

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

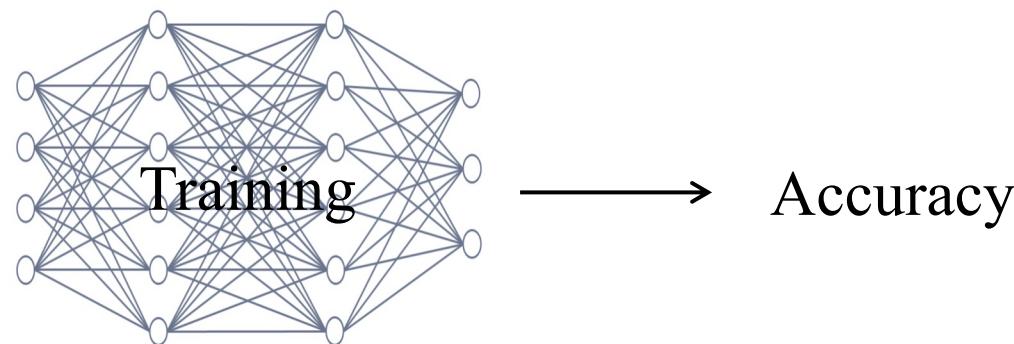
Qian Xie 谢倩 (Cornell ORIE)

TTAP Job Talk

# Motivation: World of Optimization under Uncertainty

ML model training:

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



# Motivation: World of Optimization under Uncertainty

ML model training:

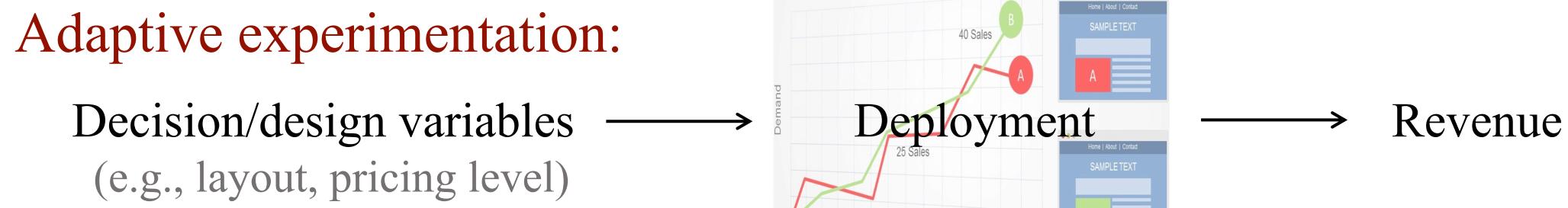
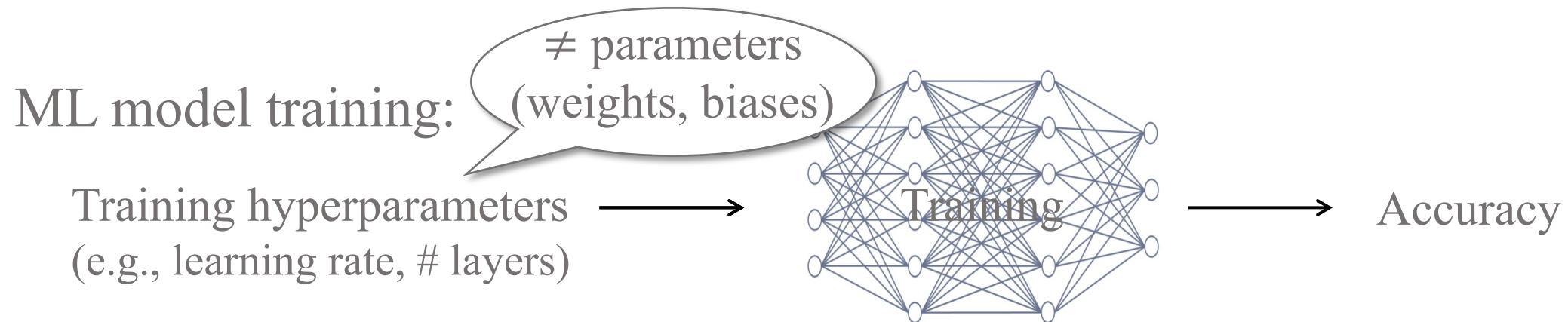
Training hyperparameters  
(e.g., learning rate, # layers)

$\neq$  parameters  
(weights, biases)



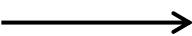
→ Accuracy

# Motivation: World of Optimization under Uncertainty



# Motivation: World of Optimization under Uncertainty

Design choices  $x$



non-analytical &  
no gradient info

Performance metric  $f(x)$

ML model training:

$\neq$  parameters  
(weights, biases)

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  $x$   $\longrightarrow$



non-analytical &  
no gradient info

Observed outcome  $f(x)$

ML model training:

$\neq$  parameters  
(weights, biases)

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



$\longrightarrow$  Accuracy

Adaptive experimentation:

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



$\longrightarrow$  Revenue

# Background: Black-Box Optimization

Black-box optimization:

(gradient-based methods not applicable)

Input  $x$  →



expensive-to-evaluate

Observed outcome  $f(x)$

ML model training:

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



Training

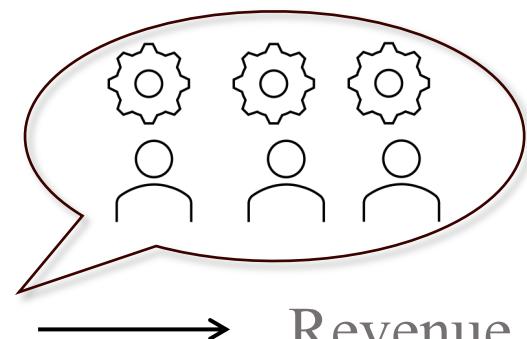
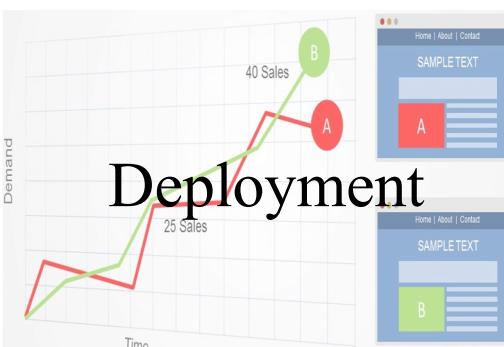
→ Accuracy

Training time

Compute credits

Adaptive experimentation:

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



→ Revenue

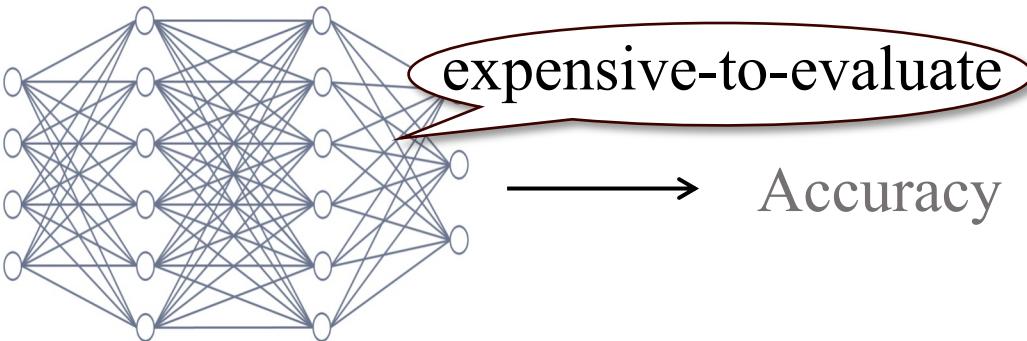
Operational cost

User experience

# Naïve (Non-Adaptive) Approach: Grid Search

ML model training:

Training hyperparameters

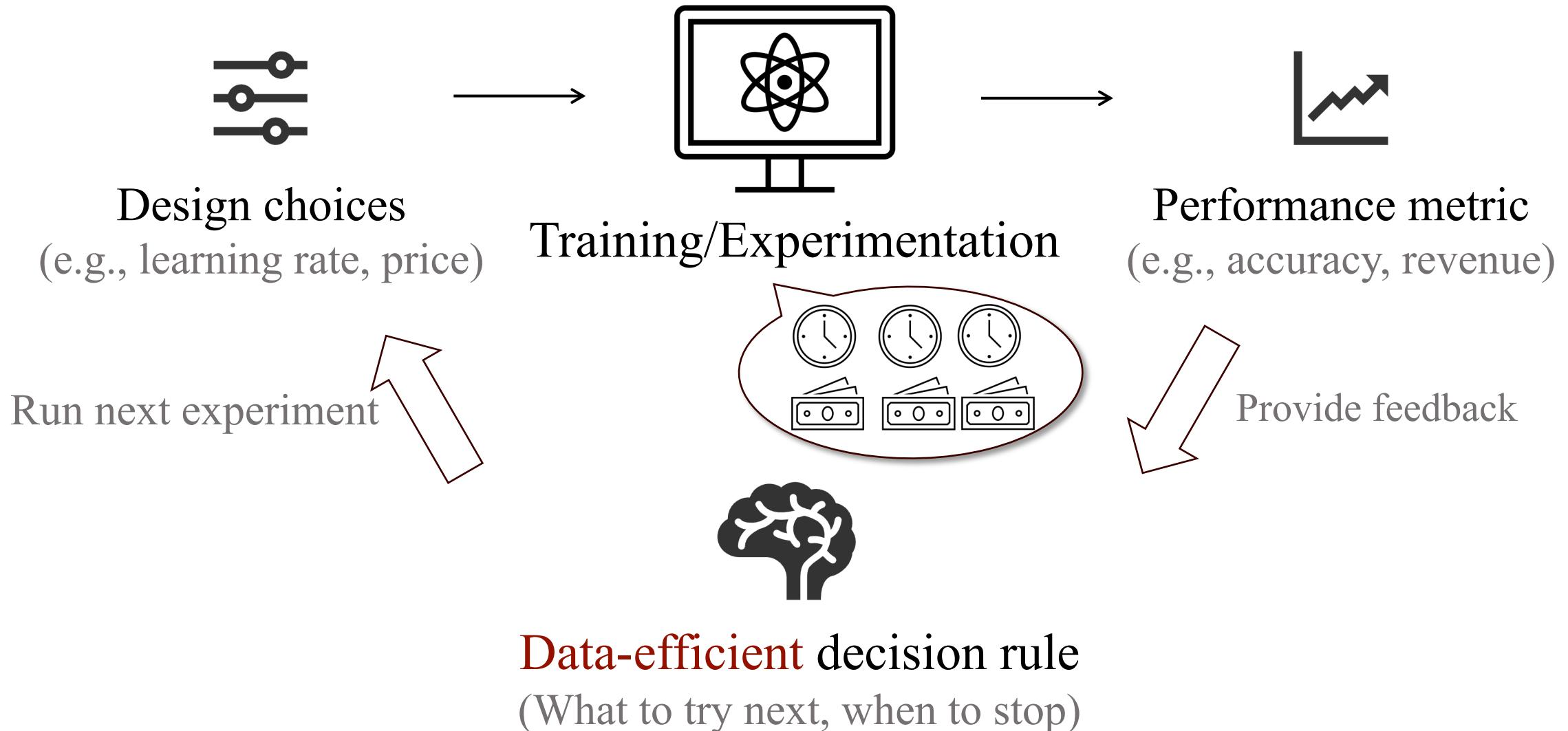


Accuracy

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!

# Data-Driven (Adaptive) Approach



# 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-based 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-based 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

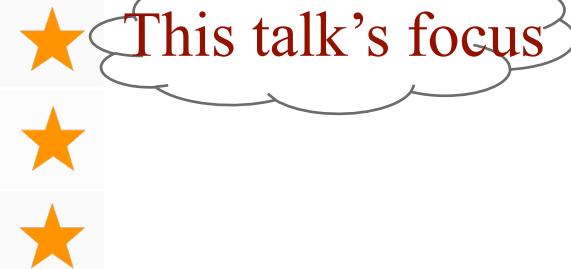
# New Methods for Black-Box Optimization

## Naïve approaches:

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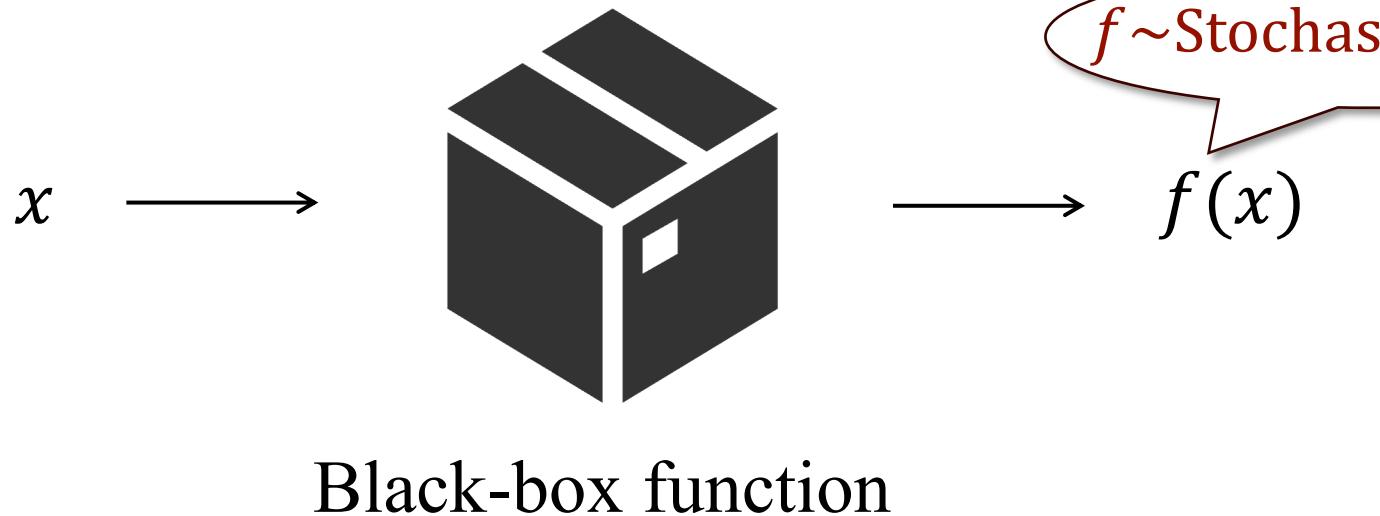


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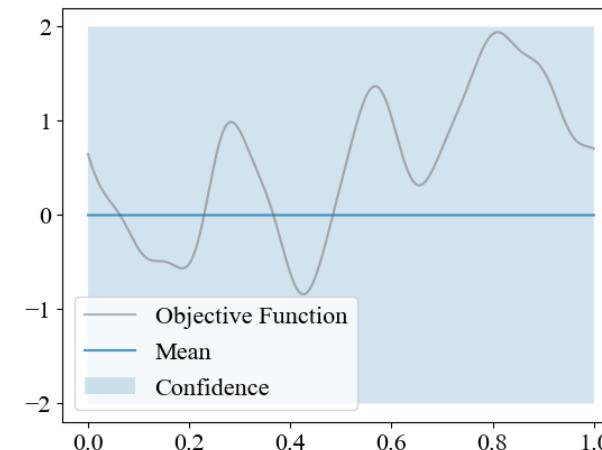
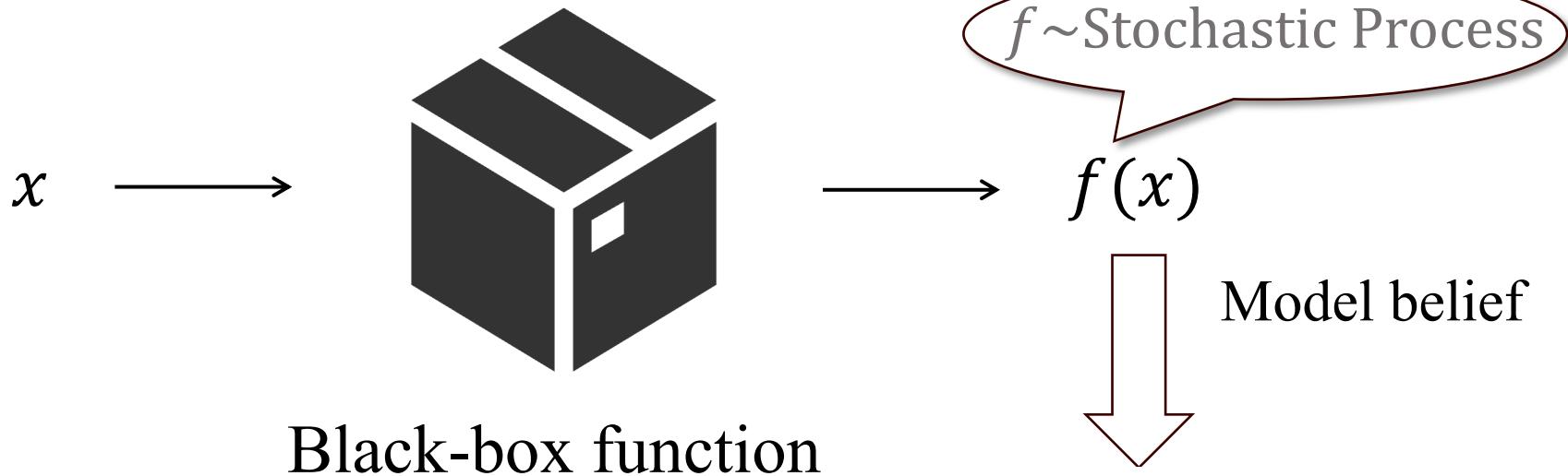
★ New methods under this umbrella

