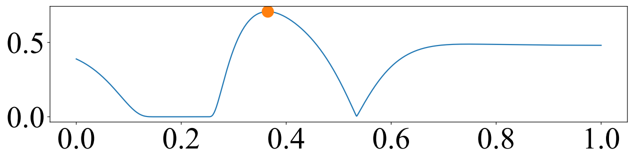


Decision rule
(e.g., EI, UCB, TS)

Decide next input
(gradient-based optimization)

Bayesian Optimization

Time $t + 1$

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

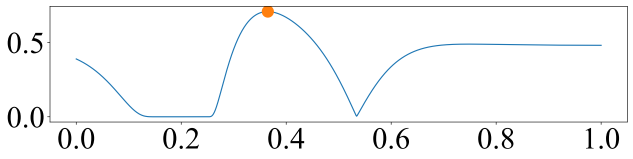
Black-box function

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

Update belief
(Bayes' rule)

Probabilistic model
(e.g., Gaussian process)

scoring (worth of each point

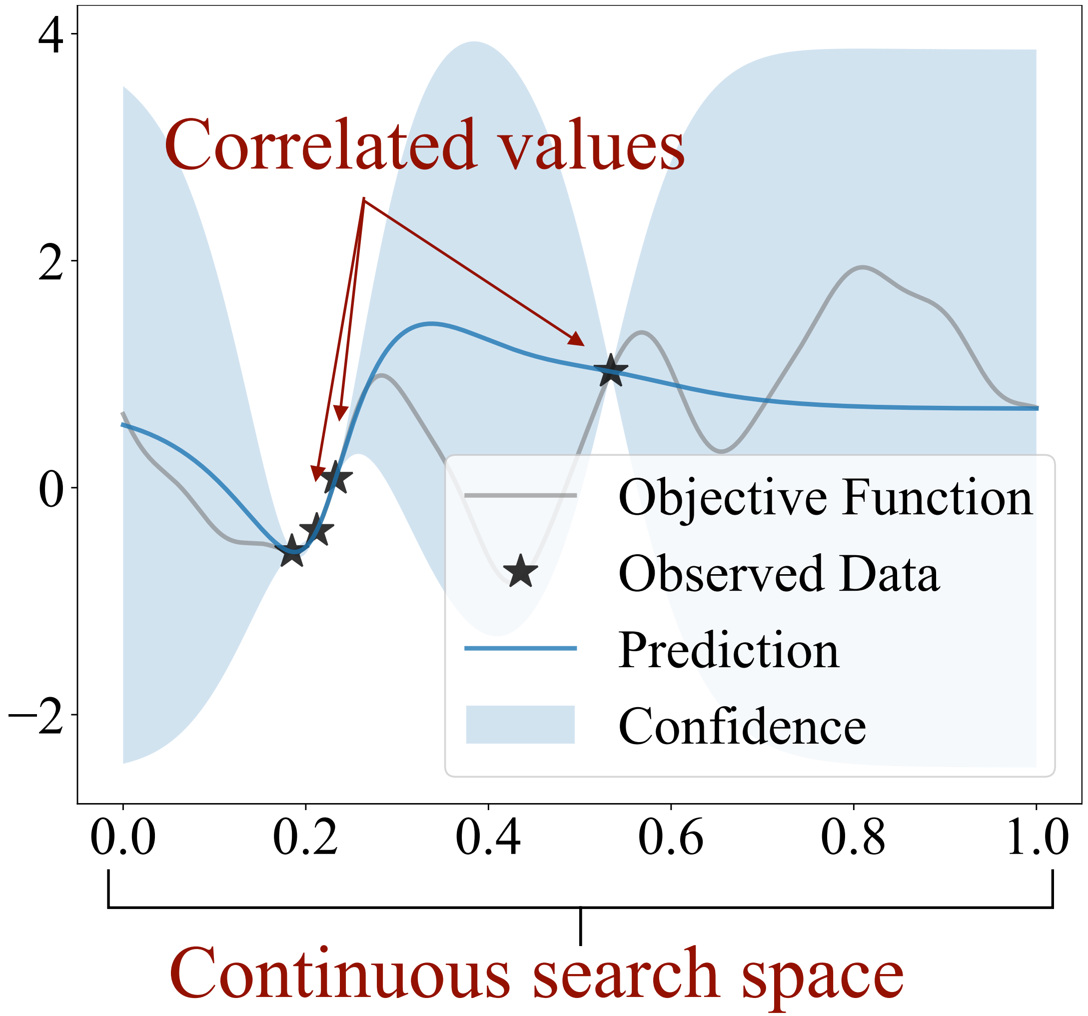


My focus

Decision rule
(e.g., EI, UCB, TS)

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

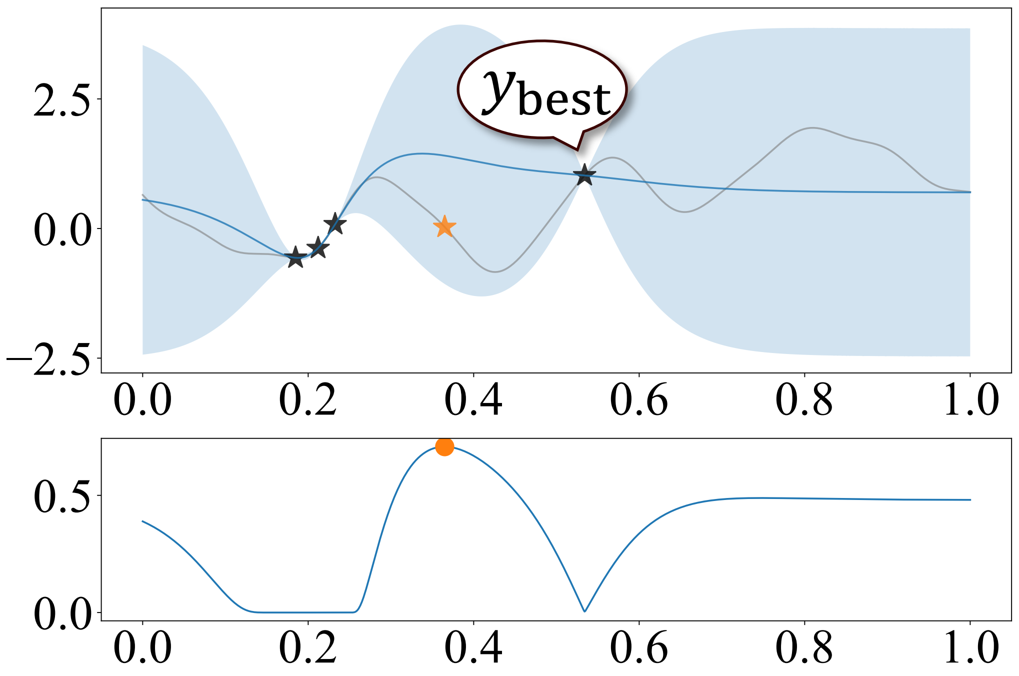
current best observed

data D

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

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

posterior distribution



One-step approximation to MDP

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

Popular Decision Rule: Expected Improvement

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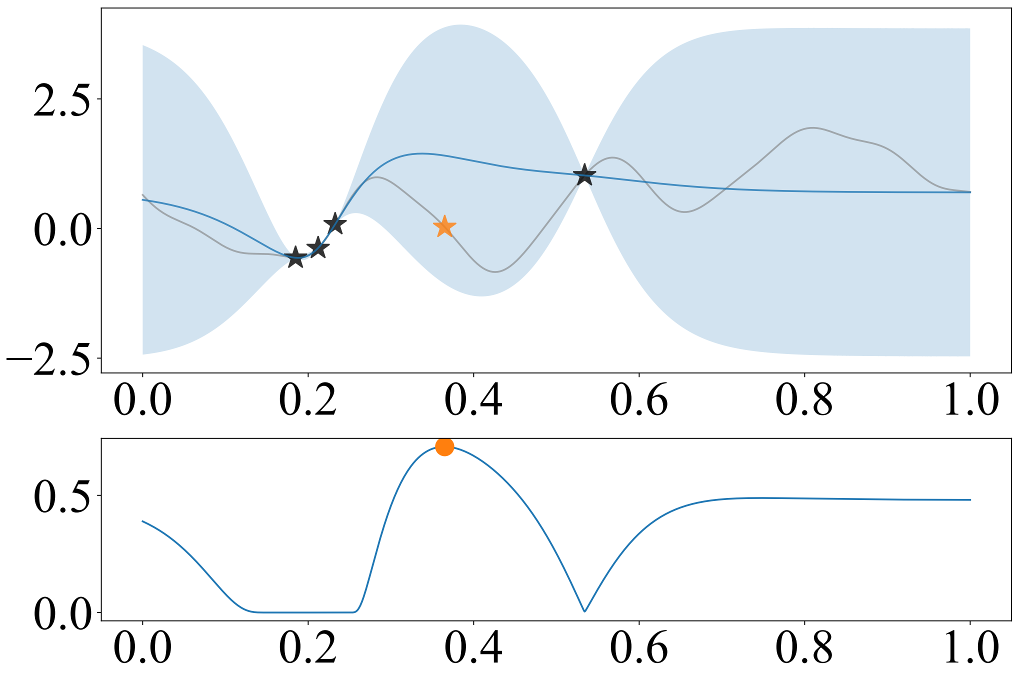
posterior distribution

