

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) \longrightarrow



\longrightarrow Accuracy

Motivation: World of Optimization under Uncertainty

ML model training:

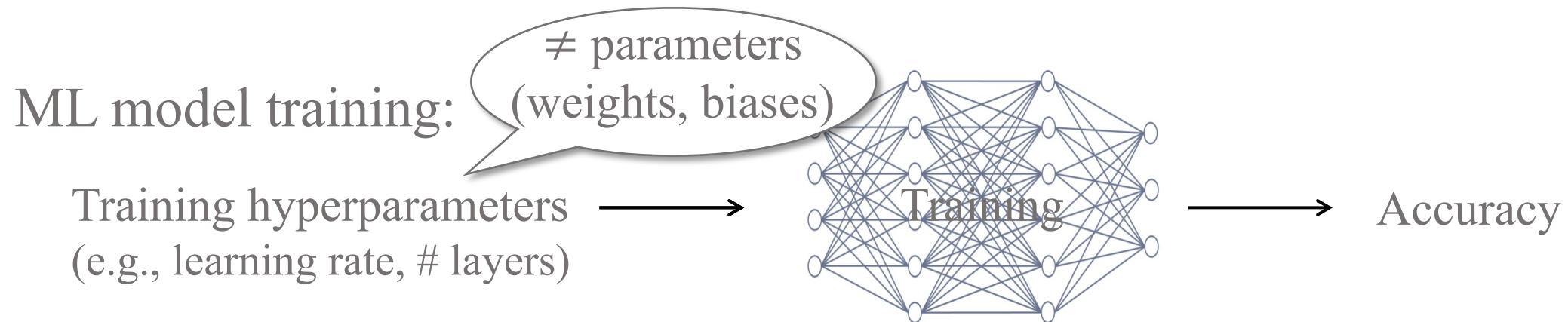
Training hyperparameters
(e.g., learning rate, # layers)

≠ parameters
(weights, biases)