# Bayesian Optimization



# Bayesian Optimization

Time 0



Probabilistic model  
(e.g., Gaussian process)

# Bayesian Optimization

Time  $t$

$x_1, \dots, x_t$

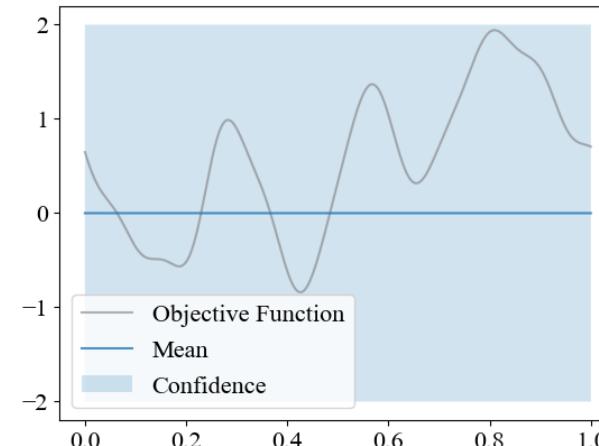


Black-box function

$f \sim \text{Stochastic Process}$

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

Model belief



Probabilistic model  
(e.g., Gaussian process)

# Bayesian Optimization

Time  $t$

$x_1, \dots, x_t$

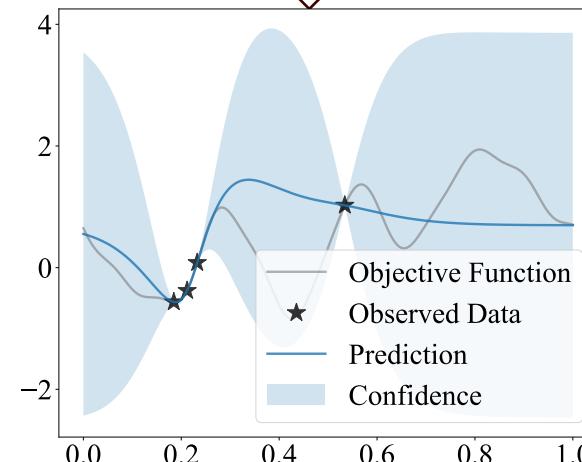


Black-box function

$f \sim \text{Stochastic Process}$

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

Update belief  
(Bayes' rule)



Probabilistic model  
(e.g., Gaussian process)

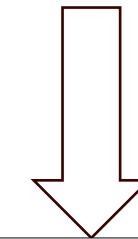
# Bayesian Optimization

Time  $t$

$x_1, \dots, x_t$

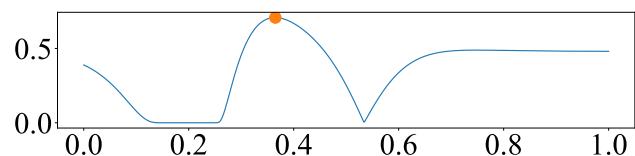


$f(x_1), \dots, f(x_t)$

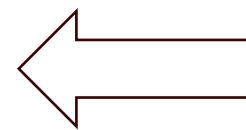


Update belief  
(Bayes' rule)

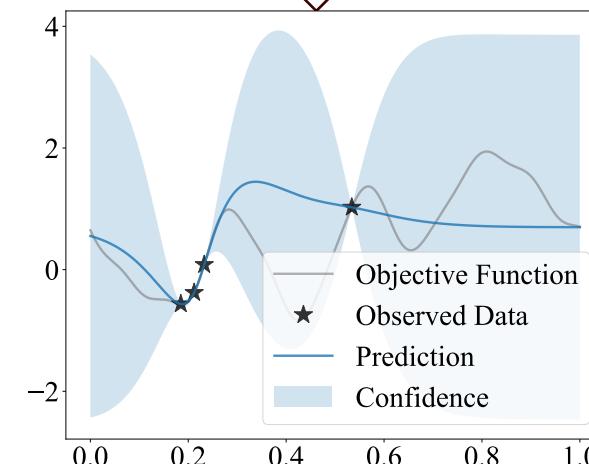
Black-box function



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

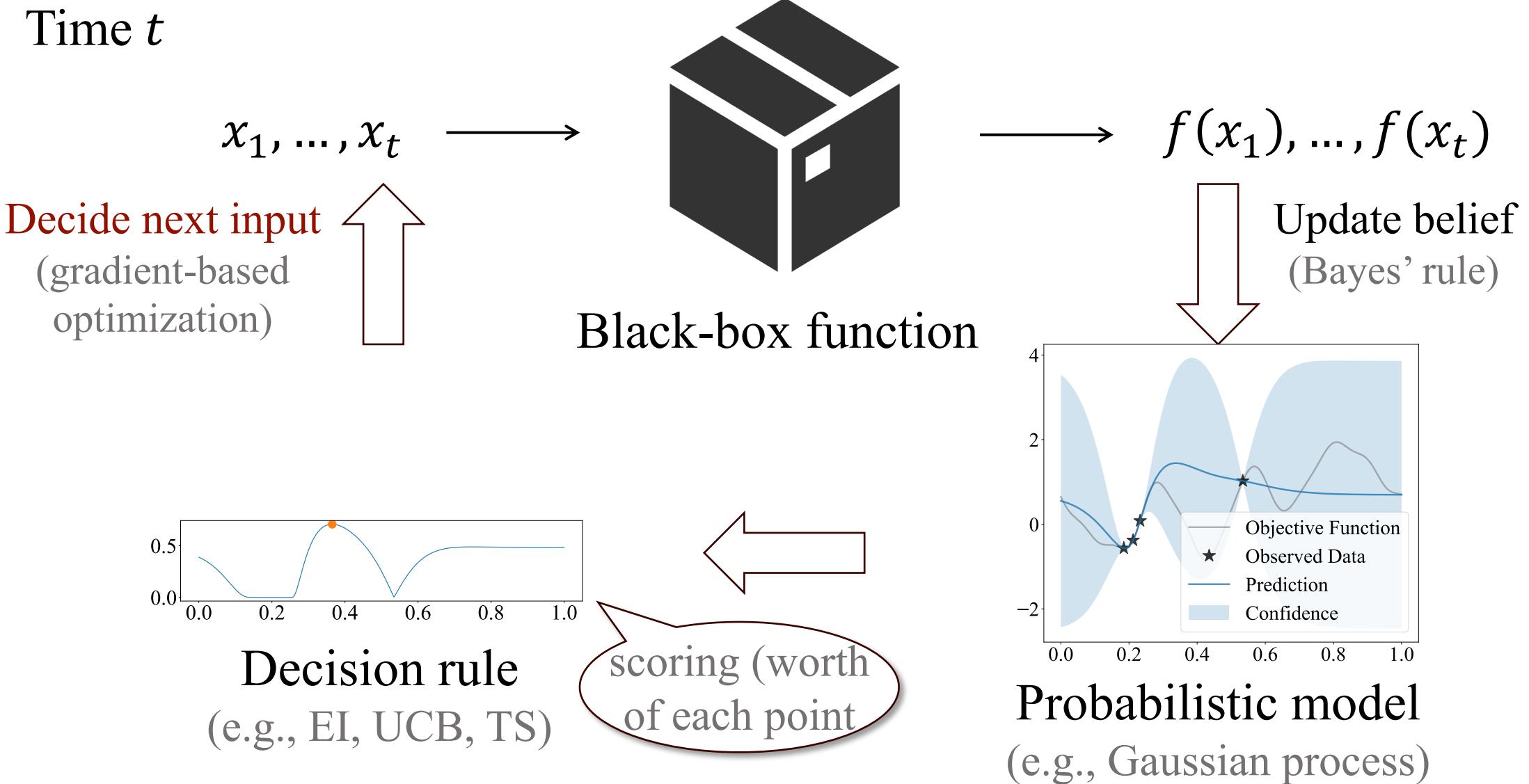


scoring (worth  
of each point)

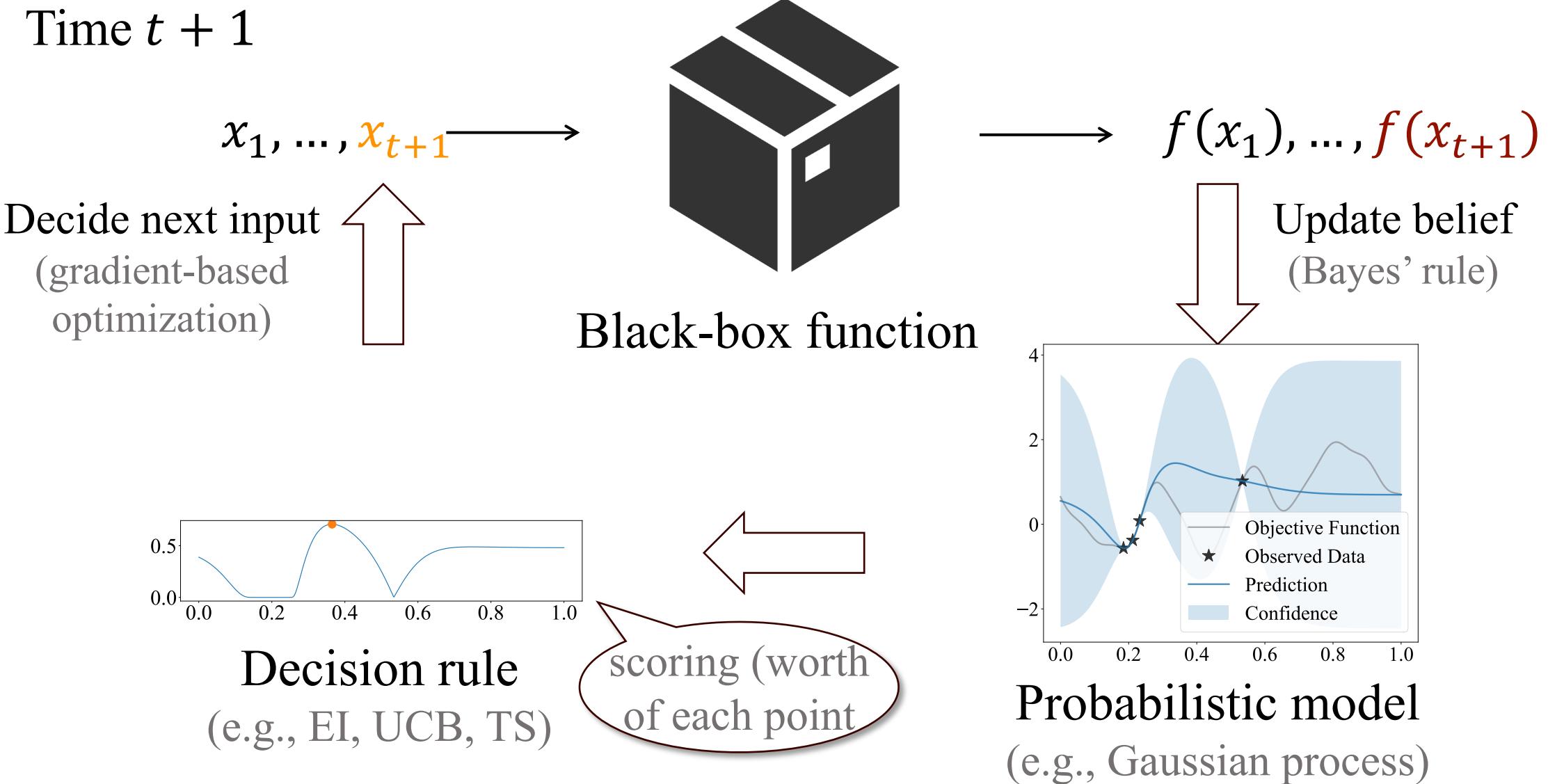


Probabilistic model  
(e.g., Gaussian process)

# Bayesian Optimization



# Bayesian Optimization



# Bayesian Optimization

Time  $t + 1$

Decide next input  
(gradient-based  
optimization)

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

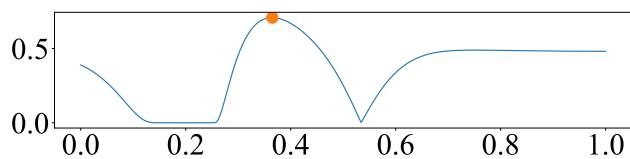


$f(x_1), \dots, f(x_{t+1})$

Update belief  
(Bayes' rule)

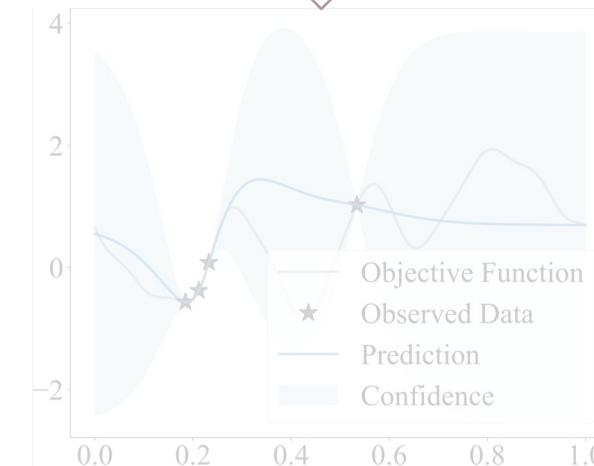
Black-box function

My focus



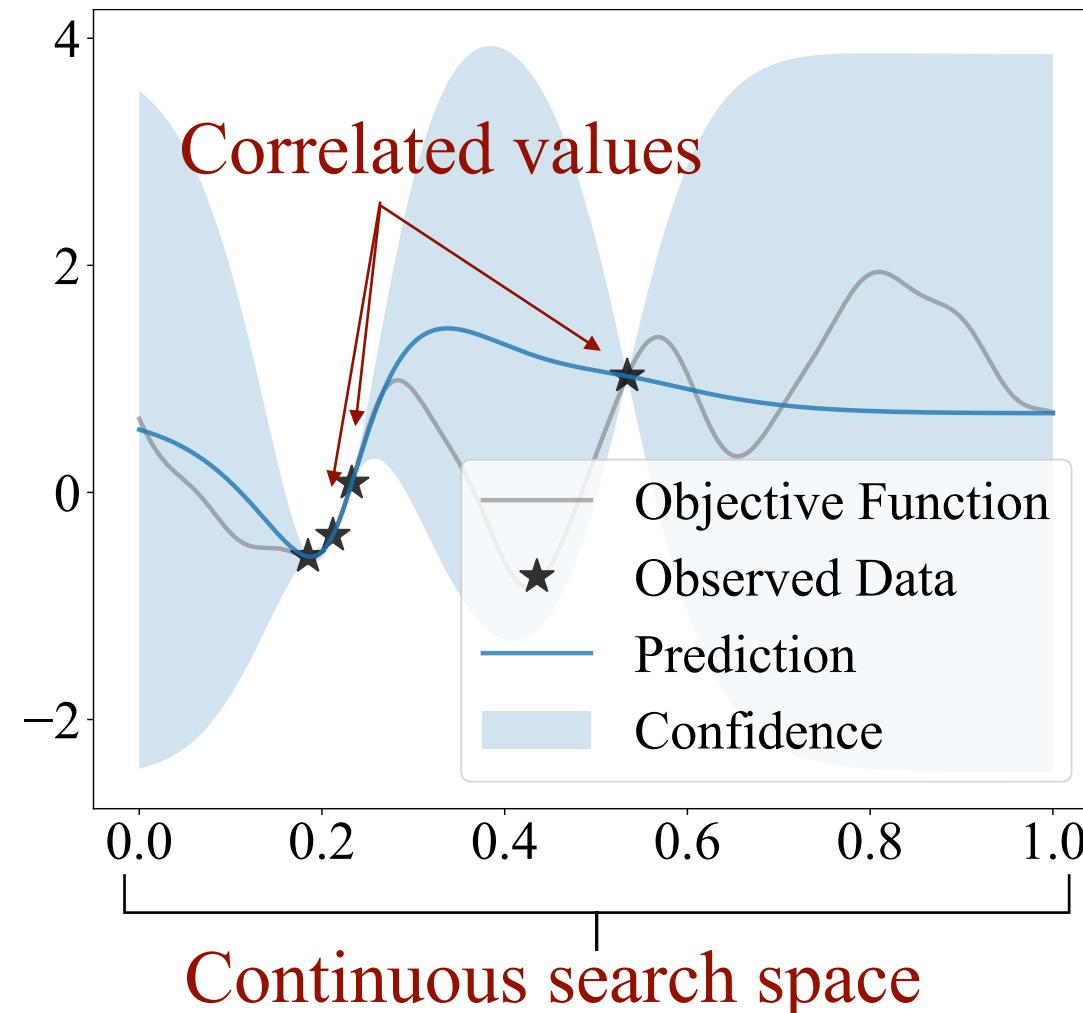
Decision rule  
(e.g., EI, UCB, TS)