One-step approximation to MDP

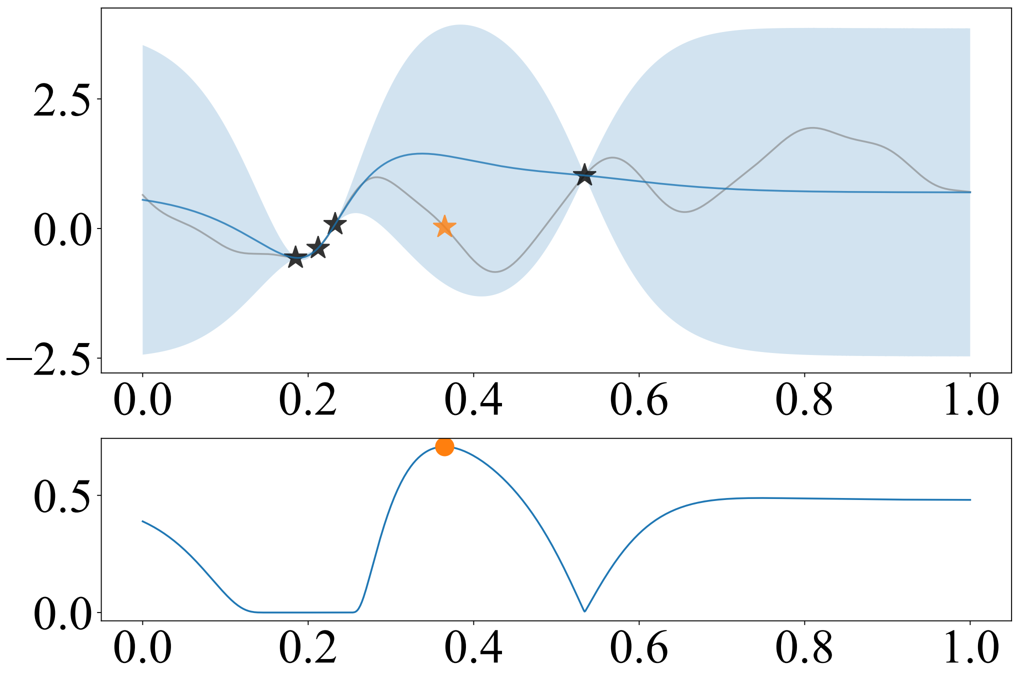


Expected improvement $\mathrm{EI}(x)$

Improvement-based design principle

Existing Design Principles

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

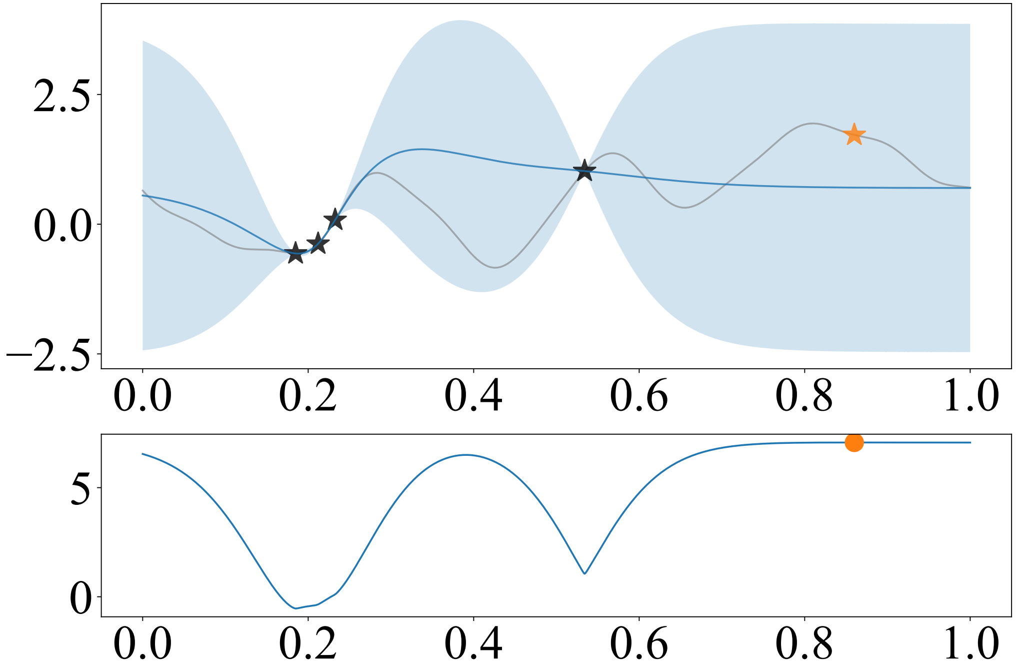


Expected improvement $\mathrm{EI}(x)$

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
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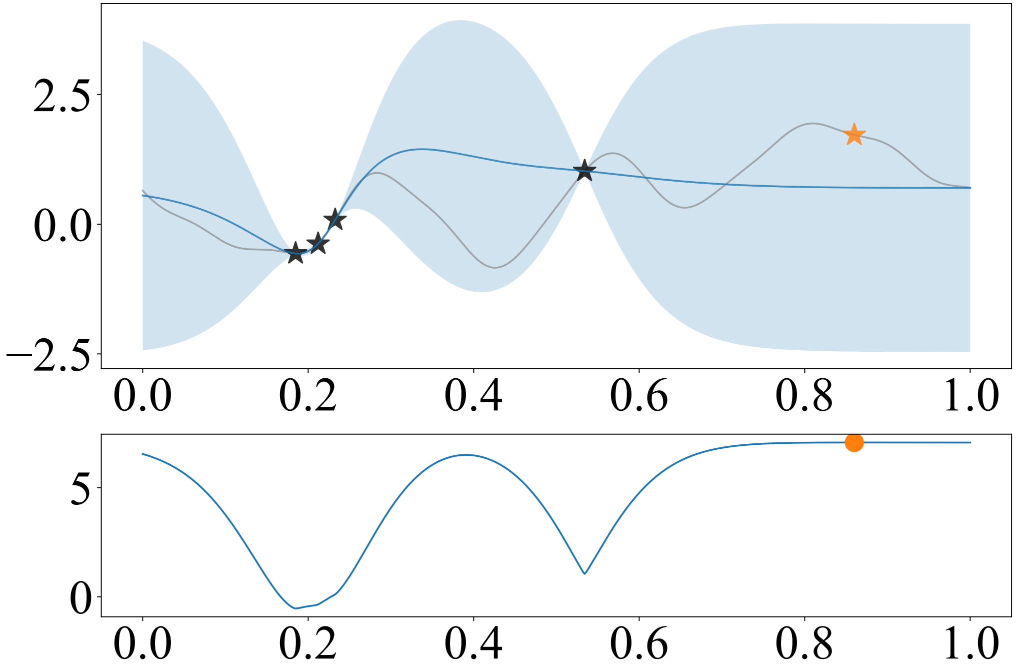
- Gittins Index

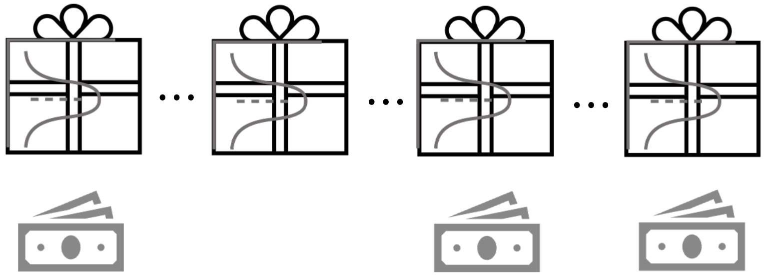


Gittins index $\mathrm{GI}(x)$

? Why another principle?

Our Contribution: Gittins Index Principle

Novel connection



Link to Pandora's Box problem
& Gittins index theory

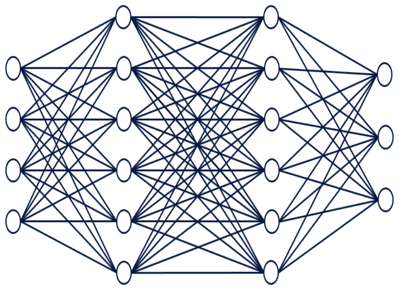
Principled decision rules

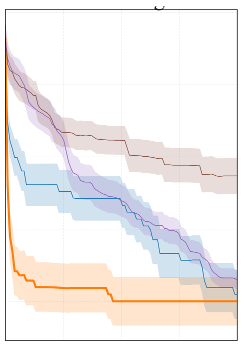
Varying evaluation costs

Adaptive stopping time

Unified framework for
selection and stopping

Competitive empirical performance





Interests from practitioners (e.g., Meta)

Future potential

Best-prompt identification

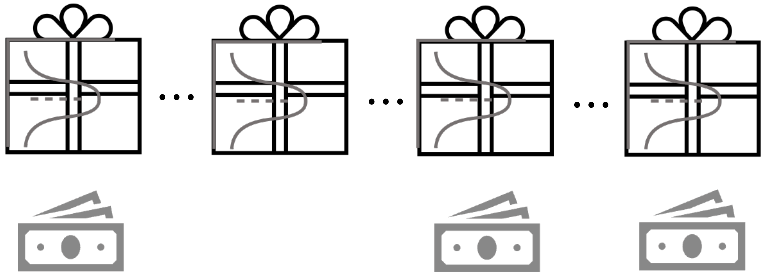
Adaptive response sampling

Chain-of-thought selection

Application to efficient LLM

Our Contribution: Gittins Index Principle

Novel connection



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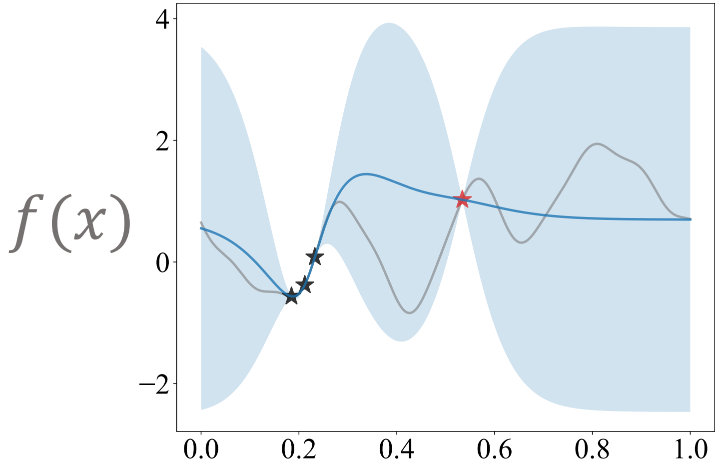
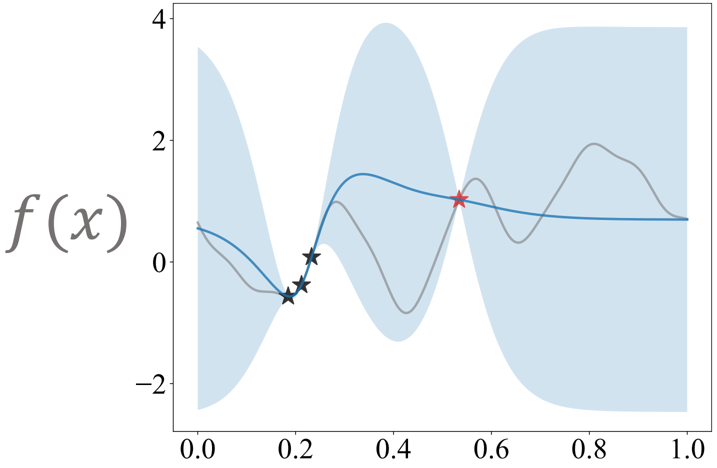
Bayesian Optimization



Continuous search space

Correlated function values

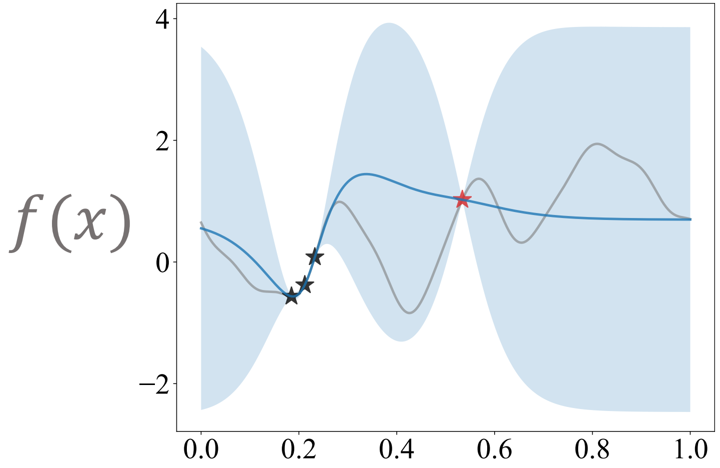
Bayesian Optimization



Continuous search space $\Longrightarrow$ Discrete

Correlated function values $\Longrightarrow$ Independent

Bayesian Optimization

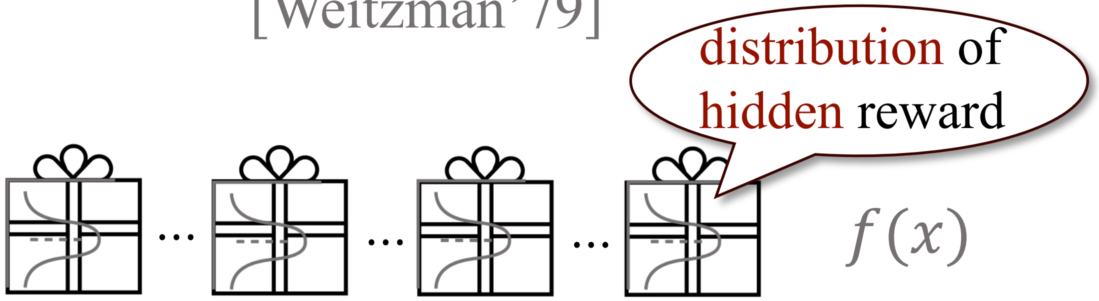


Continuous search space

Correlated function values

Pandora's Box

[Weitzman'79]

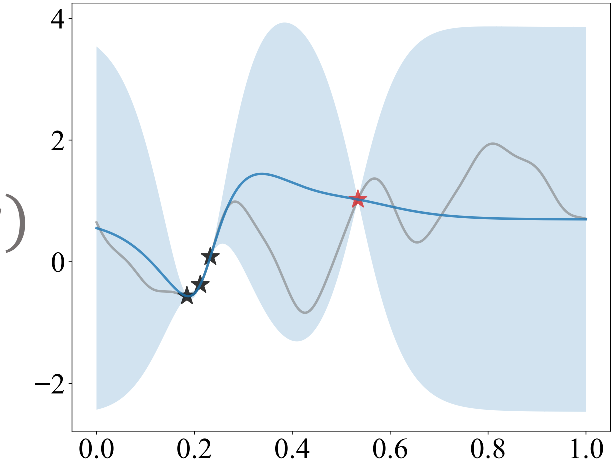


Discrete

Independent

Bayesian Optimization

$f(x)$



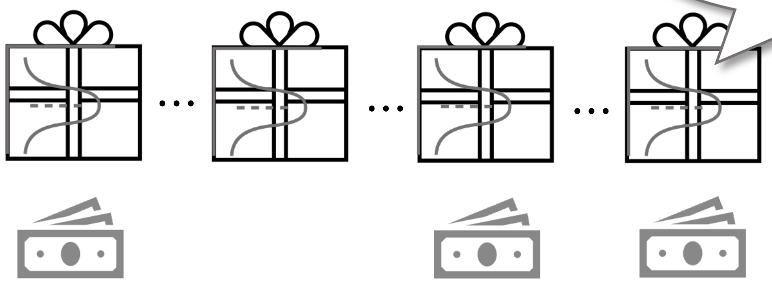
Continuous search space

Correlated function values

Pandora's Box

[Weitzman'79]

distribution of hidden reward



$f(x)$

$c(x)$

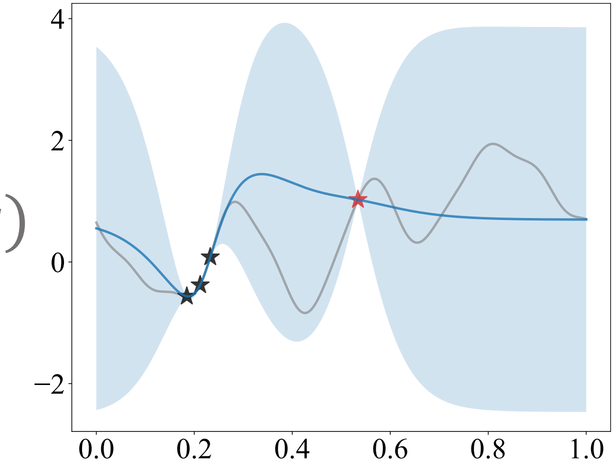
costs to open

Discrete

Independent

Bayesian Optimization

$f(x)$



Continuous search space

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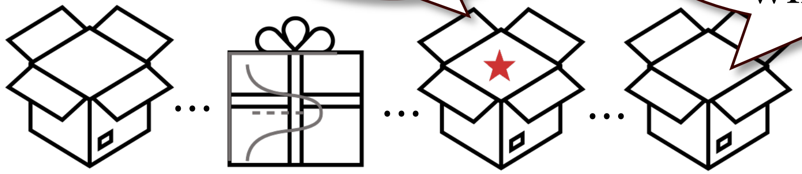

$f(x)$

$c(x)$

costs to open

Discrete

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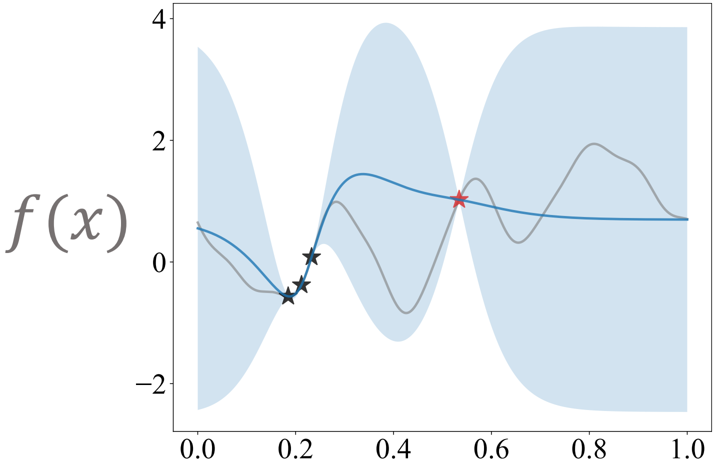
Bayesian Optimization

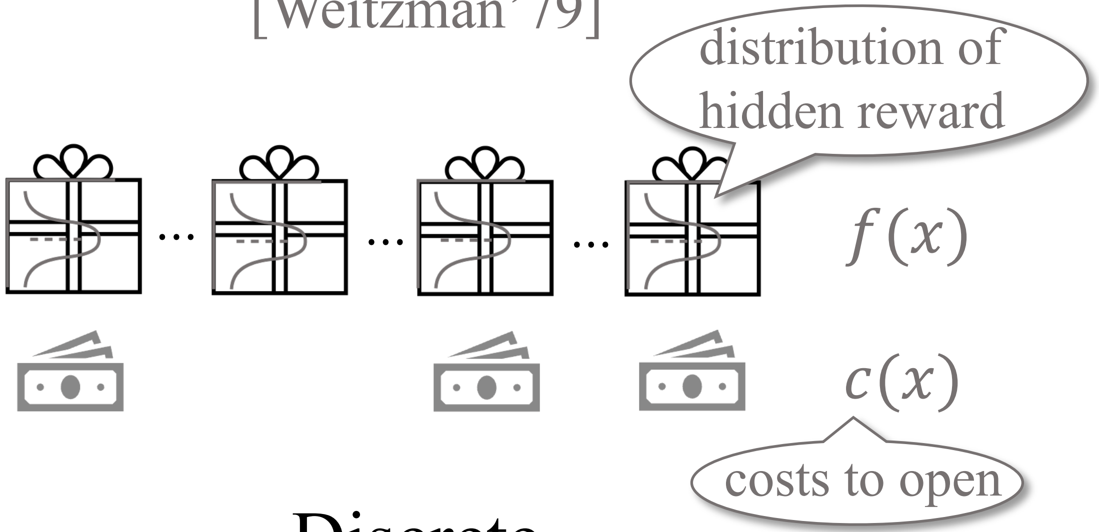


Continuous search space

Correlated function values

Pandora's Box

[Weitzman'79]



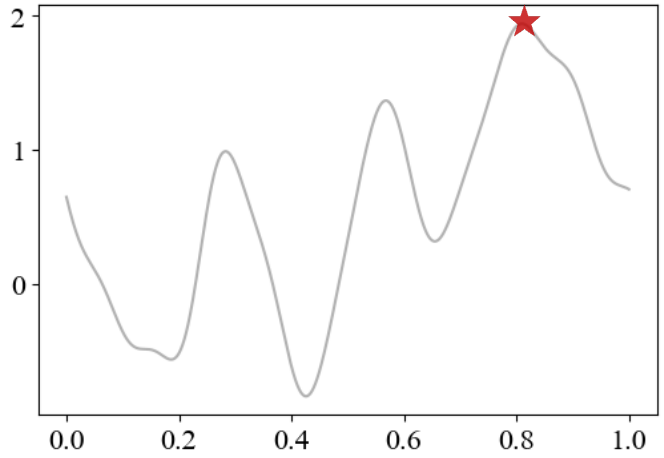
Discrete

Independent

Optimal policy: Gittins index

Bayesian Optimization

$f(x)$



Continuous

Correlated

Pandora's Box

[Weitzman'79]