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

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

“improvement”

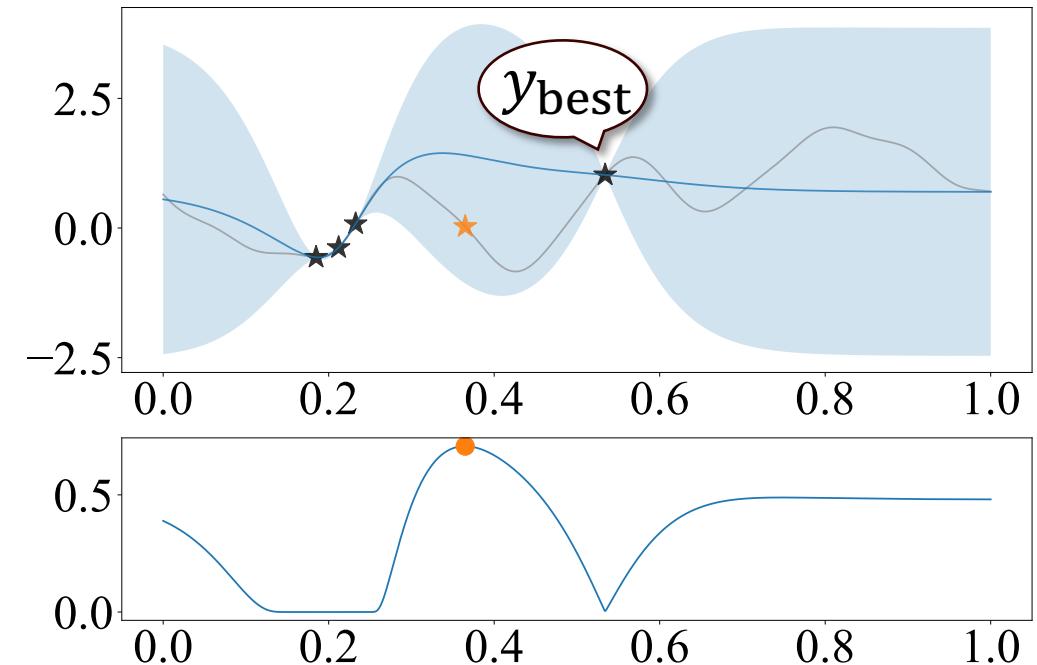
current best observed

data  $D$

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

posterior distribution

One-step approximation to MDP



Expected improvement  $EI(x)$

# Popular Decision Rule: Expected Improvement

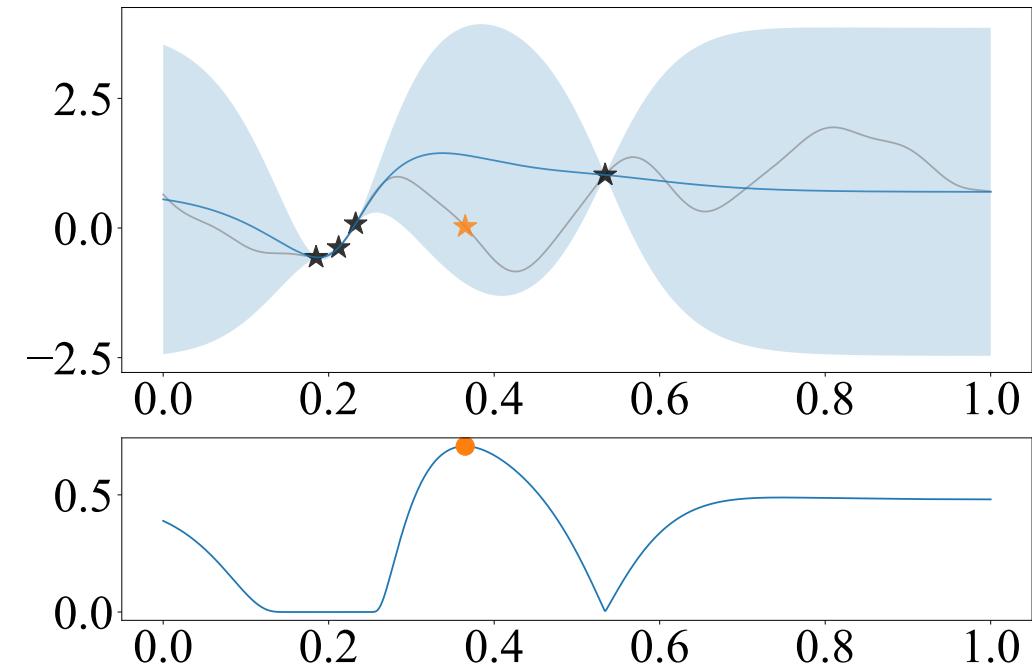
$$EI(x) = \mathbb{E}[\max(f(x) - y_{\text{best}}, 0) \mid x_1, \dots, x_t]$$

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

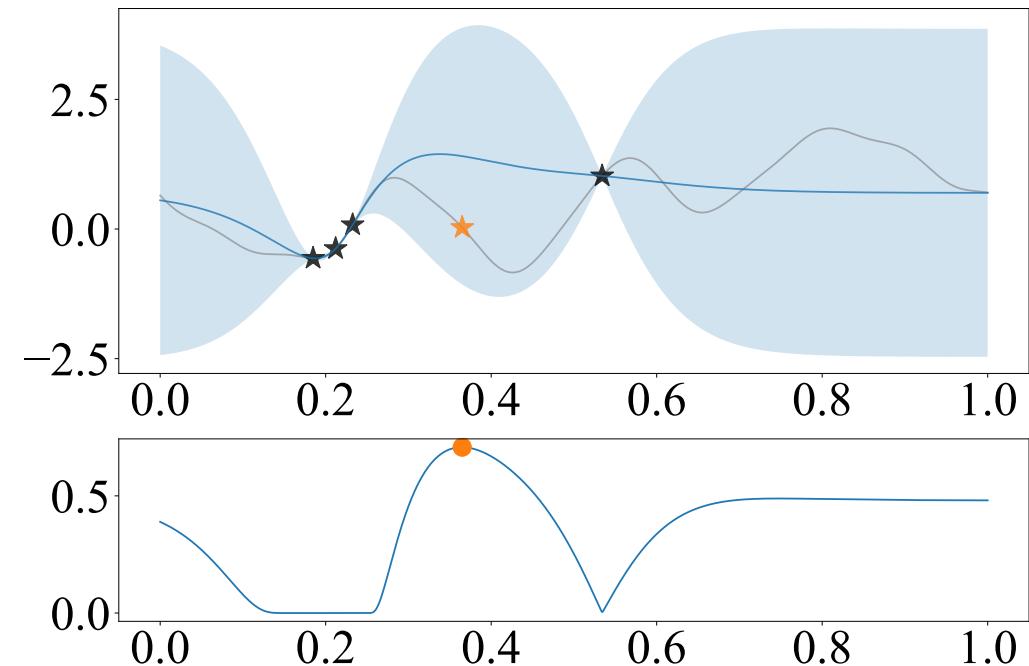


Expected improvement  $EI(x)$

Improvement-based  
design principle

# Existing Design Principles

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

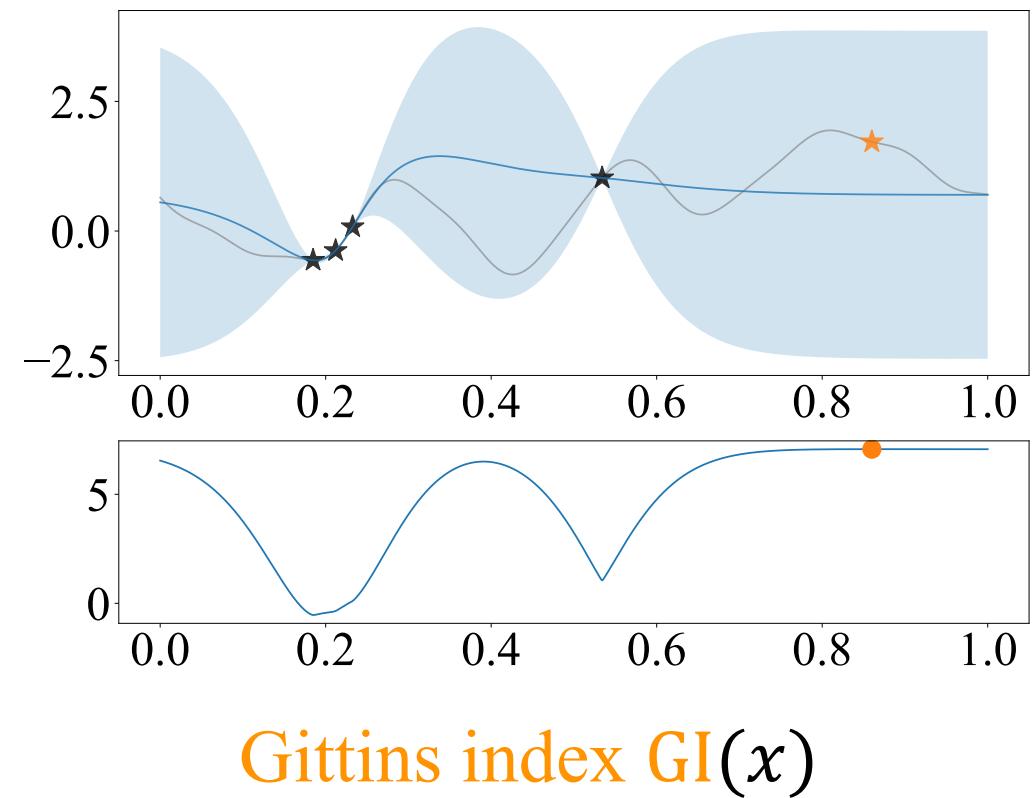


Expected improvement  $EI(x)$

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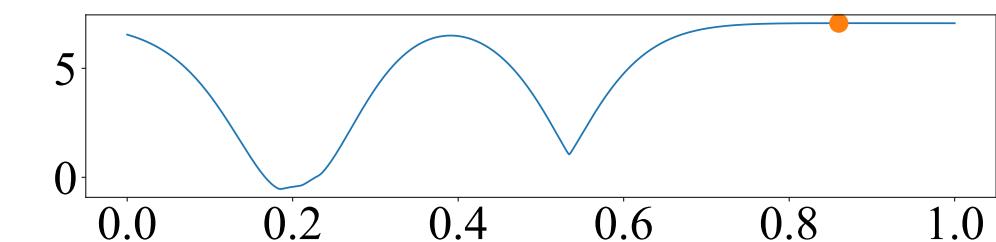
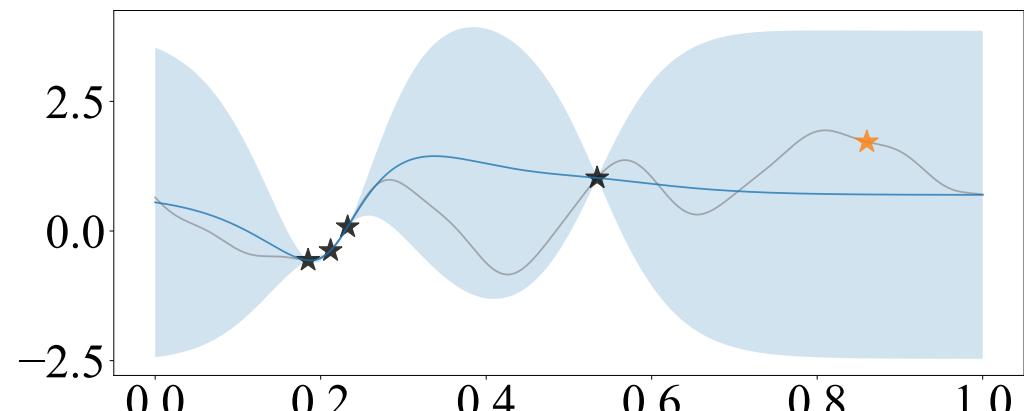
# New Design Principle: Gittins Index

- 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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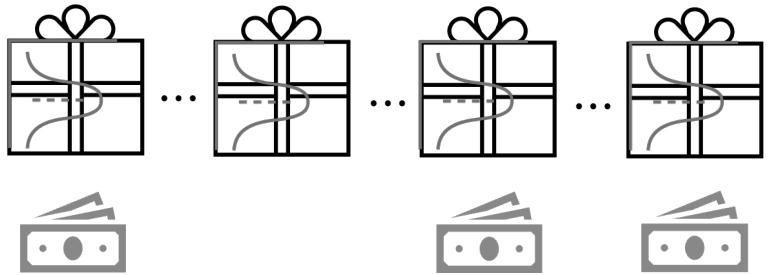


Gittins index  $GI(x)$

? Why another principle?