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

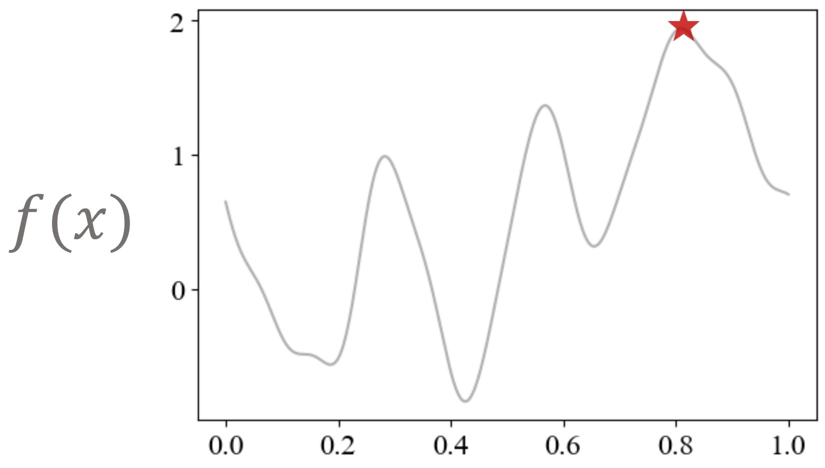
Step 1: Assign each box a Gittins index

Discrete

Independent

Optimal policy: Gittins index

Bayesian Optimization



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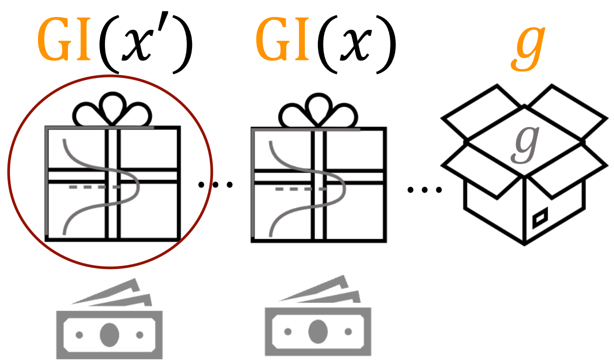


Step 2: Act on the box with the highest index

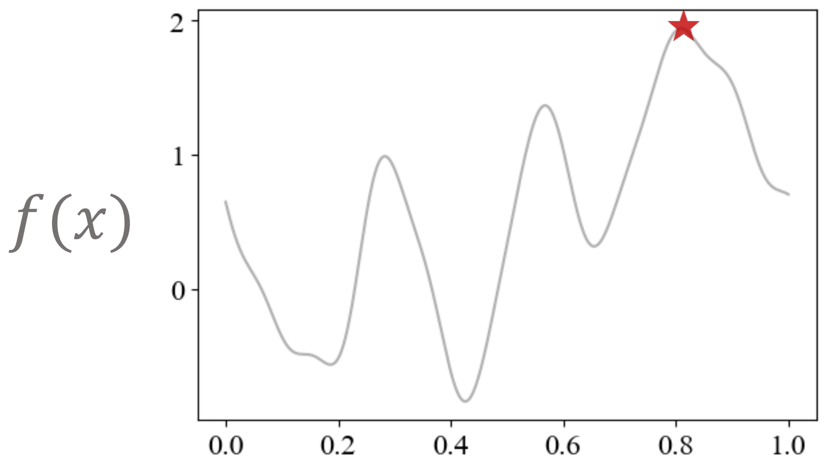
- *Closed*: open it
- *Opened*: select & stop

Discrete

Independent

Optimal policy: Gittins index

Bayesian Optimization

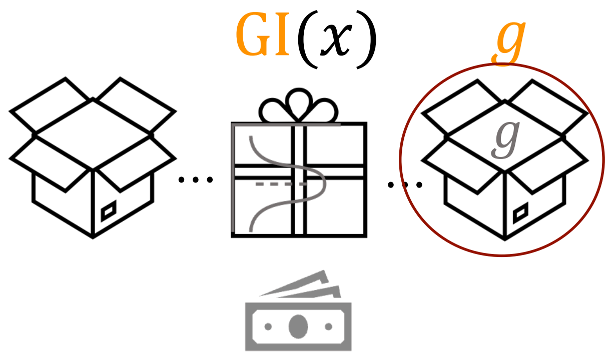


Continuous

Correlated

Pandora's Box

[Weitzman'79]



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

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

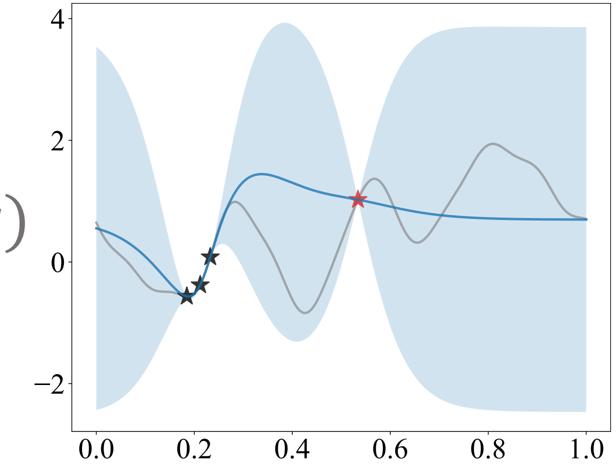
Discrete

Independent

Optimal policy: Gittins index

Bayesian Optimization

$f(x)$

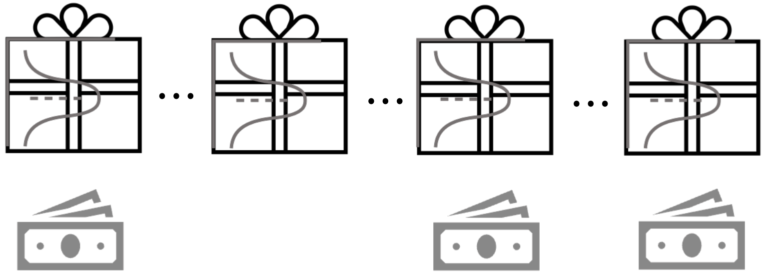


Continuous search space

Correlated function values

Pandora's Box

[Weitzman'79]



$f(x)$

$c(x)$

costs to open

Discrete

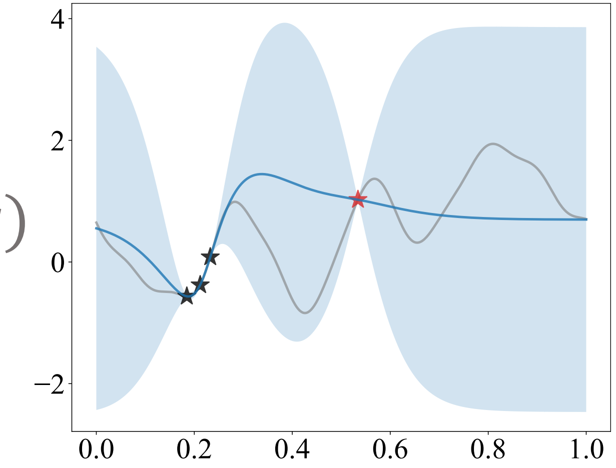
Independent

How to translate?

$\Leftarrow$ Optimal policy: Gittins index

Bayesian Optimization

$f(x)$



Continuous search space

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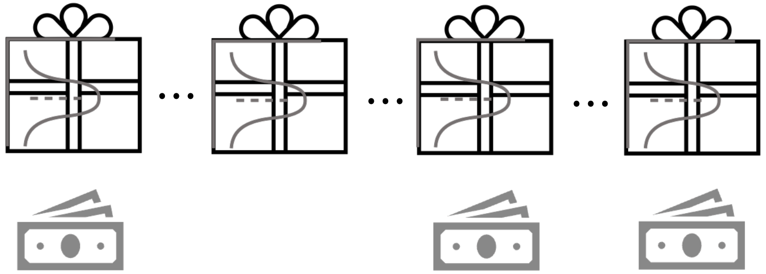


$f(x)$

$c(x)$

costs to open

Discrete

Independent

New!

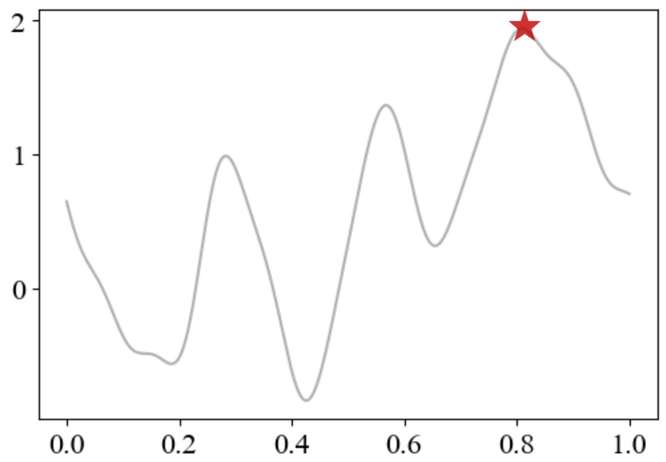
Our policy: $\mathrm{GI}_{f|D}(x;c)$ $\xLeftarrow[\text{take continuum limit}]{\text{incorporate posterior}}$ Optimal policy: $\mathrm{GI}_f(x;c)$

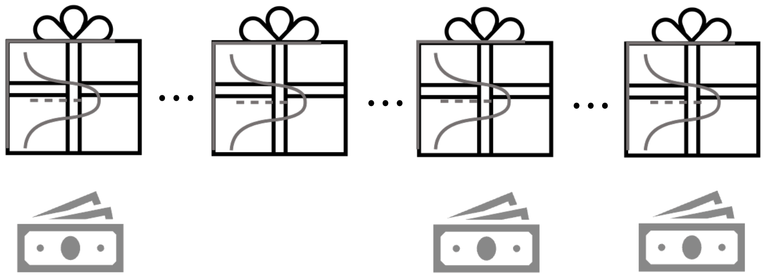
Bayesian Optimization

Pandora's Box

[Weitzman'79]

$f(x)$





$f(x)$

$c(x)$

costs to open

Continuous | Discrete

Correlated | Independent

incorporate posterior

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

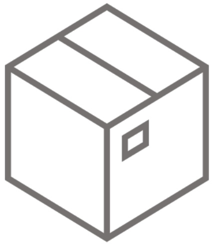
take continuum limit

How to compute?

Intuition

Exploration | Exploitation

$f(x)$



vs.

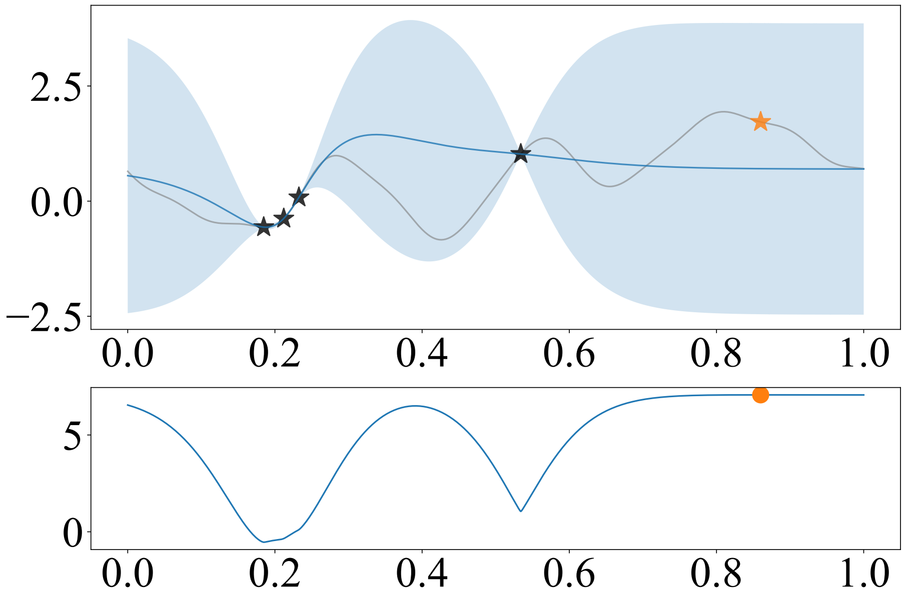
$c(x)$

Open closed box | Take opened box

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

Should one open box? Depend on 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.