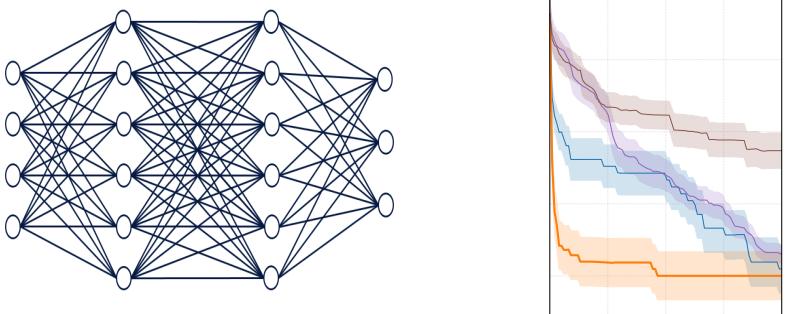
# Our Contribution: Gittins Index Principle

## Novel connection



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

## Competitive empirical performance



Interests from practitioners (e.g., Meta)

## Principled decision rules

- Varying evaluation costs
- Adaptive stopping time

Unified framework for selection and stopping

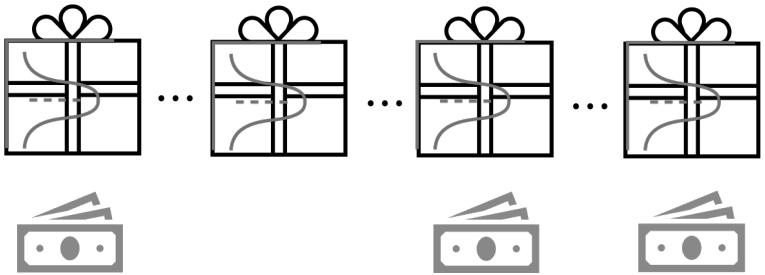
## Future potential

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

Application to **efficient LLM**

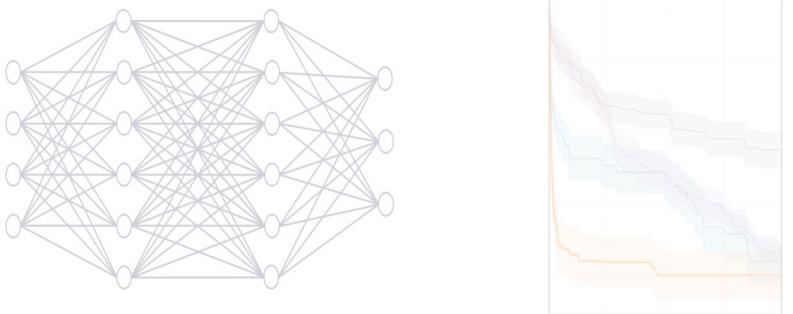
# Our Contribution: Gittins Index Principle

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Competitive empirical performance



Interests from practitioners (e.g., Meta)

Principled decision rules



Unified framework for cost-aware selection and stopping

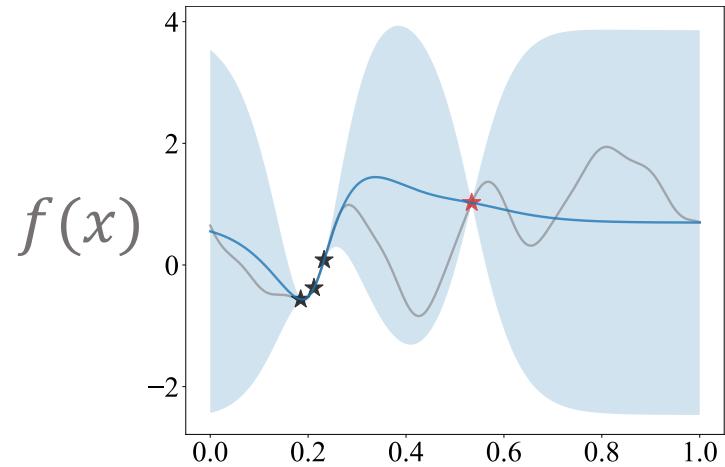
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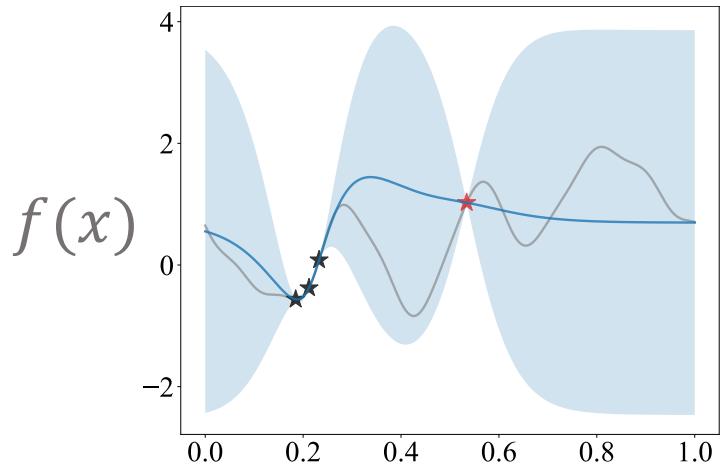
# Bayesian Optimization



Continuous search space

Correlated function values

# Bayesian Optimization



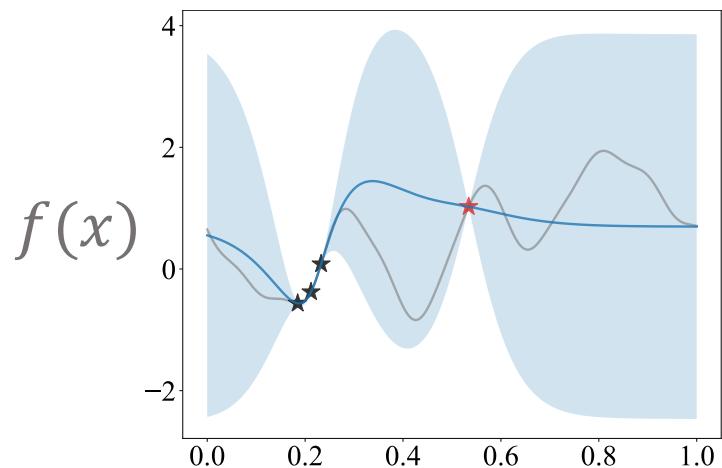
Continuous search space  $\Rightarrow$

Discrete

Correlated function values  $\Rightarrow$

Independent

# Bayesian Optimization



Continuous search space

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# Pandora's Box

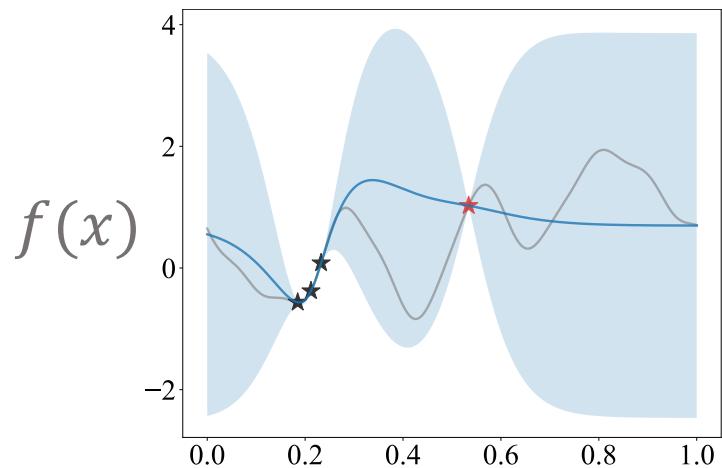
[Weitzman'79]



Discrete

Independent

# Bayesian Optimization

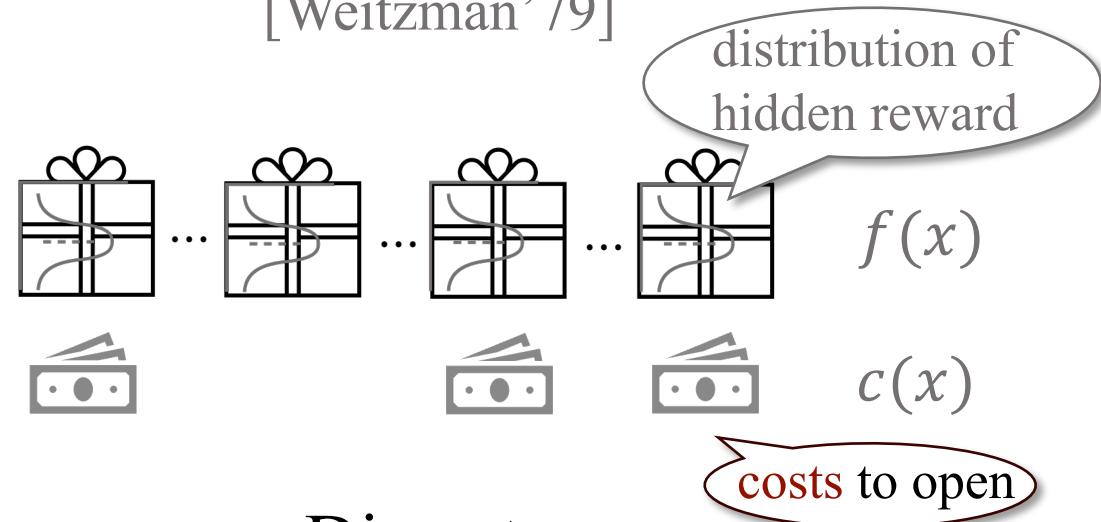


Continuous search space

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# Pandora's Box

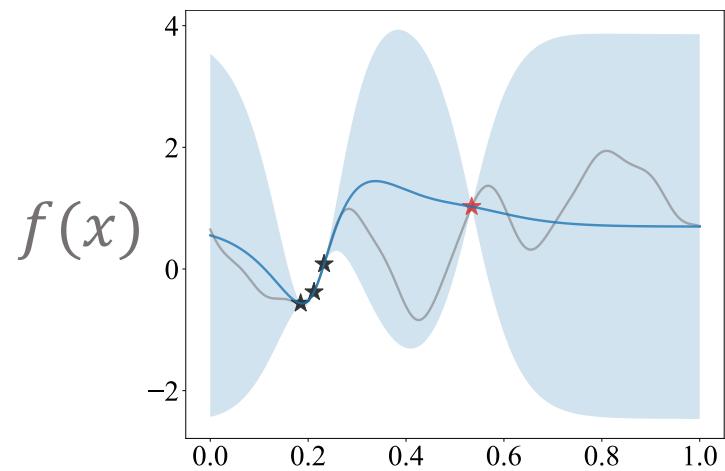
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Discrete

Independent

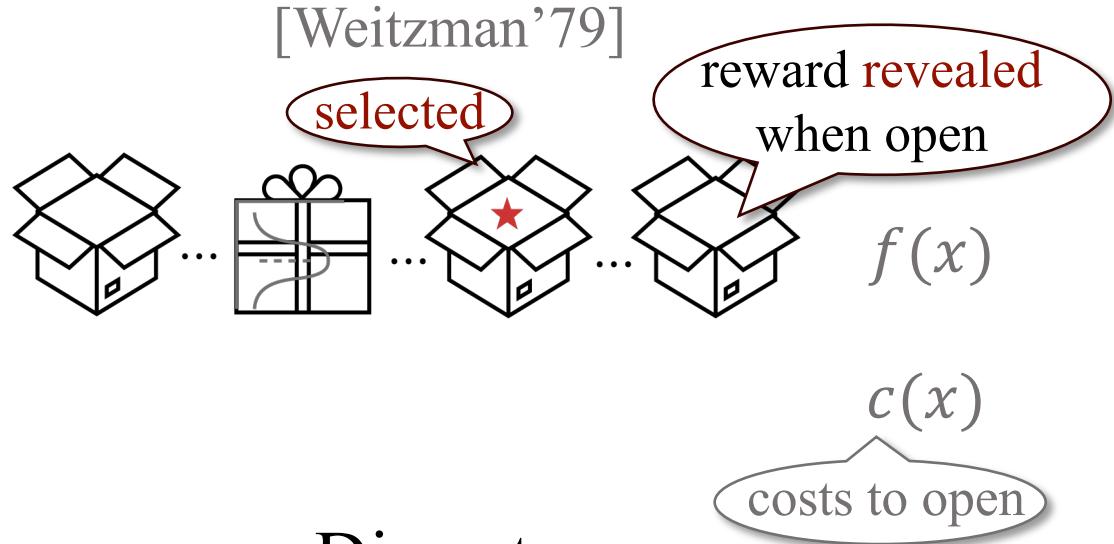
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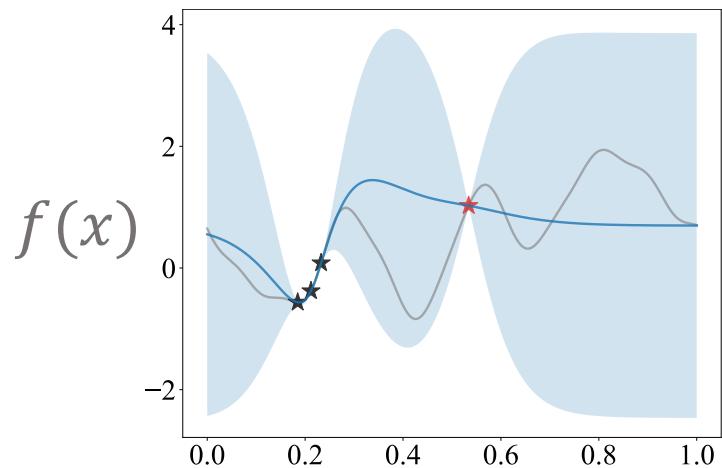
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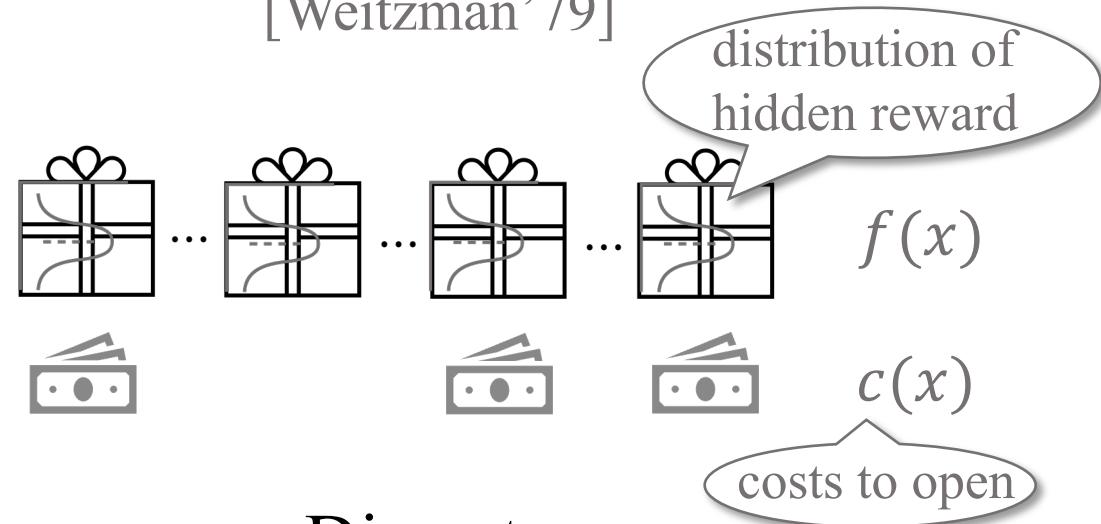


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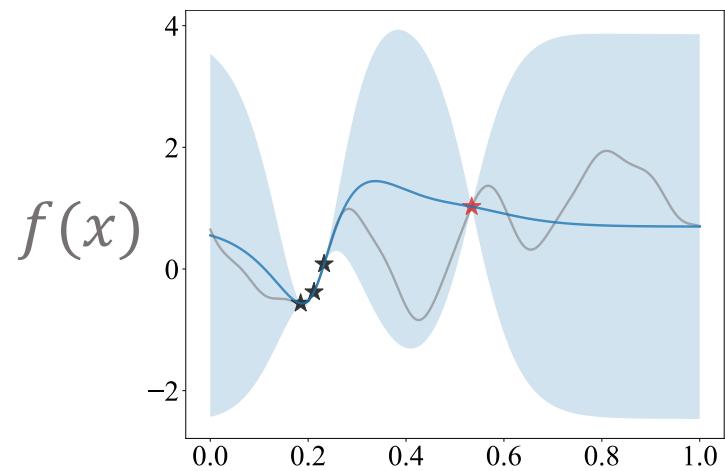


Discrete

Independent

Optimal policy: Gittins index

# Bayesian Optimization

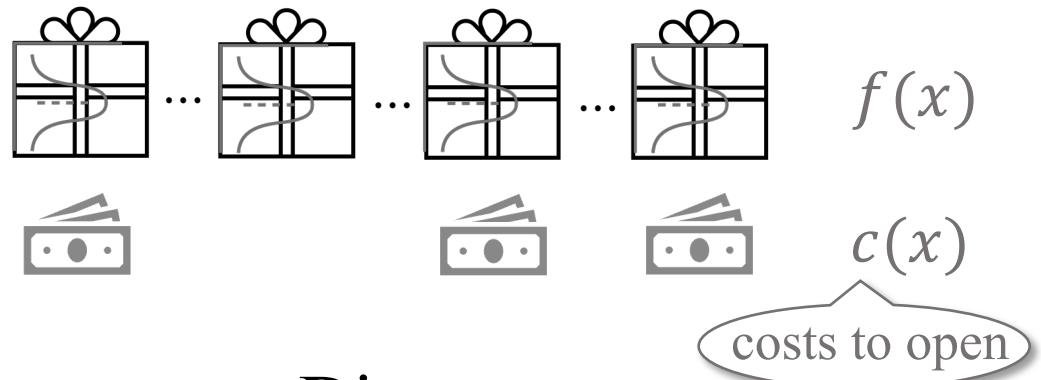


Continuous search space

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# Pandora's Box

[Weitzman'79]



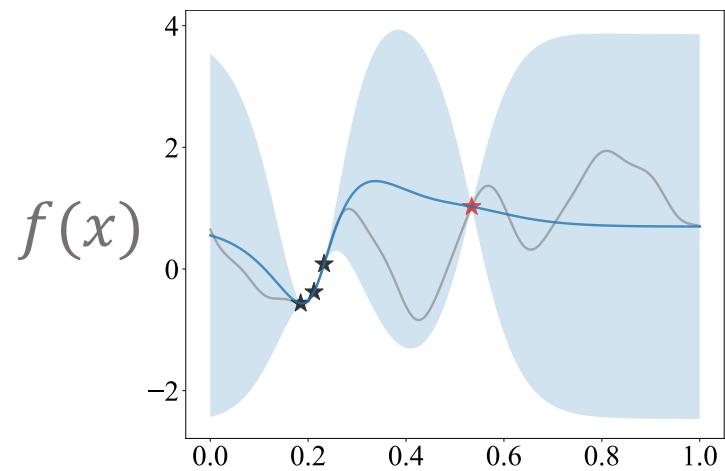
Discrete

Independent

How to translate?

Optimal policy: Gittins index

# Bayesian Optimization

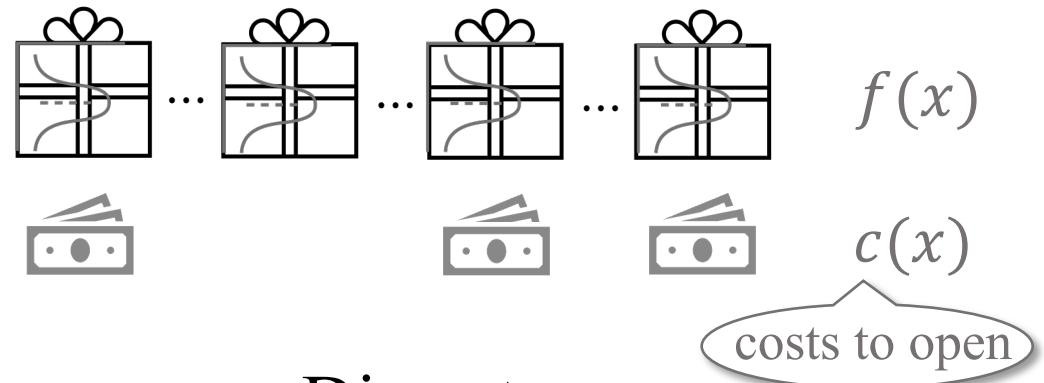


Continuous search space

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# Pandora's Box

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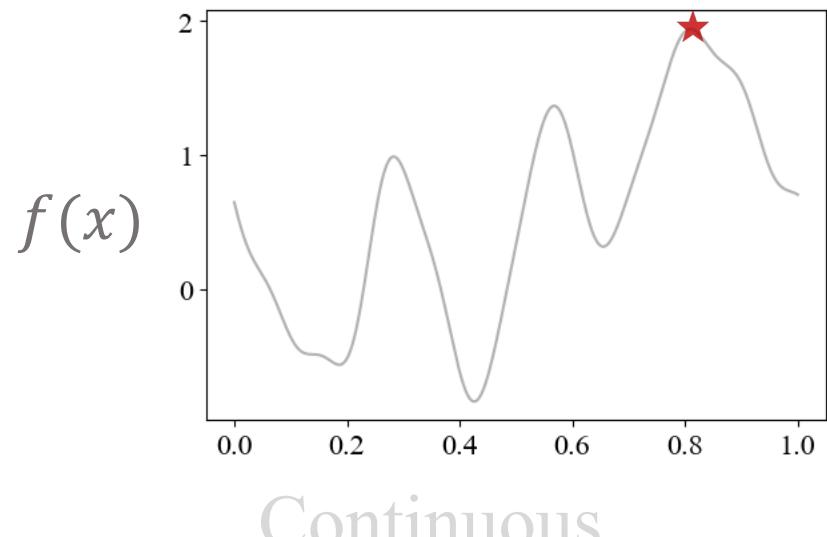
Discrete

Independent

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

incorporate posterior      New!  
take continuum limit

# Bayesian Optimization

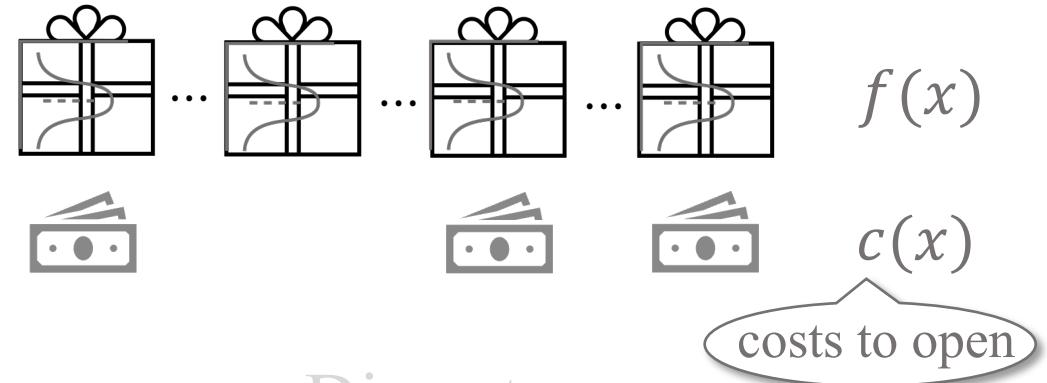


Correlated

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

# Pandora's Box

[Weitzman'79]



Discrete

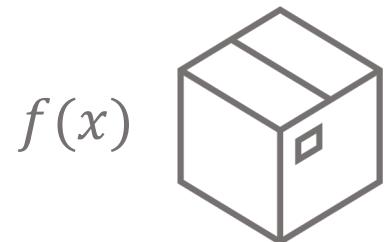
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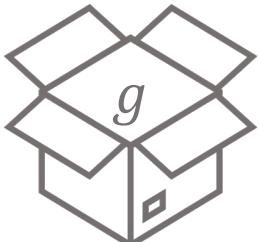
Optimal policy:  $\text{GI}_f(x; c(x))$

# Intuition

Exploration



Exploitation



vs.

Open closed box

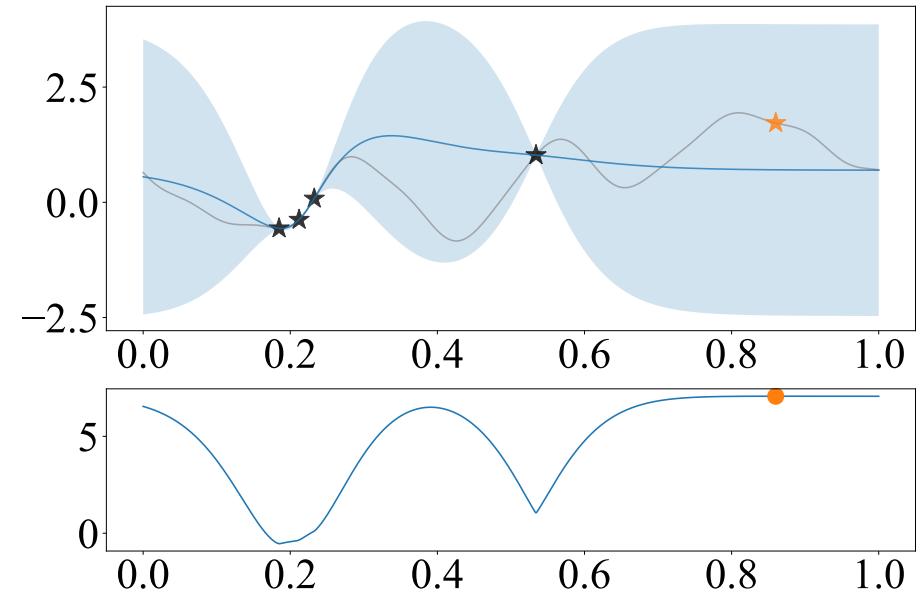
Take opened box

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

$$g$$

Should one open box? Depend on  $g$ !

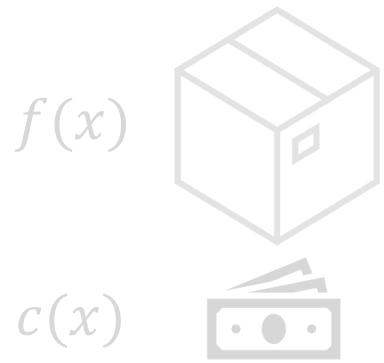
# Gittins Index



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

# Intuition

Exploration



vs.

Exploitation



Open closed box

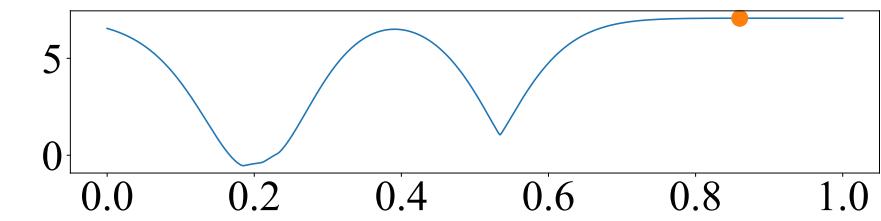
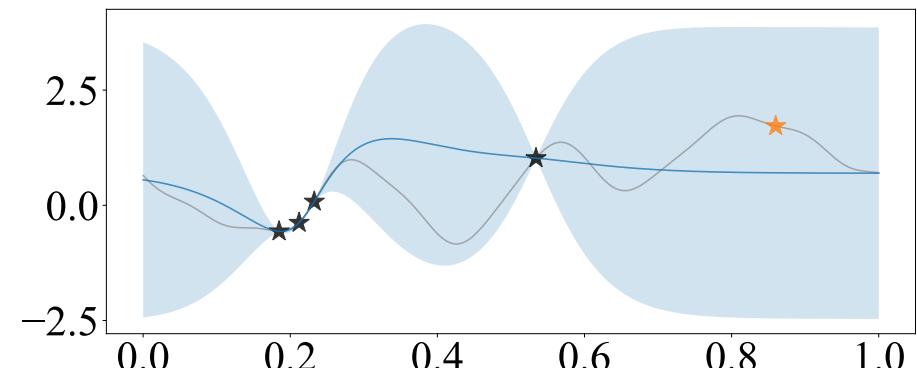
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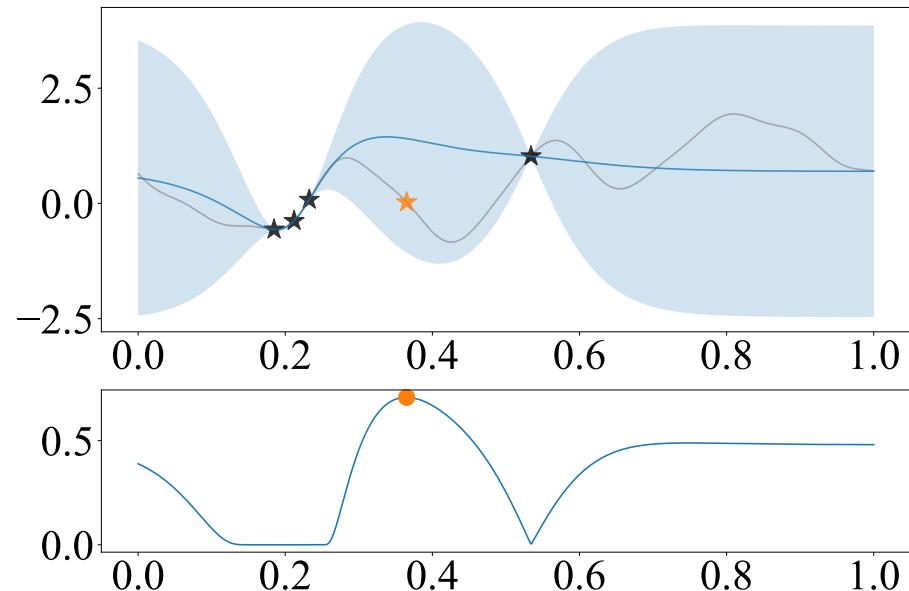
# Gittins Index



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

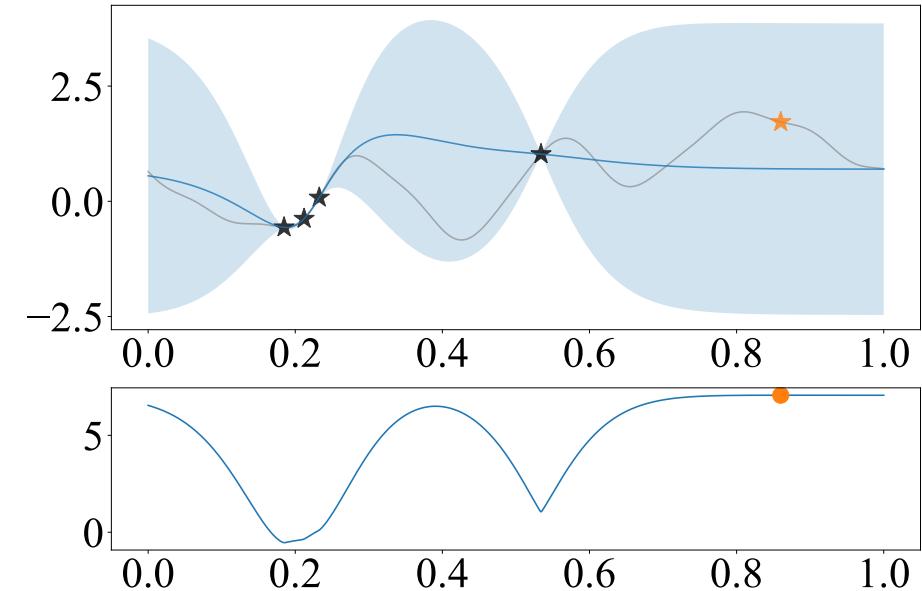
$$\text{EI}_{f|D}(x; g)$$

# Expected Improvement

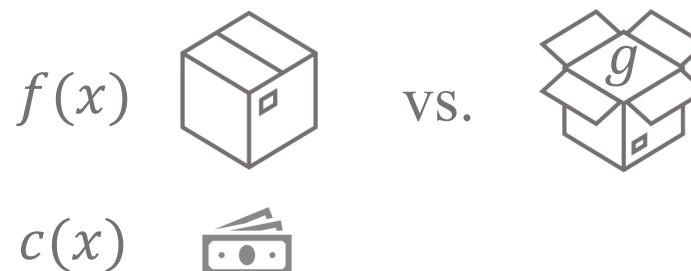


$$\text{EI}_{f|D}(x) := \mathbb{E}[\max(f(x) - y_{\text{best}}, 0) \mid D]$$

# Gittins Index

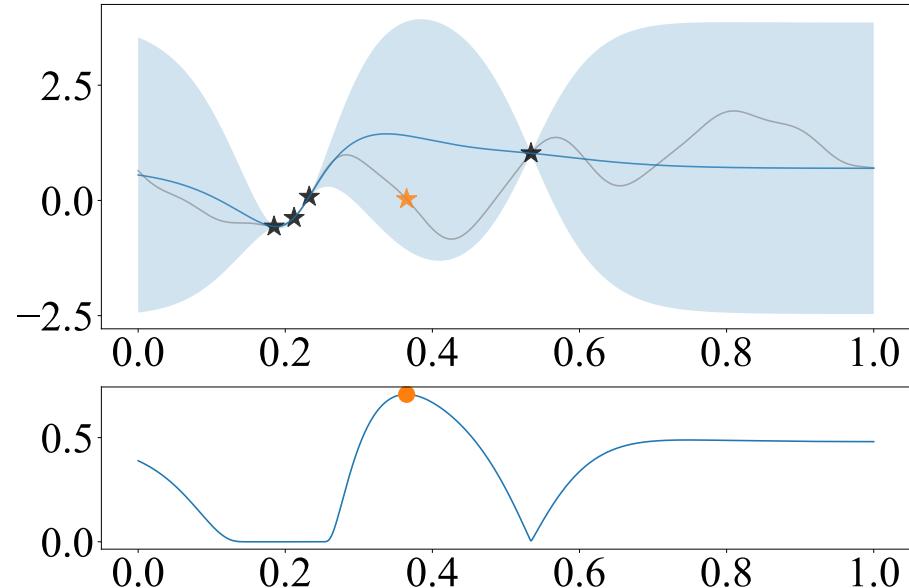


$$\begin{aligned} \text{GI}_{f|D}(x; c) &:= \text{solution } g \text{ s.t. } \text{EI}_{f|D}(x; g) = c(x) \\ \text{where } \text{EI}_{f|D}(x; g) &:= \mathbb{E}[\max(f(x) - g, 0) \mid D] \end{aligned}$$