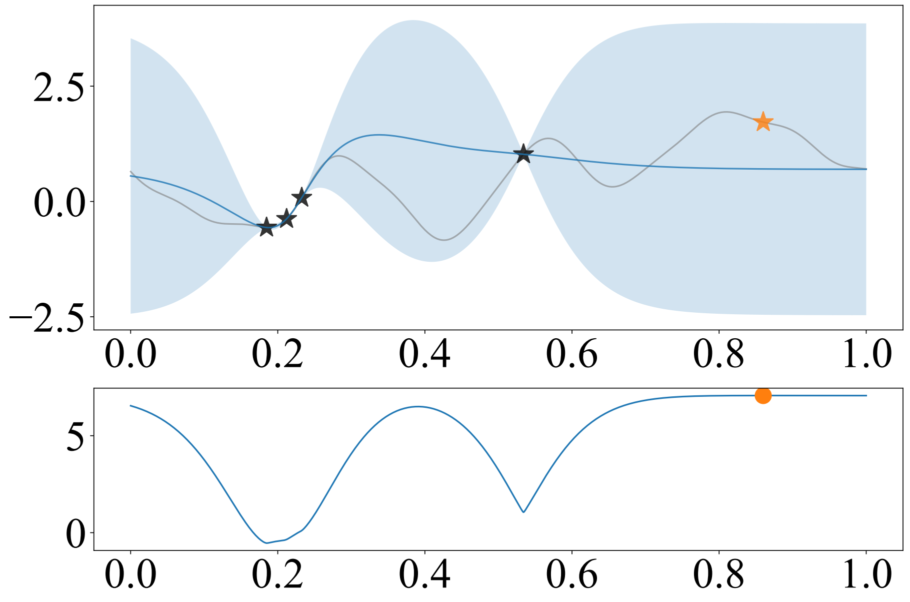
$c(x)$

Open closed box | Take opened box

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

Should one open box? Depend on g!

Gittins Index



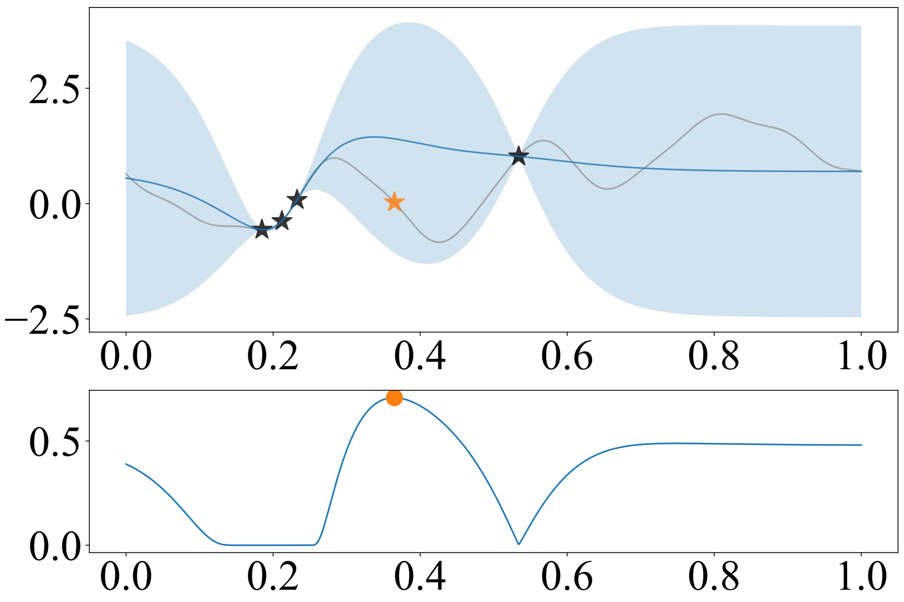
$\mathrm{GI}_{f|D}(x; c) := \text{solution } g \text{ s.t.}$

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

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

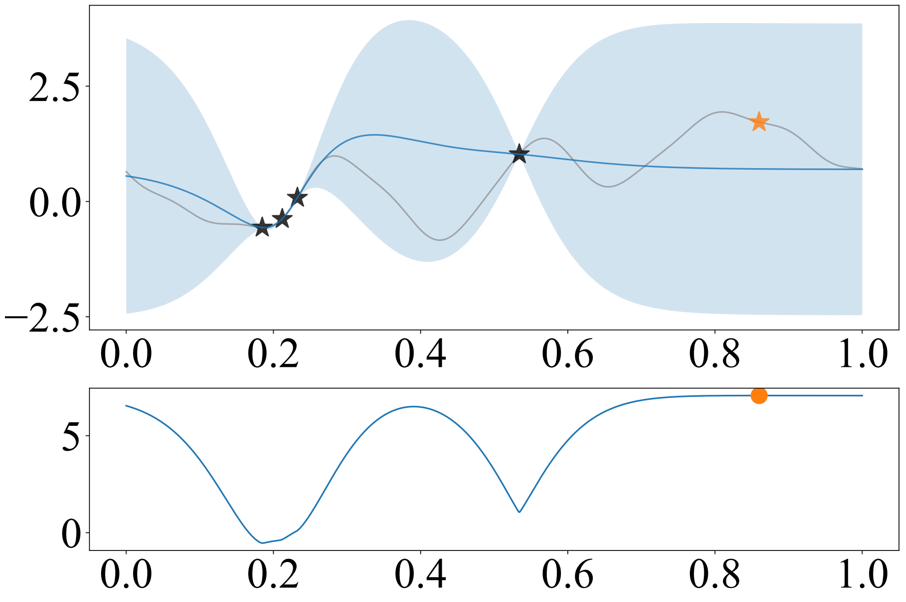
$$\Leftrightarrow \underbrace{\mathbb{E}[\max(f(x) - g, 0) \mid D]}_{\mathrm{EI}_{f|D}(x;\, g)} = c(x)$$

Expected Improvement

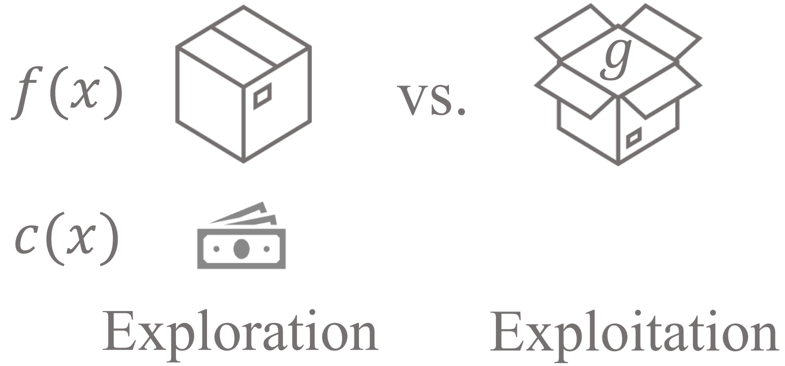


$$\mathrm{EI}_{f|D}(x) := \mathbb{E}[\max(f(x) - y_{\mathrm{best}}, 0) \mid D]$$

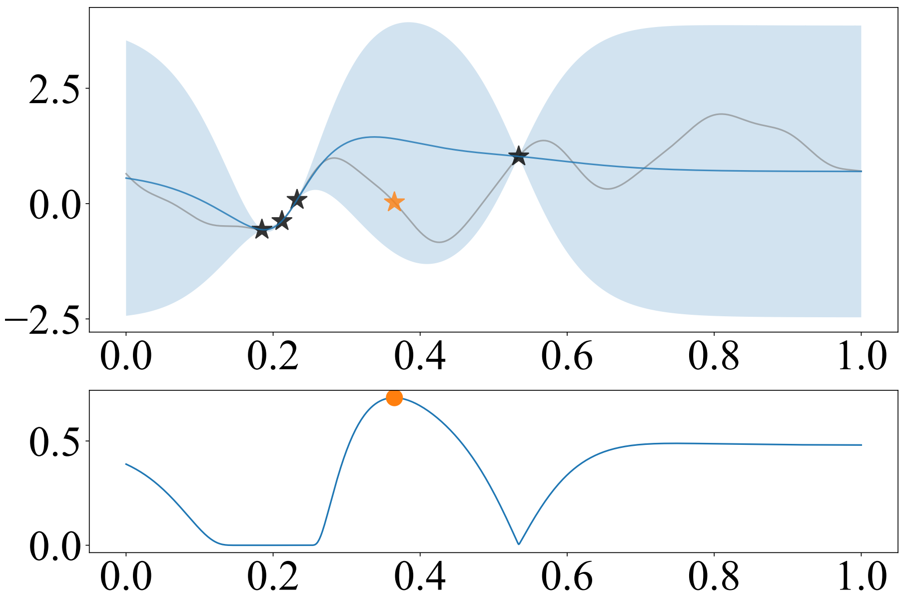
Gittins Index



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



Expected Improvement



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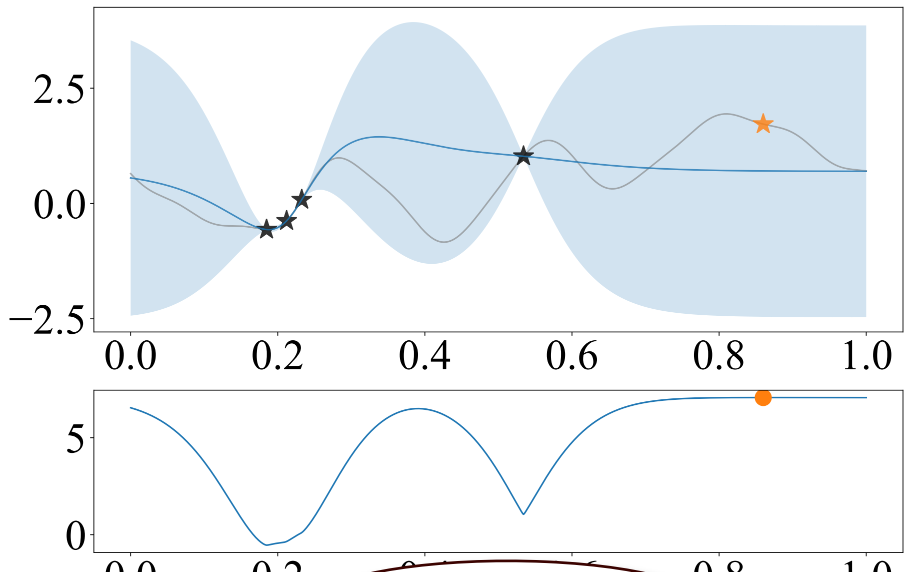
Gittins Index