Exploration      Exploitation

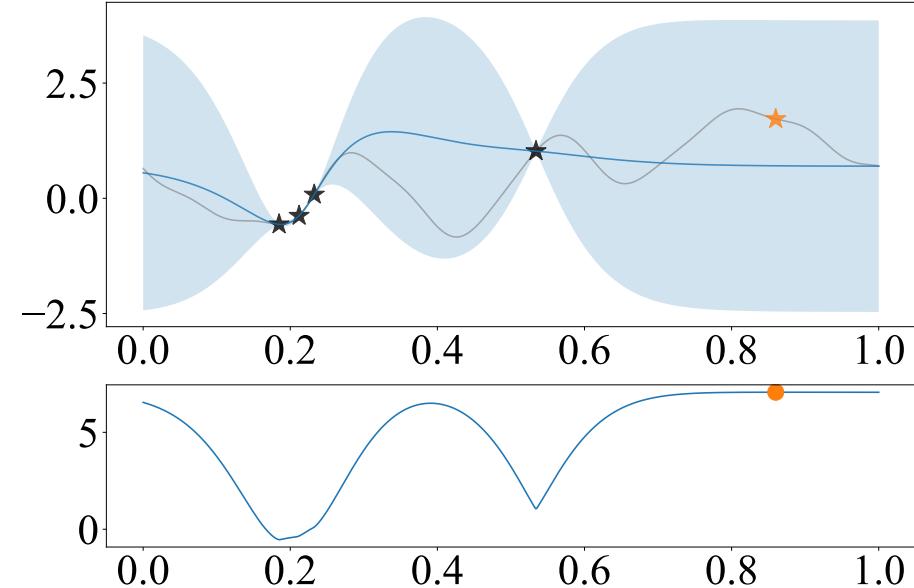
# Expected Improvement



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

Temporal simplification to MDP  
(One-step)

# Gittins Index

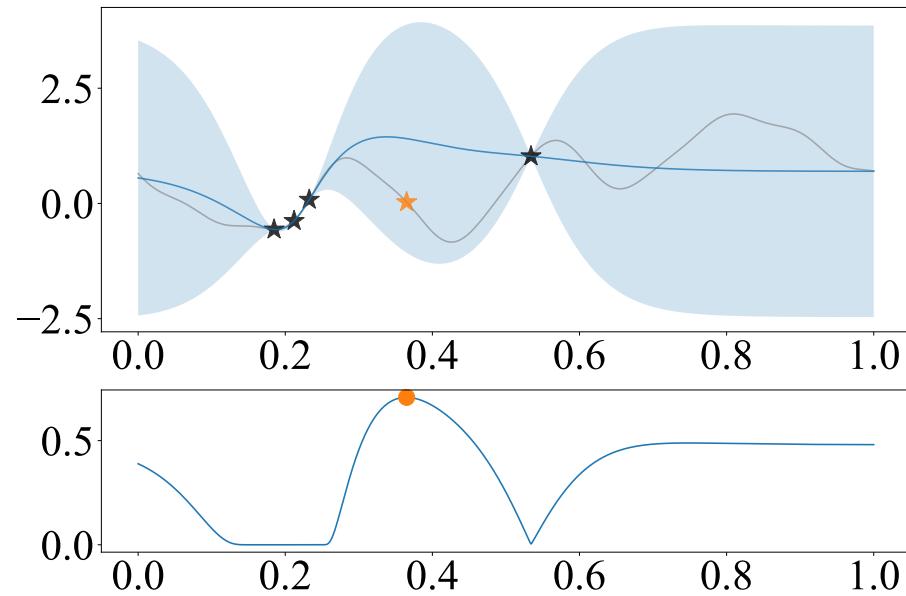


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Spatial simplification to MDP

# Expected Improvement



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

Temporal simplification to MDP

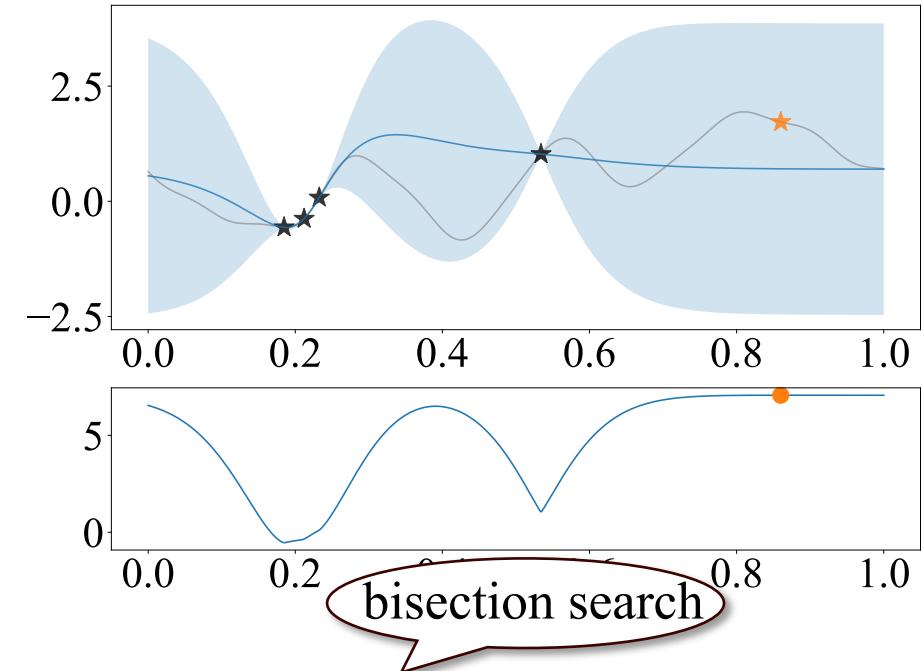


Both are principled and easy-to-compute!



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

# Gittins Index



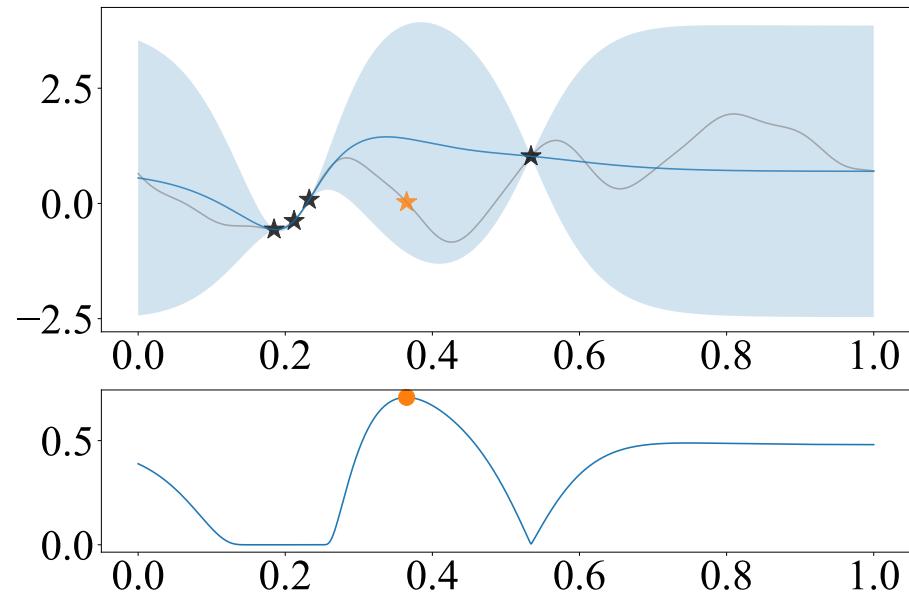
$$\text{GI}_{f|D}(x; c) := \text{solution } g \text{ s.t. } \text{EI}_{f|D}(x; g) = c(x)$$

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

analytical expression

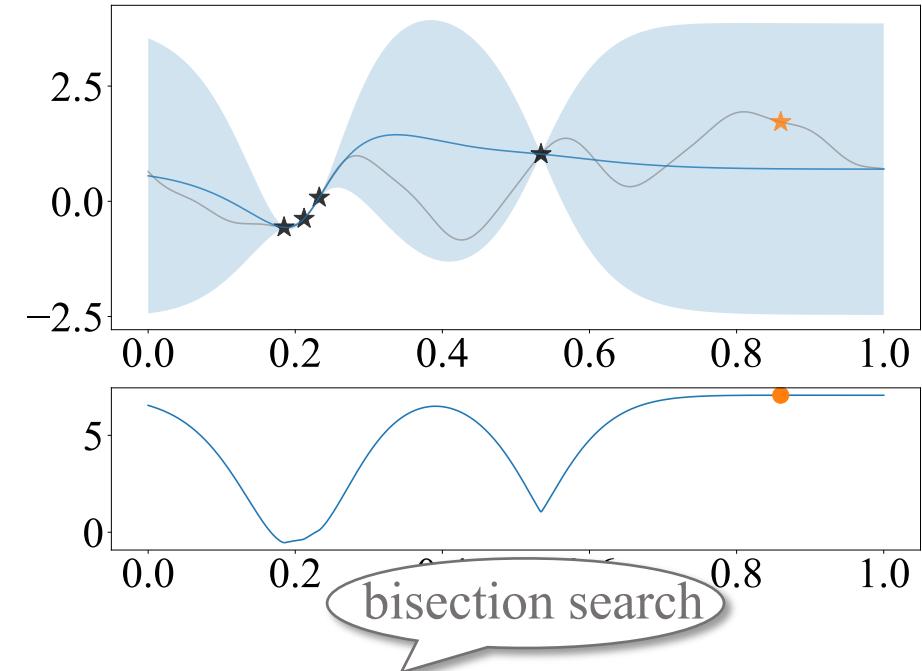
Spatial simplification to MDP

# 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

hard to discover GI

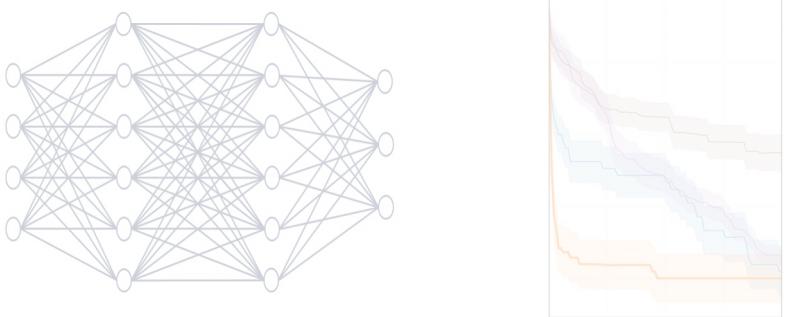
# Our Contribution: Gittins Index Principle

Novel connection



Link to Pandora's Box problem  
& Gittins index theory

Competitive empirical performance



Interests from practitioners (e.g., Meta)

Principled decision rules

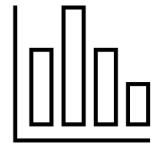
- Varying evaluation costs
- Adaptive stopping time

Unified framework for  
selection and stopping

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

Application to efficient LLM

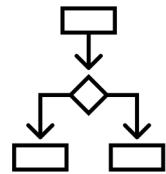
# Under-explored Information for Better Decisions



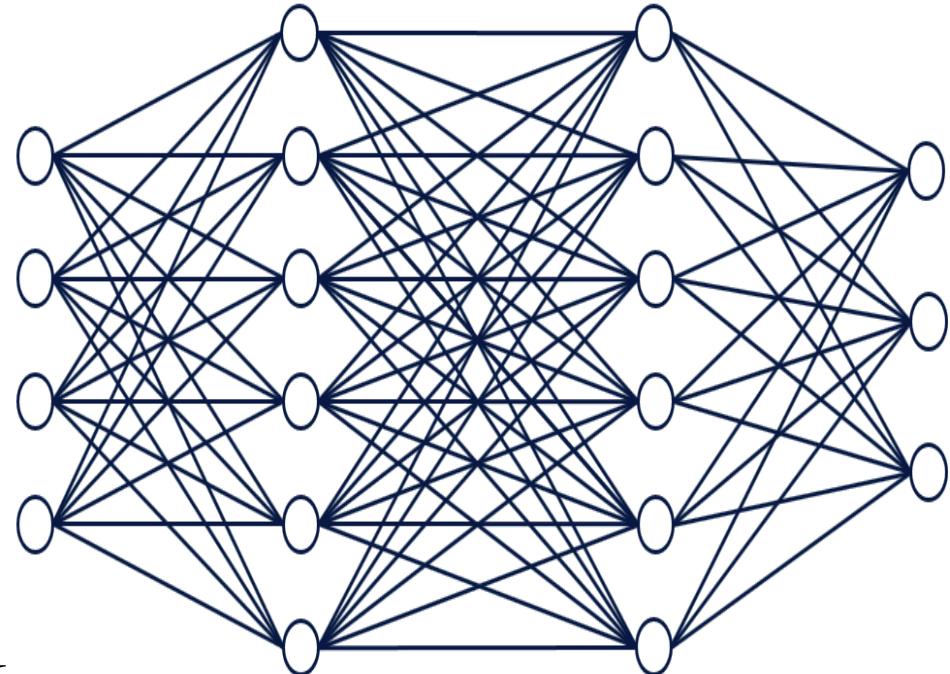
Varying evaluation costs



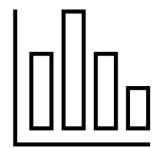
Smart stopping time



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

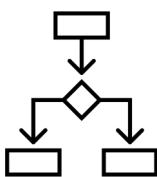
$$\tau: \text{EI}(x_\tau) \leq \theta$$

[Locatelli'97,

Nguyen et al.'17,

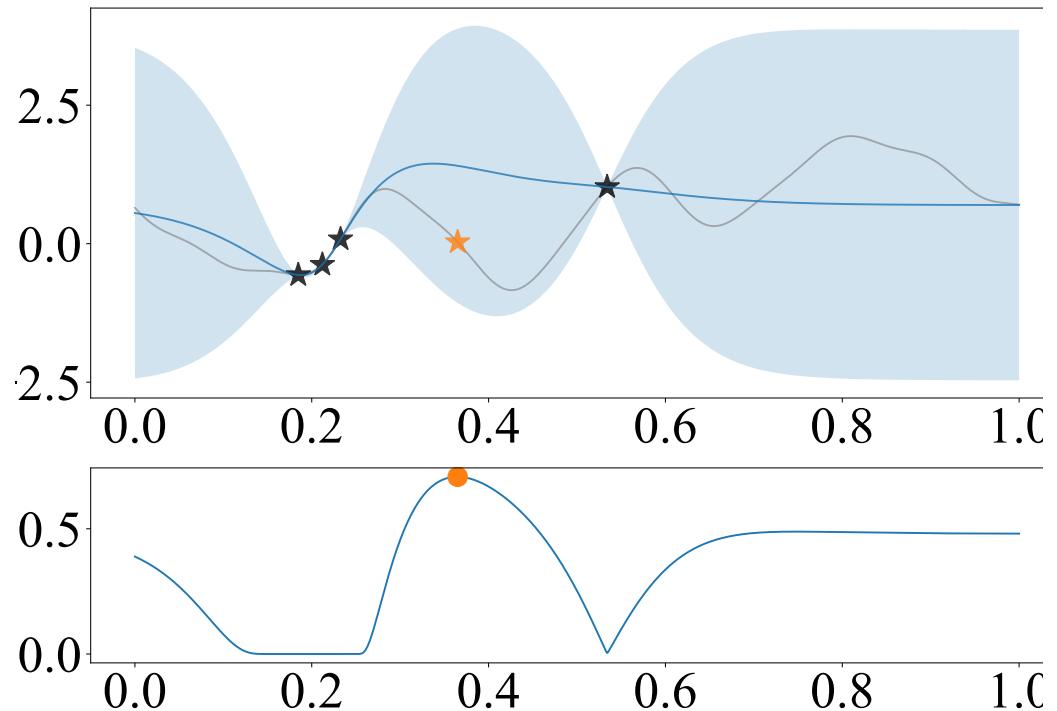
Ishibashi et al.'23]

Which threshold?



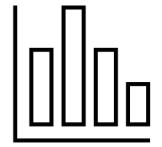
Observable multi-stage feedback

?



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

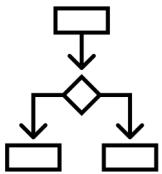
# Under-explored Information for Better Decisions



Varying evaluation costs



Smart stopping time



Observable multi-stage feedback



New design principle:  
**Gittins index**

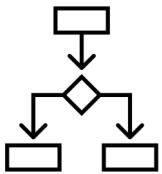
# Why Gittins index?



Varying evaluation costs



Smart stopping time

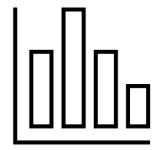


Observable multi-stage feedback

New design principle:  
Gittins index

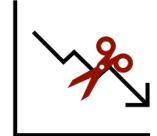
**Optimal** in related sequential  
decision problems

# Why Gittins index?



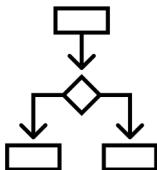
Varying evaluation costs

Features in **Pandora's box**



Smart stopping time

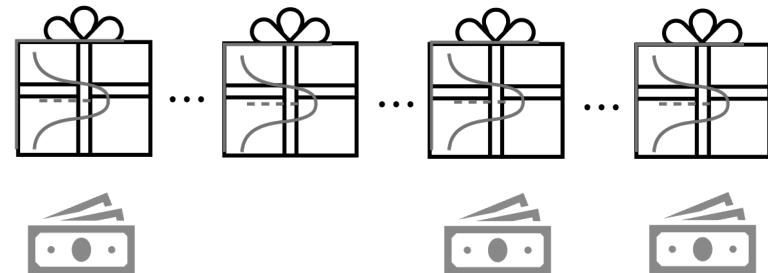
Features in **Pandora's box**



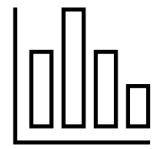
Observable multi-stage feedback

New design principle:  
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Optimal in related sequential  
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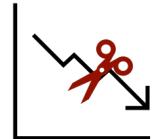


# Why Gittins index?



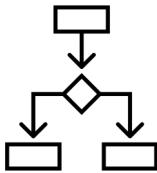
Varying evaluation costs

Features in Pandora's box



Smart stopping time

Features in Pandora's box

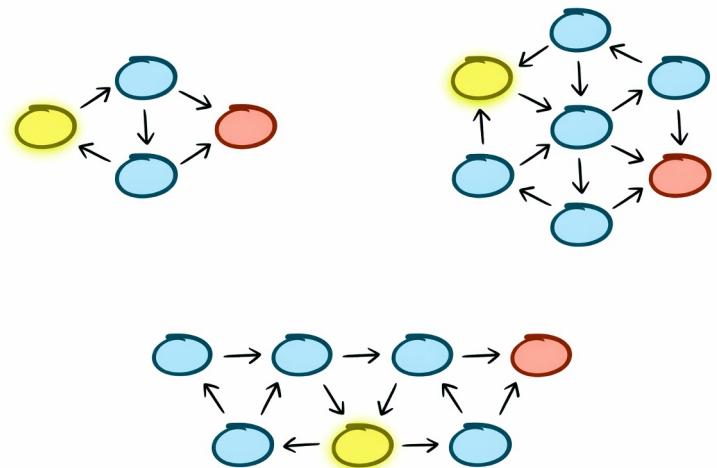


Observable multi-stage feedback

Features in Markov chain selection

New design principle:  
Gittins index

Optimal in related sequential  
decision problems

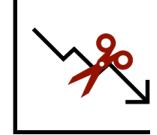


# Why Gittins index?



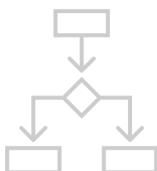
Varying evaluation costs

Features in **Pandora's box**



Smart stopping time

Features in **Pandora's box**



Observable multi-stage feedback

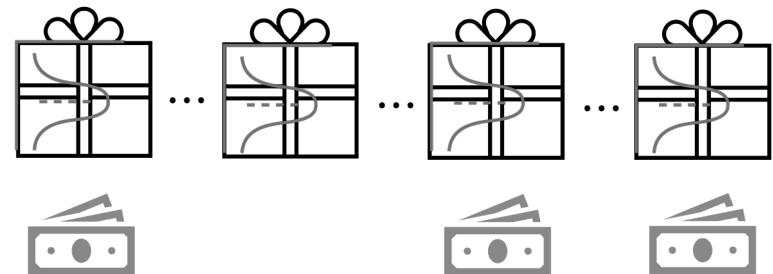
Features in Markov chain selection



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

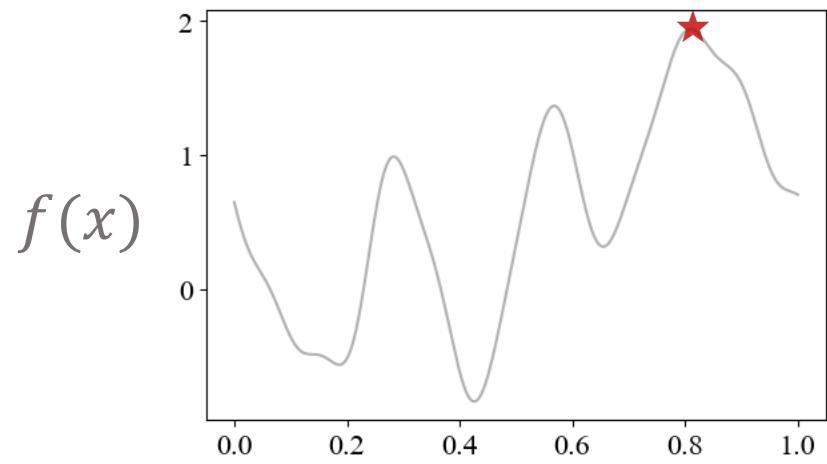
New design principle:  
Gittins index

Optimal in related sequential  
decision problems



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

# Bayesian Optimization



Continuous

Correlated

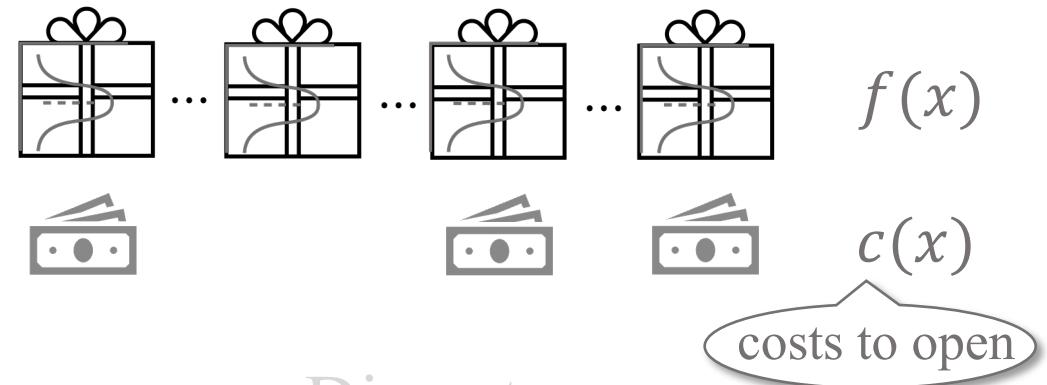
Cost-unaware

Fixed-iteration

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

# Pandora's Box

[Weitzman'79]



Discrete

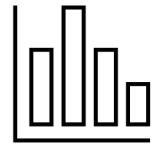
Independent

Cost-aware

Flexible-stopping

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

# Expected Improvement vs Gittins Index



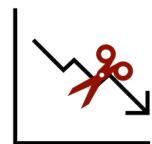
Varying evaluation costs

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

Arbitrarily bad

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

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:

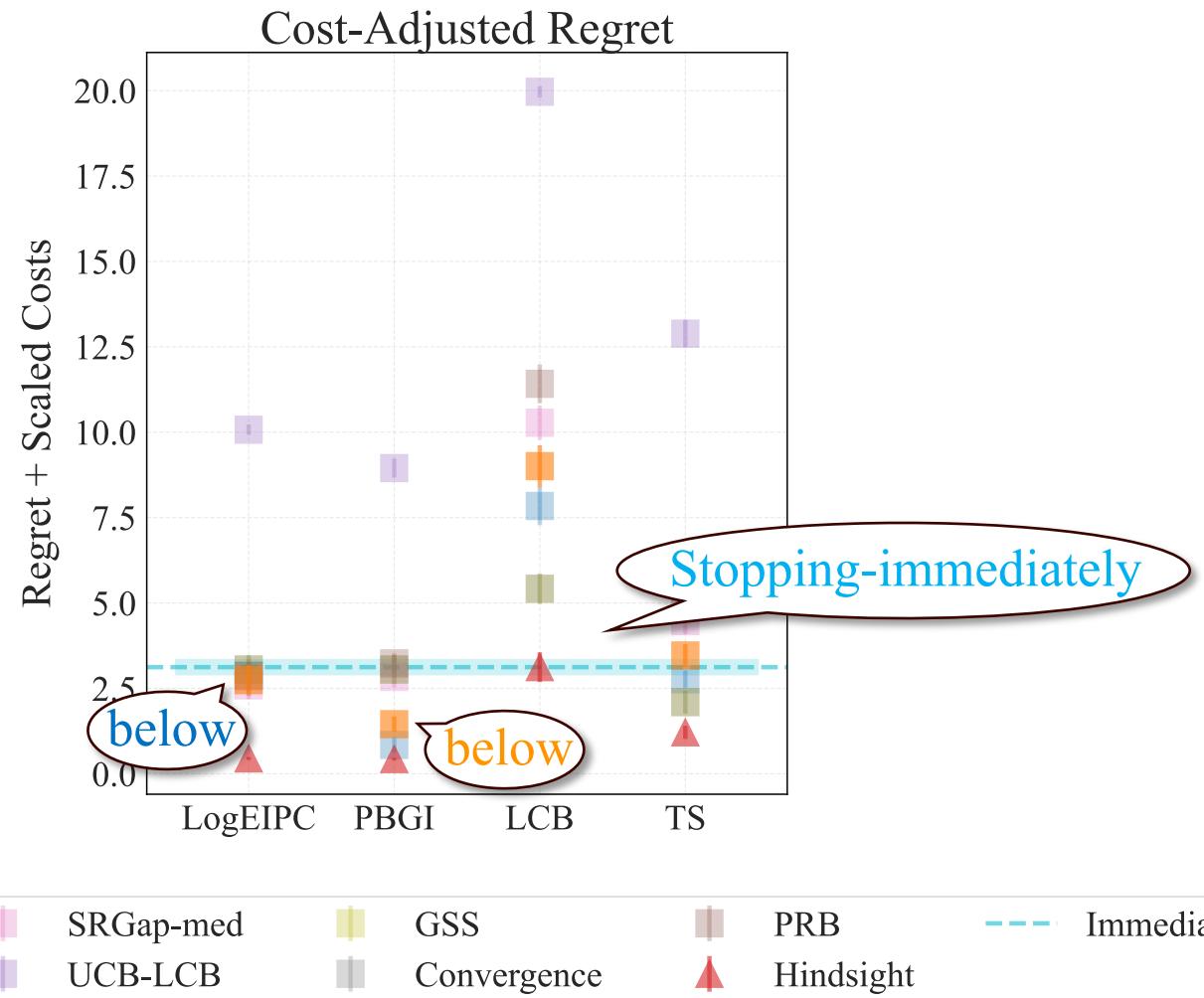
- Matches the **best achievable performance in the worst case** (evaluations are all very costly).
- Avoids **over-spending** — a property many cost-unaware stopping rules lack.

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



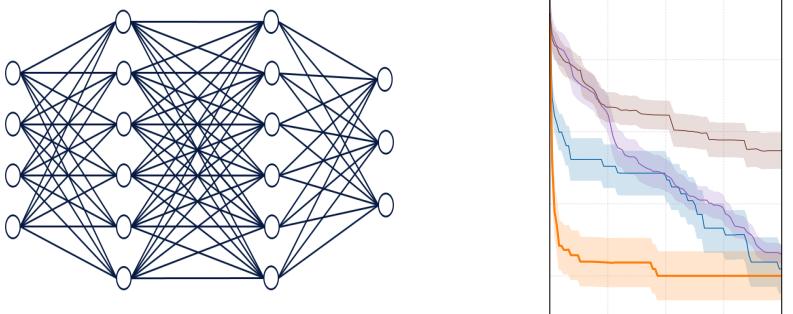
Link to Pandora's Box problem  
& Gittins index theory

Principled decision rules

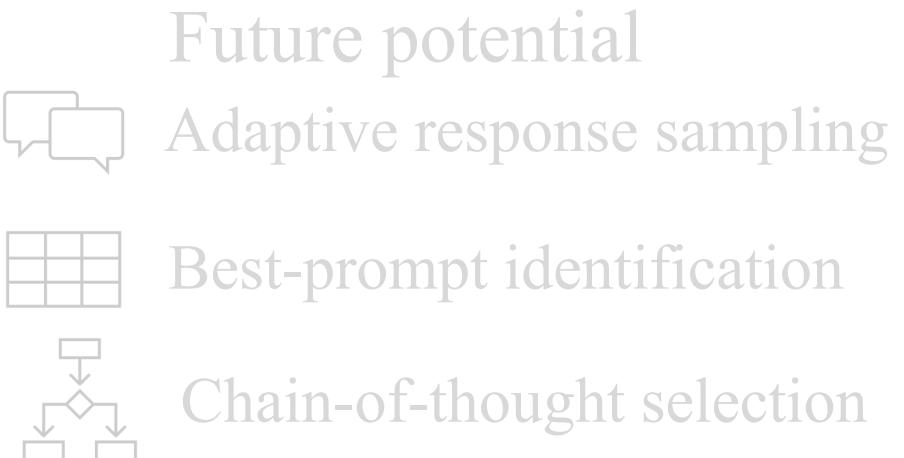


Unified framework for  
selection and stopping

## Competitive empirical performance

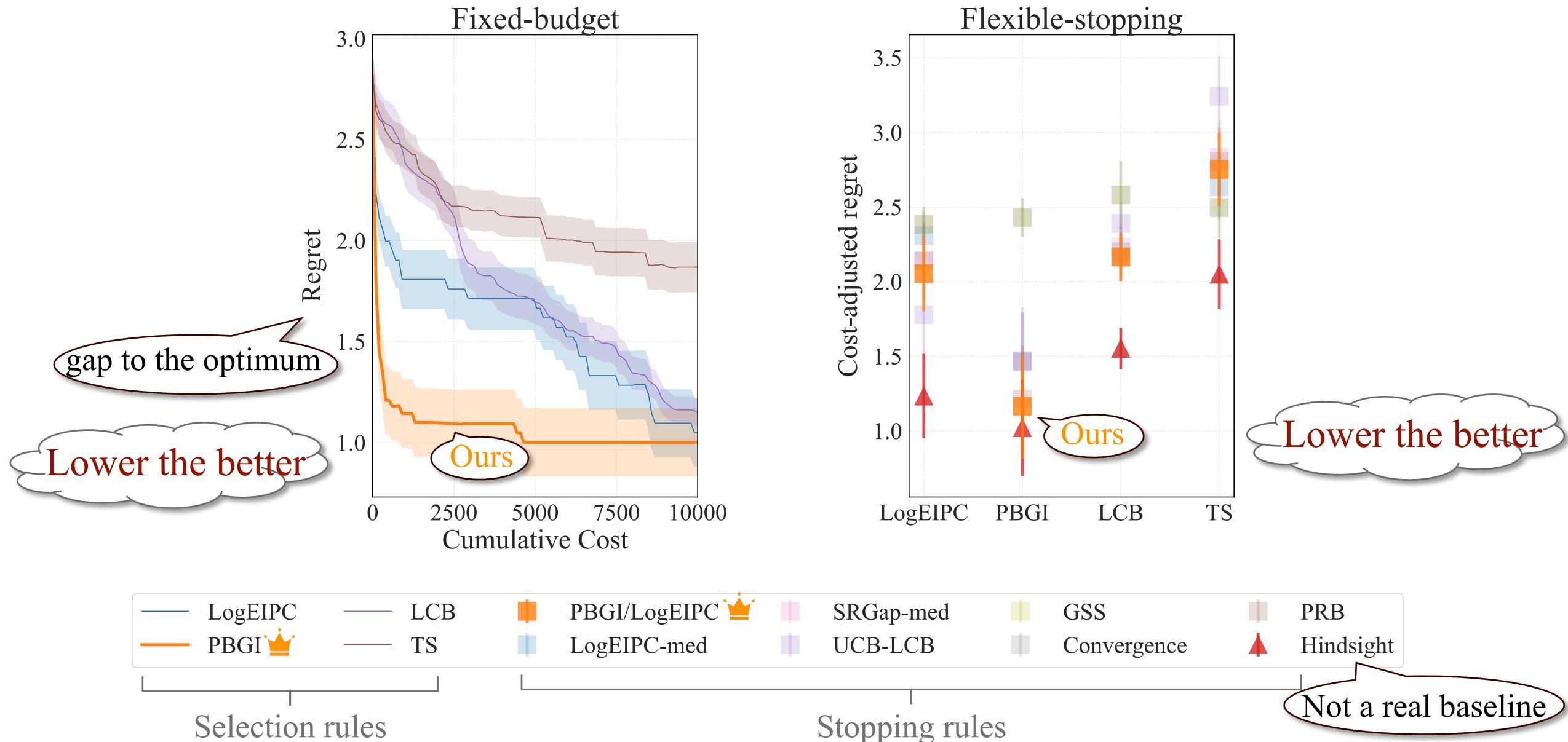


Interests from practitioners (e.g., Meta)