bisection search

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

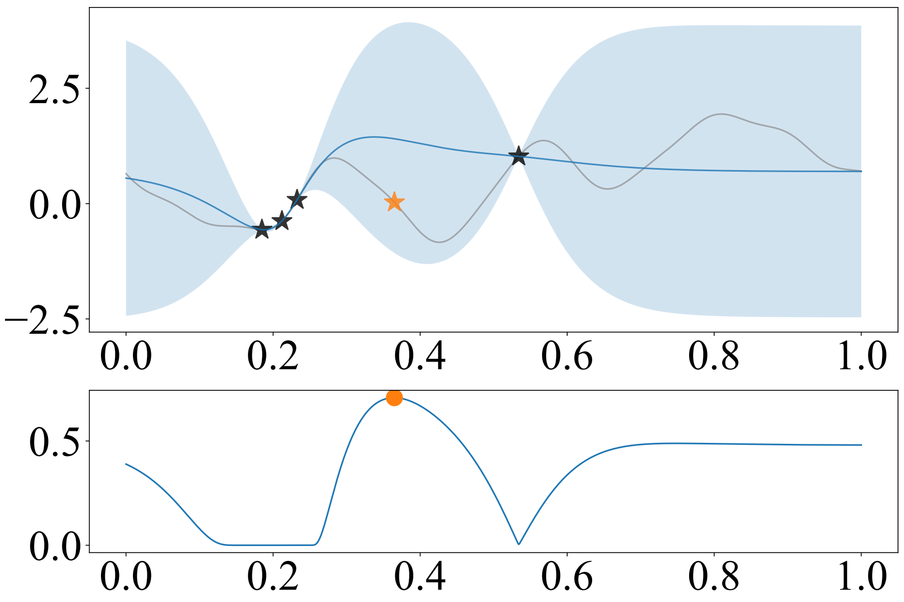
where $\mathrm{EI}_{f|D}(x; g) := \mathbb{E}[\max(f(x) - g, 0) \mid D]$

analytical expression

Easy-to-compute decision rule!

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

Expected Improvement



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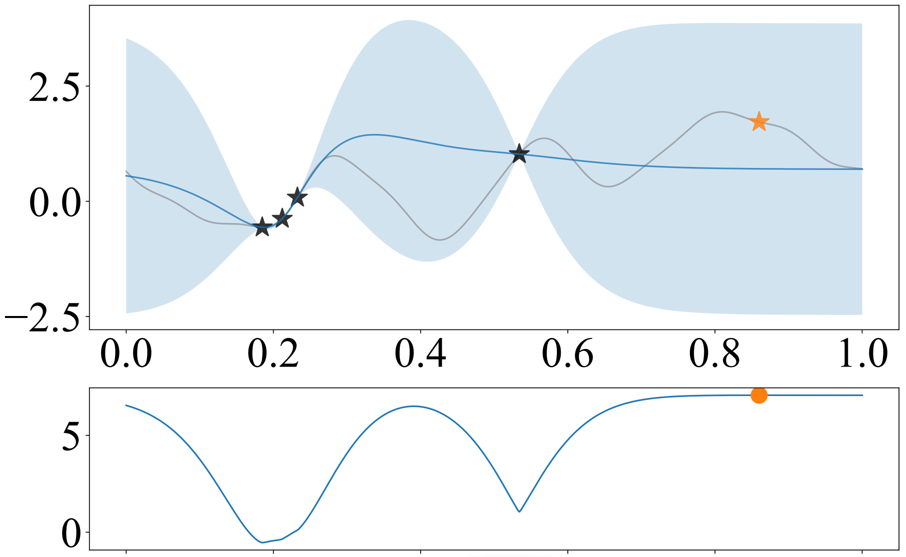
Gittins Index



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

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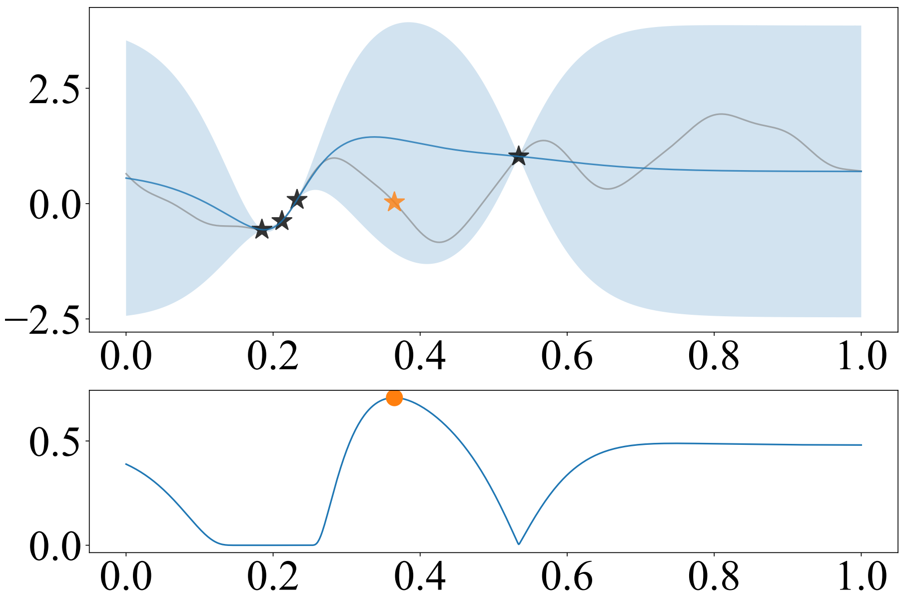
Google DeepMind

FunBO: Discovering new acquisition functions for Bayesian Optimization with FunSearch

hard to discover GI

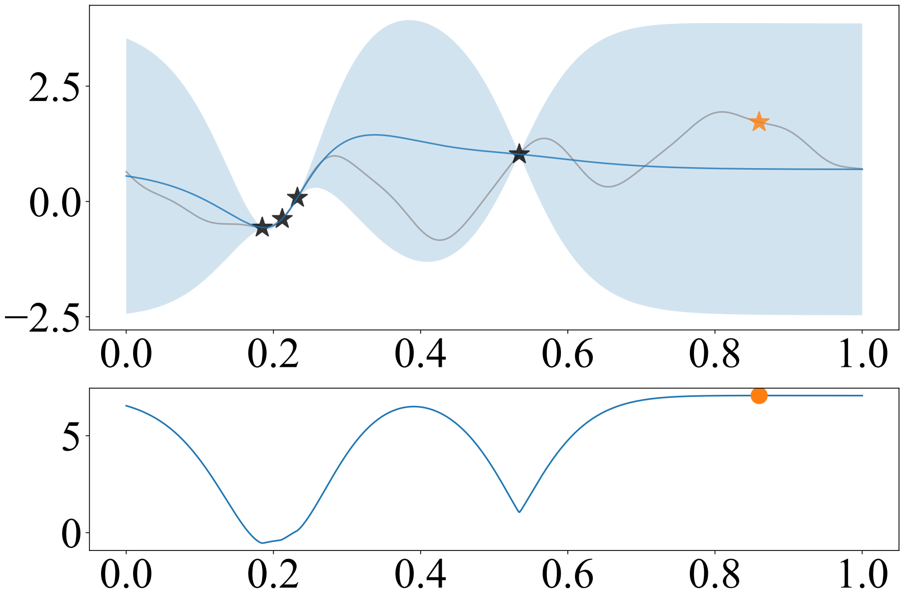
Expected Improvement



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

Temporal simplification to MDP
(One-step)

Gittins Index



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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