Application to efficient LLM

# Gittins Index vs Baselines on AutoML Benchmark



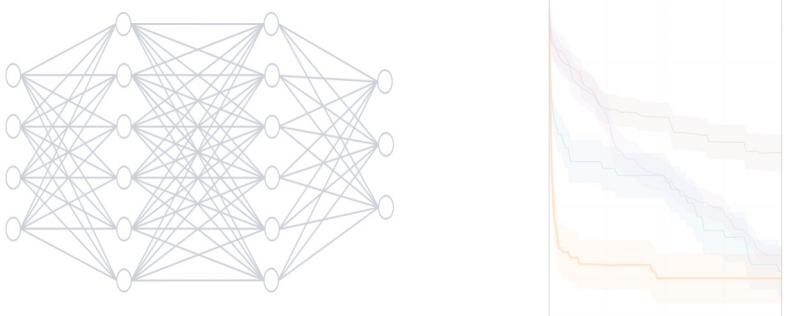
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Link to Pandora's Box problem  
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Competitive empirical performance



Interests from practitioners (e.g., Meta)

Principled decision rules

- Varying evaluation costs
- Adaptive stopping time

Unified framework for cost-aware selection and stopping

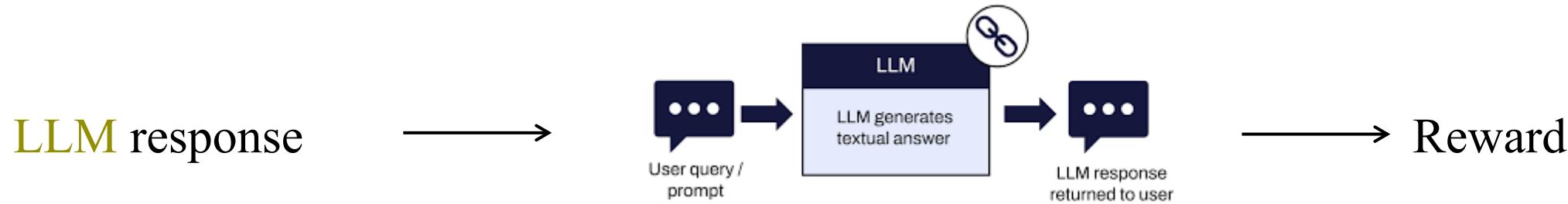
Future potential

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

Application to efficient LLM

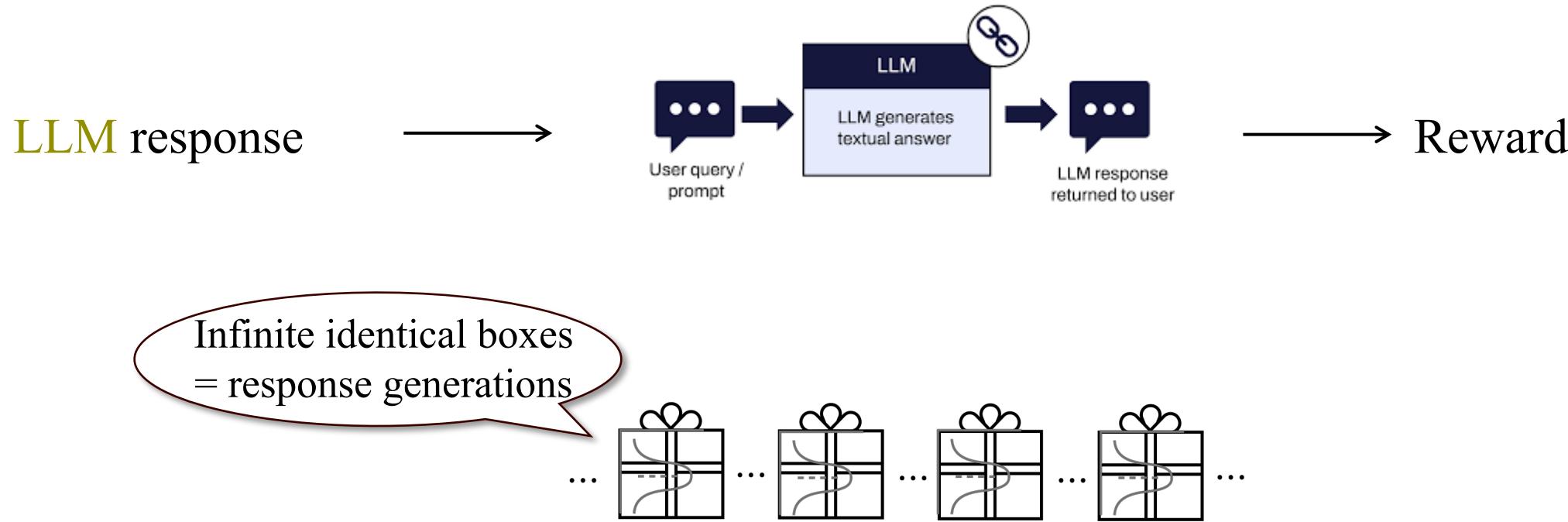
# Adaptive Response Sampling in LLM Inference

LLM inference time alignment (optimization):



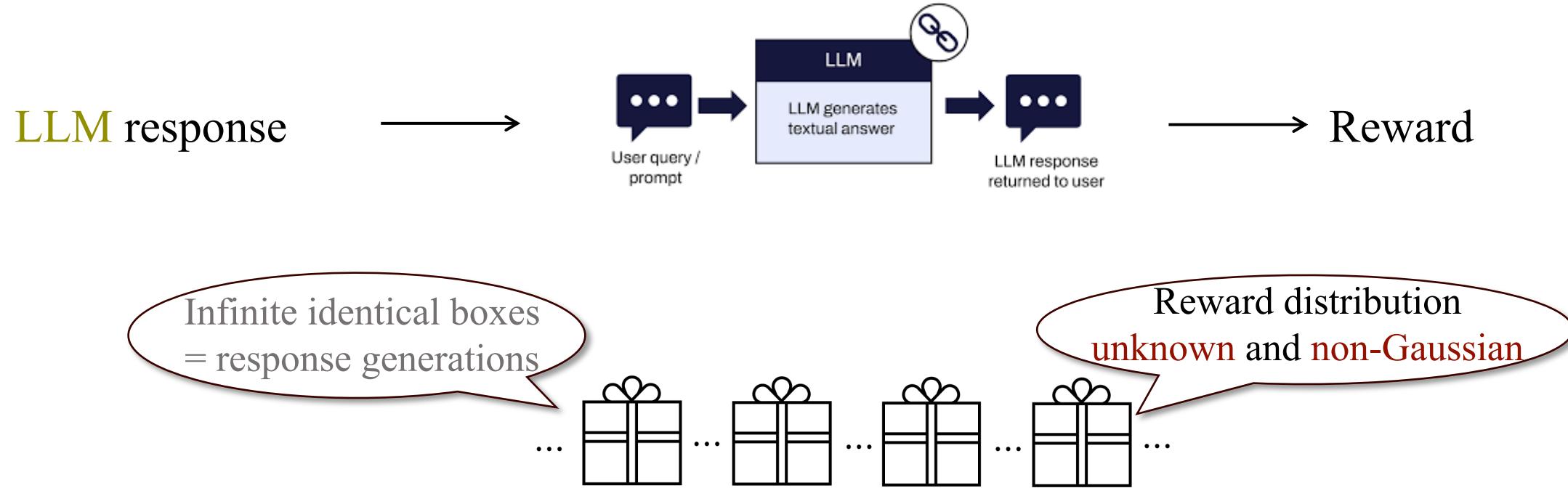
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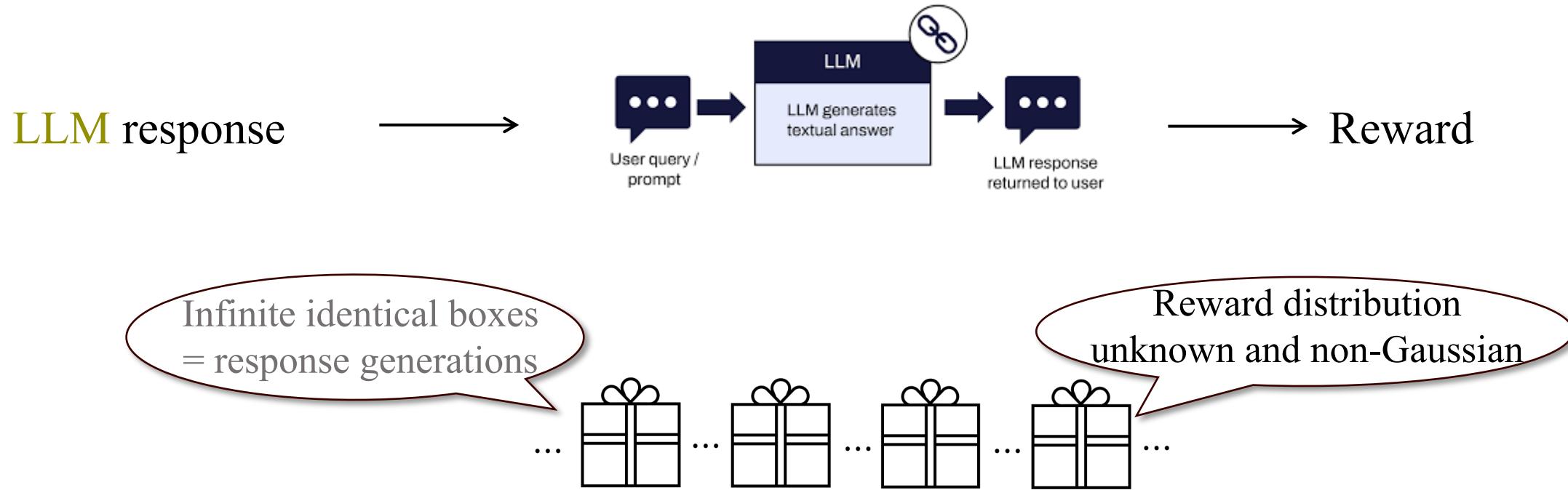
Adaptive stopping vs. fixed budget (best-of- $N$ )  
(Kalayci et al. 2025)

# Adaptive Response Sampling in LLM Inference



Adaptive stopping vs. fixed budget (best-of- $N$ )  
(Kalayci et al. 2025)

# Adaptive Response Sampling in LLM Inference



Adaptive stopping vs. fixed budget (best-of- $N$ )  
(Kalayci et al. '25)

Ours: model-free stopping  
via meta learning

# Best-prompt Identification in LLM Evaluation

LLM multi-prompt evaluation:

Prompt template  
for each LLM



	Zero-shot	Few-shot	CoT	RAG	Revise
ChatGPT (GPT-4.1)	★★★★★	★★★★★	★★★★★	★★★★★	★★★★★
Claude 3.5 Sonnet	★★★★★	★★★★★	★★★★★		★★★★★
Gemini 1.5 Pro	★★★★★	★★★	?	★★★★	★★★★★
deepseek	?	?	★★★★	?	★★★★
Llama 3.1-70B	?	?	★★★★	?	★★★
Mistral Large	?	?	★★★	?	★

Average performance  
of (LLM, prompt) pairs

# Best-prompt Identification in LLM Evaluation

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Gemini 1.5 Pro	★★★★★	★★★	?	★★★	★★★★★
deepseek	?	?	★★★	?	★★★
Llama 3.1-70B	?	?	★★★	?	★★★
Mistral Large	?	?	★★★	?	★

Average performance  
of (LLM, prompt) pairs

Prompt/ Question	Q1	Q2	Q3	...	Predicted avg performance
Prompt 1	1	$\hat{P}_{12}$	$\hat{P}_{13}$	...	$\widehat{\text{perf}}_1$
Prompt 2	$\hat{P}_{21}$	1	$\hat{P}_{23}$	...	$\widehat{\text{perf}}_2$
Prompt 3	1	$\hat{P}_{32}$	$\hat{P}_{33}$	...	$\widehat{\text{perf}}_3$
...	...	...	...	...	...

Matrix completion  
(Polo et al. NeurIPS'24)

# Best-prompt Identification in LLM Evaluation

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Gemini 1.5 Pro	★★★★★	★★★	?	★★★	★★★★★
deepseek	?	?	★★★	?	★★★
Llama 3.1-70B	?	?	★★★	?	★★★
Mistral Large	?	?	★★★	?	★

Average performance  
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Prompt 3	1	$\hat{P}_{32}$	$\hat{P}_{33}$	...	$\widehat{\text{perf}}_3$
...	...	...	...	...	...

Matrix completion  
(Polo et al. NeurIPS'24)

# Best-prompt Identification in LLM Evaluation

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Gemini 1.5 Pro	★★★★★	★★★	?	★★★	★★★★★
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Llama 3.1-70B	?	?	★★★	?	★★★
Mistral Large	?	?	★★★	?	★

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Prompt 3	1	$\hat{P}_{32}$	$\hat{P}_{33}$	...	$\widehat{\text{perf}}_3$
...	...	...	...	...	...

How about tensors?

Matrix completion  
(Polo et al. NeurIPS'24)

# Best-prompt Identification in LLM Evaluation

Prompt template  
for each LLM



	Zero-shot	Few-shot	CoT	RAG	Revise
ChatGPT (GPT-4.1)	★★★★★	★★★★★	★★★★★	★★★★★	★★★★★
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Gemini 1.5 Pro	★★★★★	★★★	?	★★★	★★★★★
deepseek	?	?	★★★	?	★★★
Llama 3.1-70B	?	?	★★★	?	★★★
Mistral Large	?	?	★★★	?	★

Average performance  
of (LLM, prompt) pairs

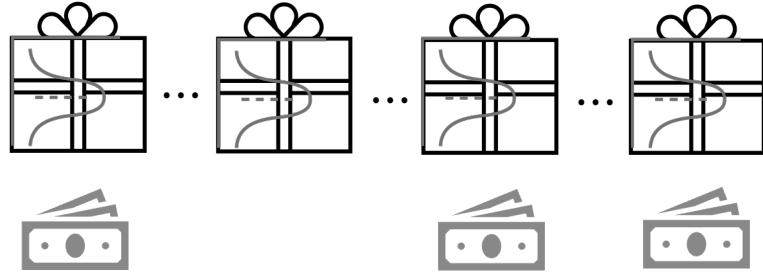
Boxes = entries



Applicable to tensors

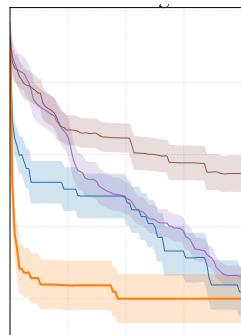
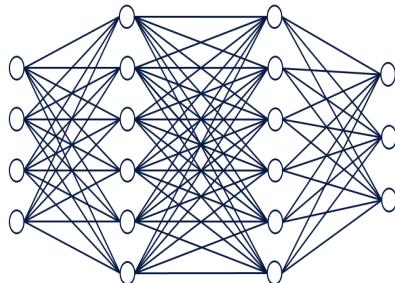
Ours: BayesOpt + Gittins  
(supports multi-selection)

## 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

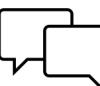


Varying evaluation costs

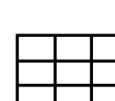


Adaptive stopping time

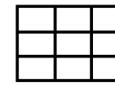
Unified framework for selection and stopping



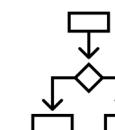
## Future potential



Adaptive response sampling



Best-prompt identification



Chain-of-thought selection



## Application to **efficient LLM**

"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.