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

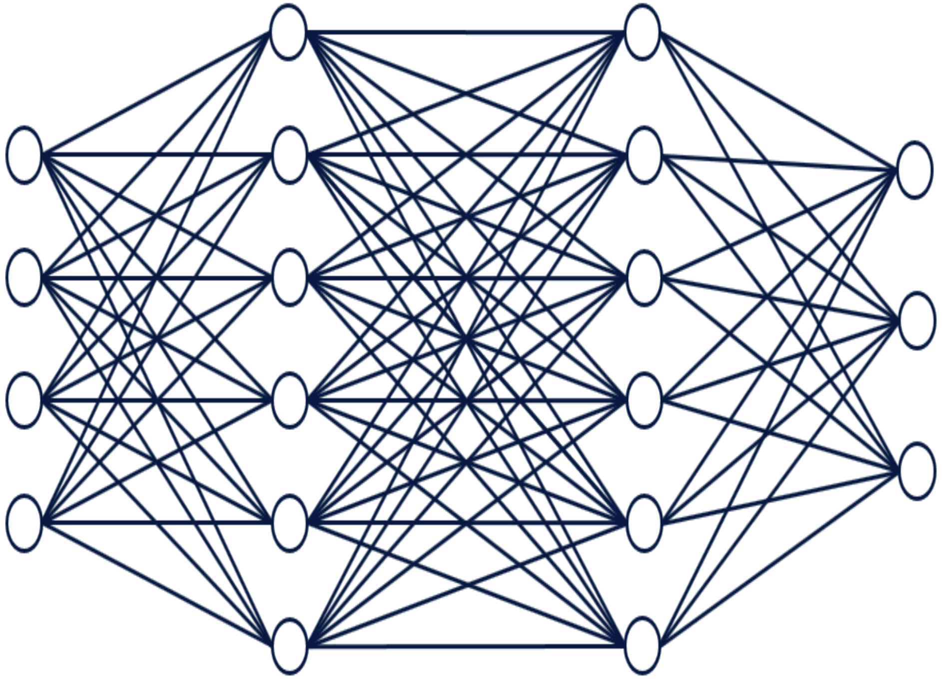
Application to efficient LLM

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

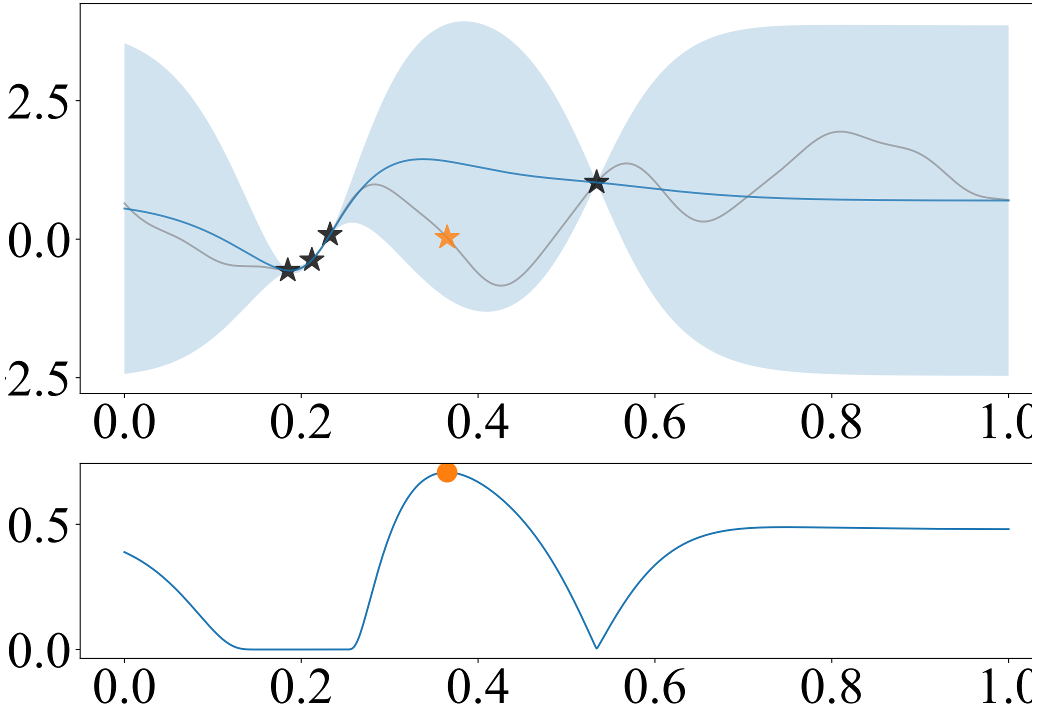
$$\tau:\ \mathrm{EI}(x_\tau) \leq \theta$$

[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

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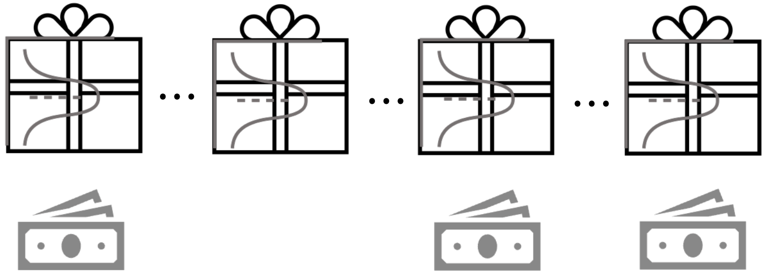

Why Gittins index?

Varying evaluation costs

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New design principle:
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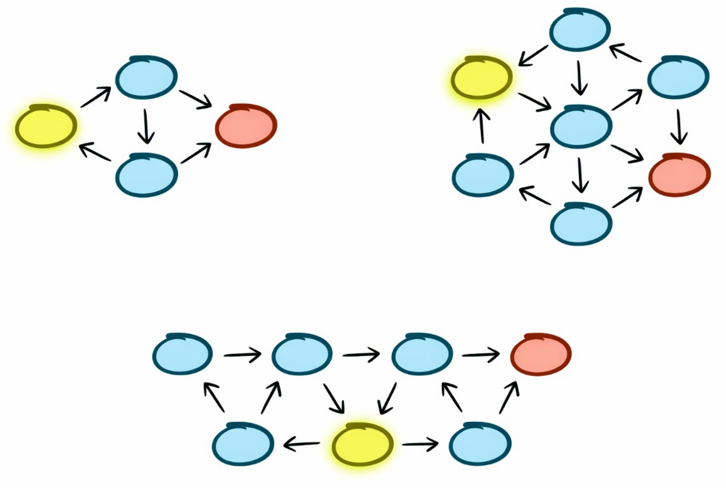

Why Gittins index?

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:
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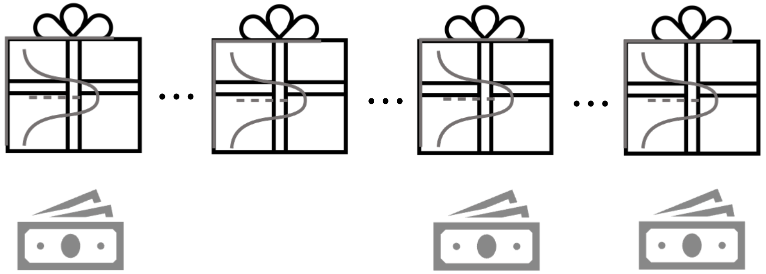
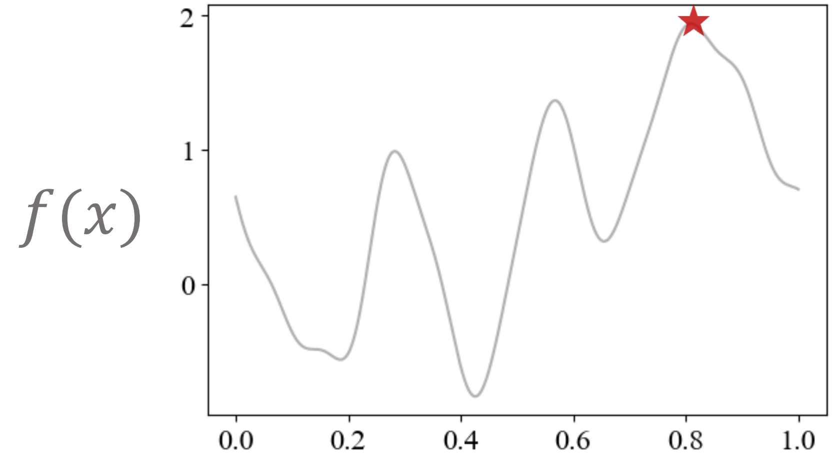
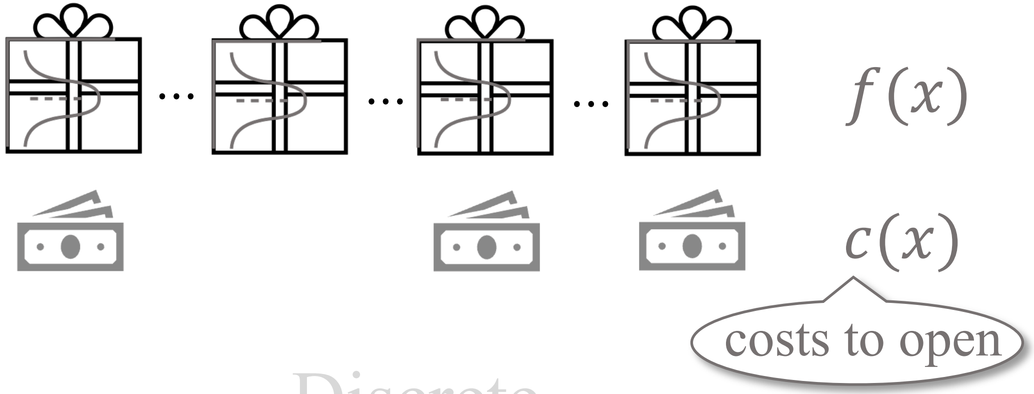


"Cost-aware Bayesian Optimization via the Pandora's Box Gittins Index." NeurIPS'24.

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

Bayesian Optimization	Pandora's Box
	[Weitzman'79]





Bayesian Optimization	Pandora's Box
Continuous	Discrete
Correlated	Independent
Cost-unaware	Cost-aware
Fixed-iteration	Flexible-stopping
$\mathbb{E} \max_{t=1,2,\ldots,T} f(x_t)$	$\mathbb{E} \max_{t=1,2,\ldots,T} f(x_t) - \mathbb{E} \sum_{t=1}^{T} c(x_t)$

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

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

Which threshold?

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

$\Leftrightarrow \tau\colon \mathrm{EIPC}(x_\tau;c) \le 1$

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

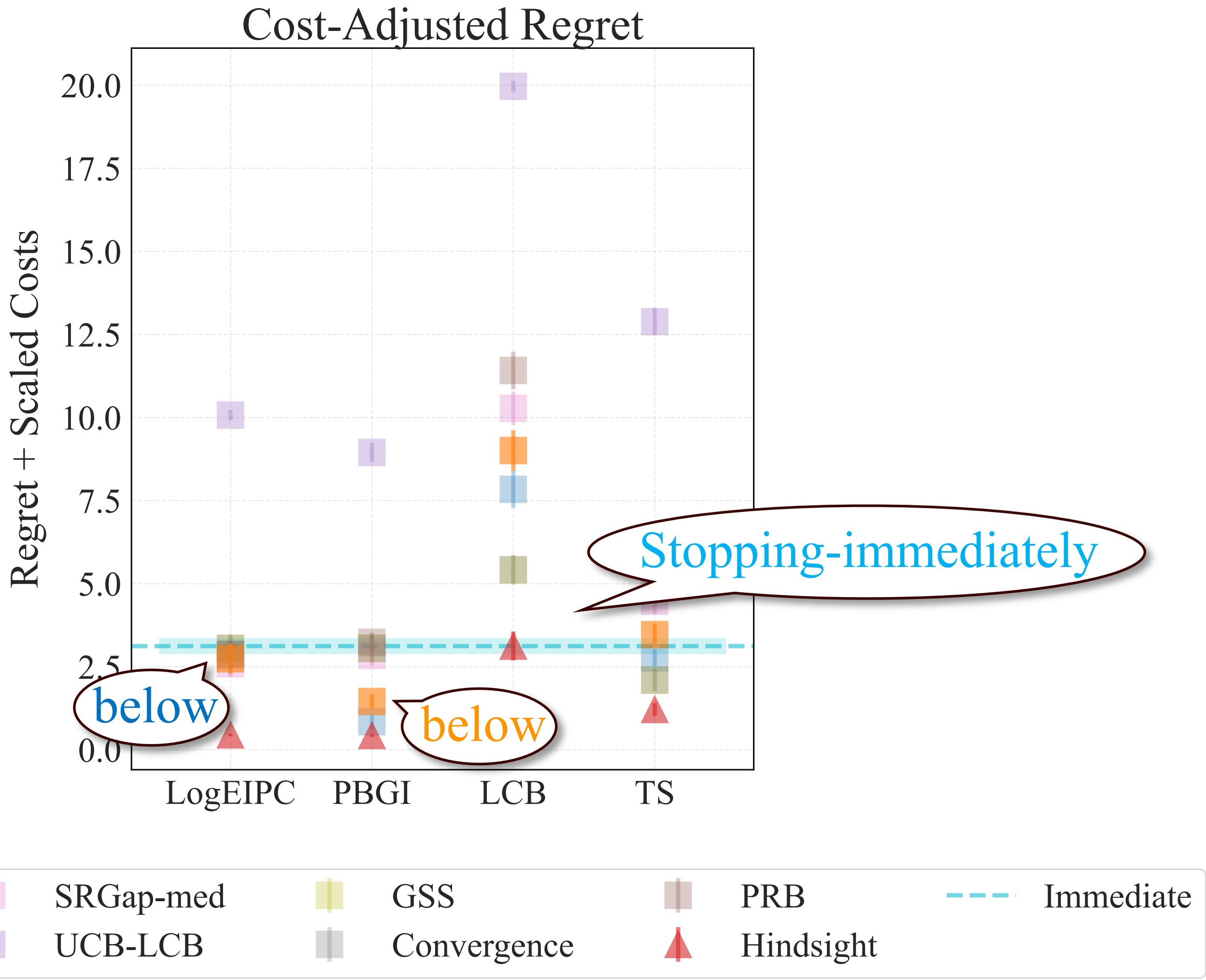
Implication:

• 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



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Link to Pandora's Box problem
& Gittins index theory

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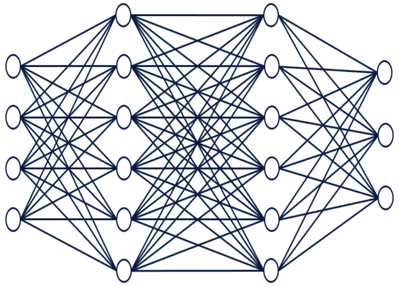
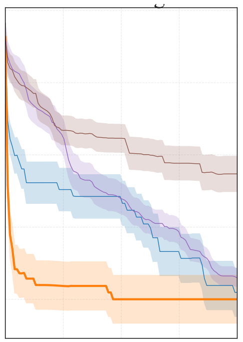




Interests from practitioners (e.g., Meta)

Future potential

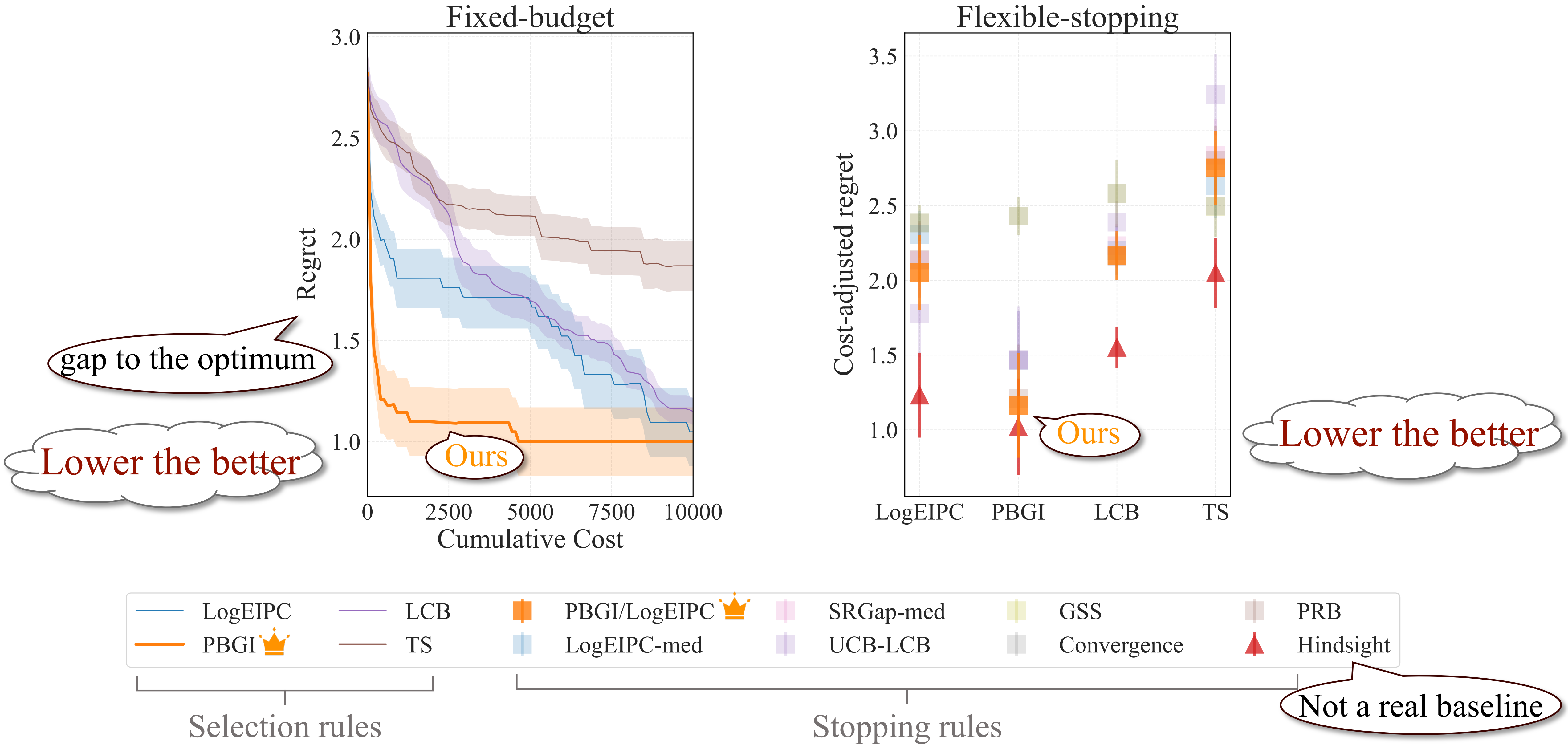
Best-prompt identification

Adaptive response sampling

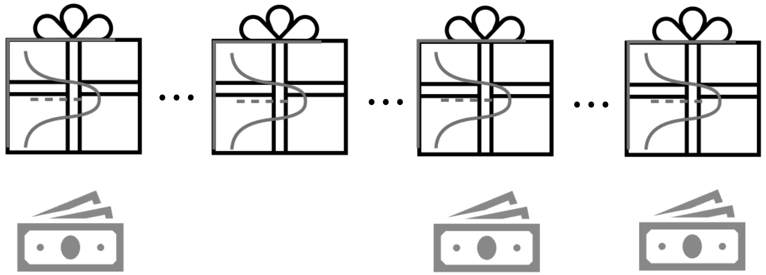
Chain-of-thought selection

Application to efficient LLM

Gittins Index vs Baselines on AutoML Benchmark



Novel connection



Link to Pandora's Box problem
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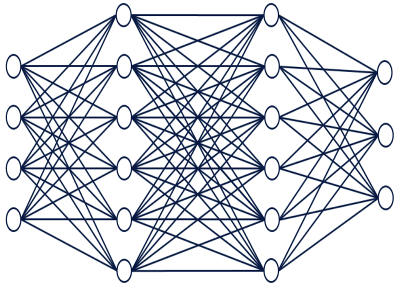
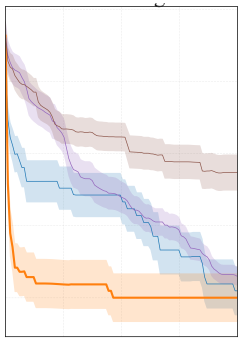
Principled decision rules

- Varying evaluation costs
- Adaptive stopping time

Unified framework for
selection and stopping

Competitive empirical performance





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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!

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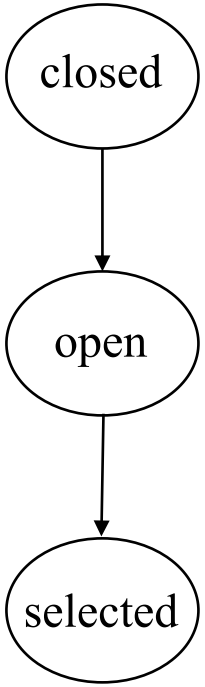
Markovian Bandits

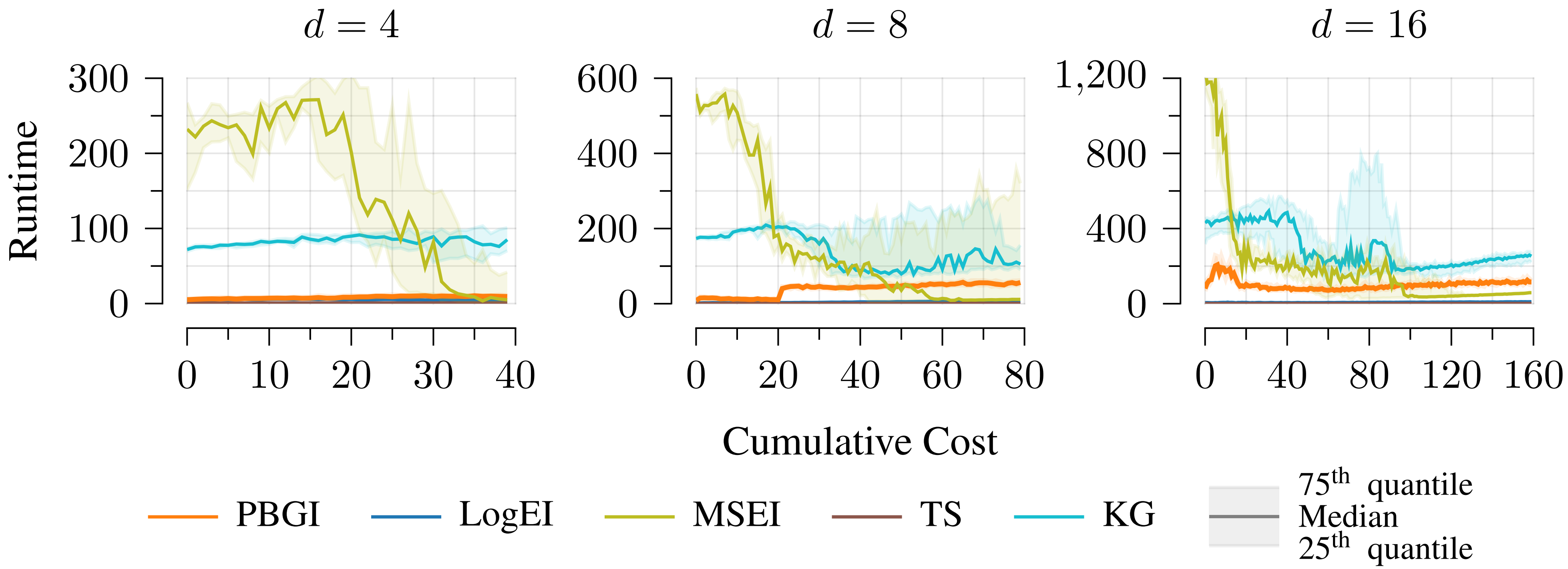
[Gittins’79]



Pandora’s Box

[Weitzman’79]

Timing Experiment: Gittins Index vs Baselines



PBGI is computationally-efficient!