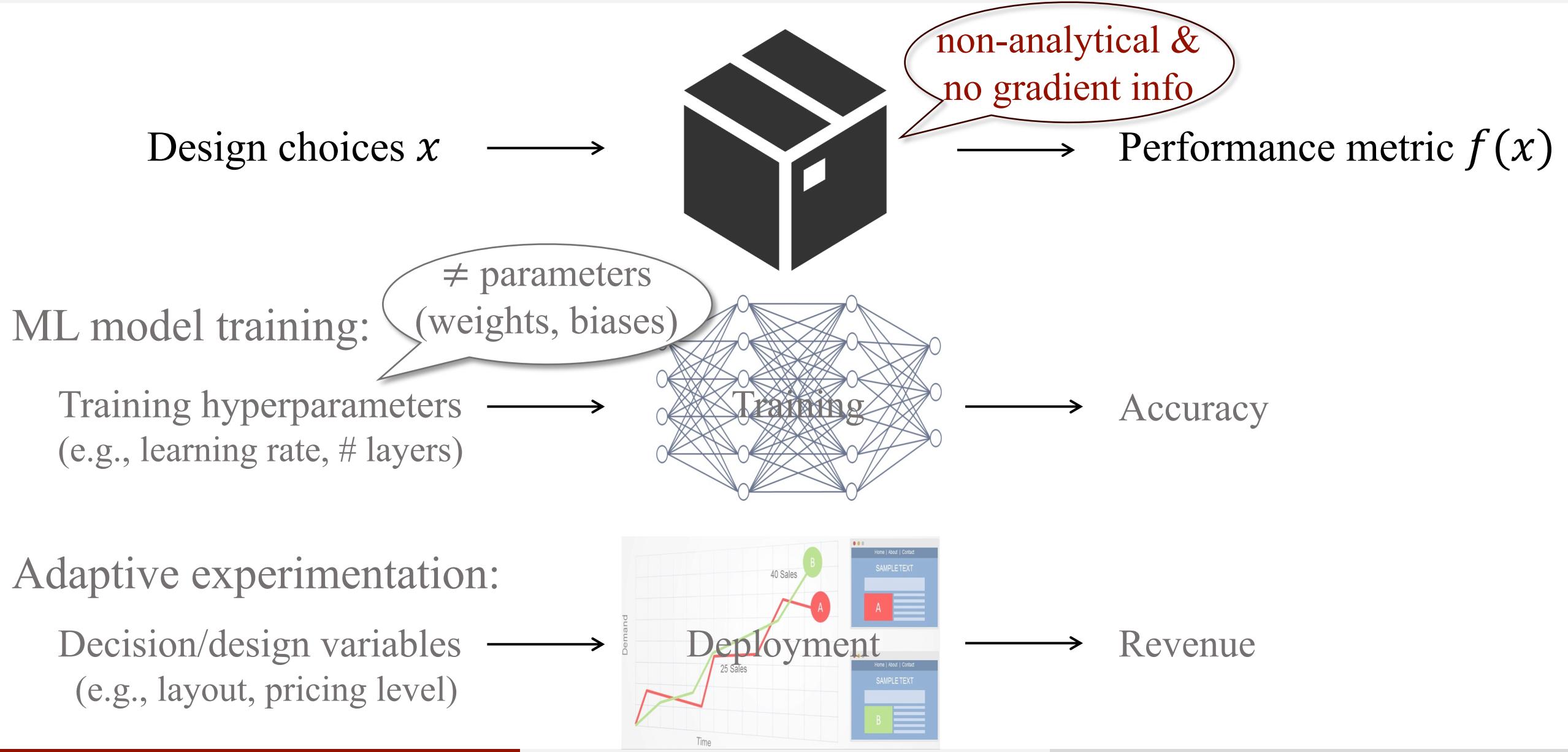


→ Accuracy

Motivation: World of Optimization under Uncertainty



Motivation: World of Optimization under Uncertainty



Motivation: World of Optimization under Uncertainty

Black-box optimization:

(gradient-based methods not applicable)

Input x \longrightarrow



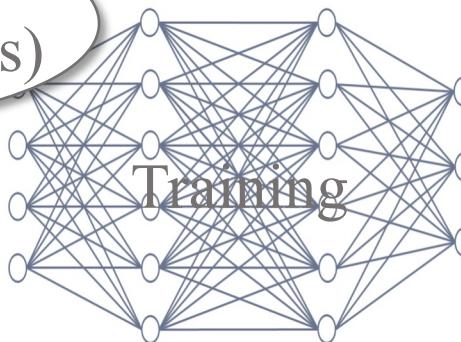
non-analytical &
no gradient info

Observed outcome $f(x)$

ML model training:

\neq parameters
(weights, biases)

Training hyperparameters
(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)

Input x →



expensive-to-evaluate

Observed outcome $f(x)$

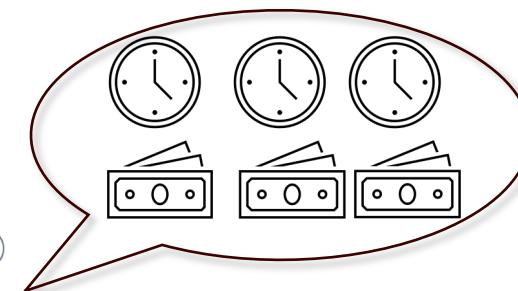
ML model training:

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



Training time

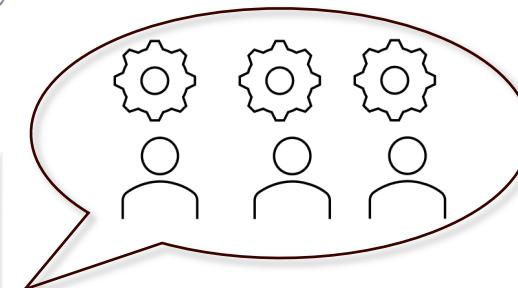
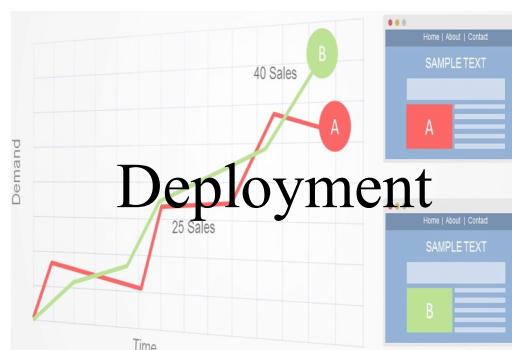
Compute credits



Accuracy

Adaptive experimentation:

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



Operational cost

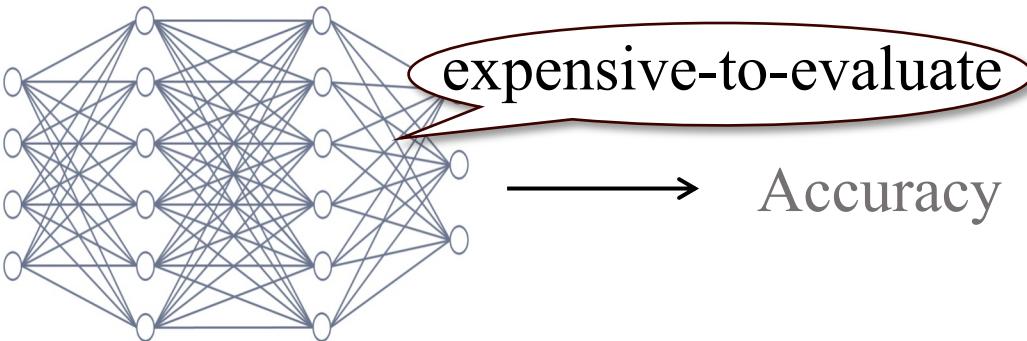
User experience

Revenue

Naïve (Non-Adaptive) Approach: Grid Search

ML model training:

Training hyperparameters

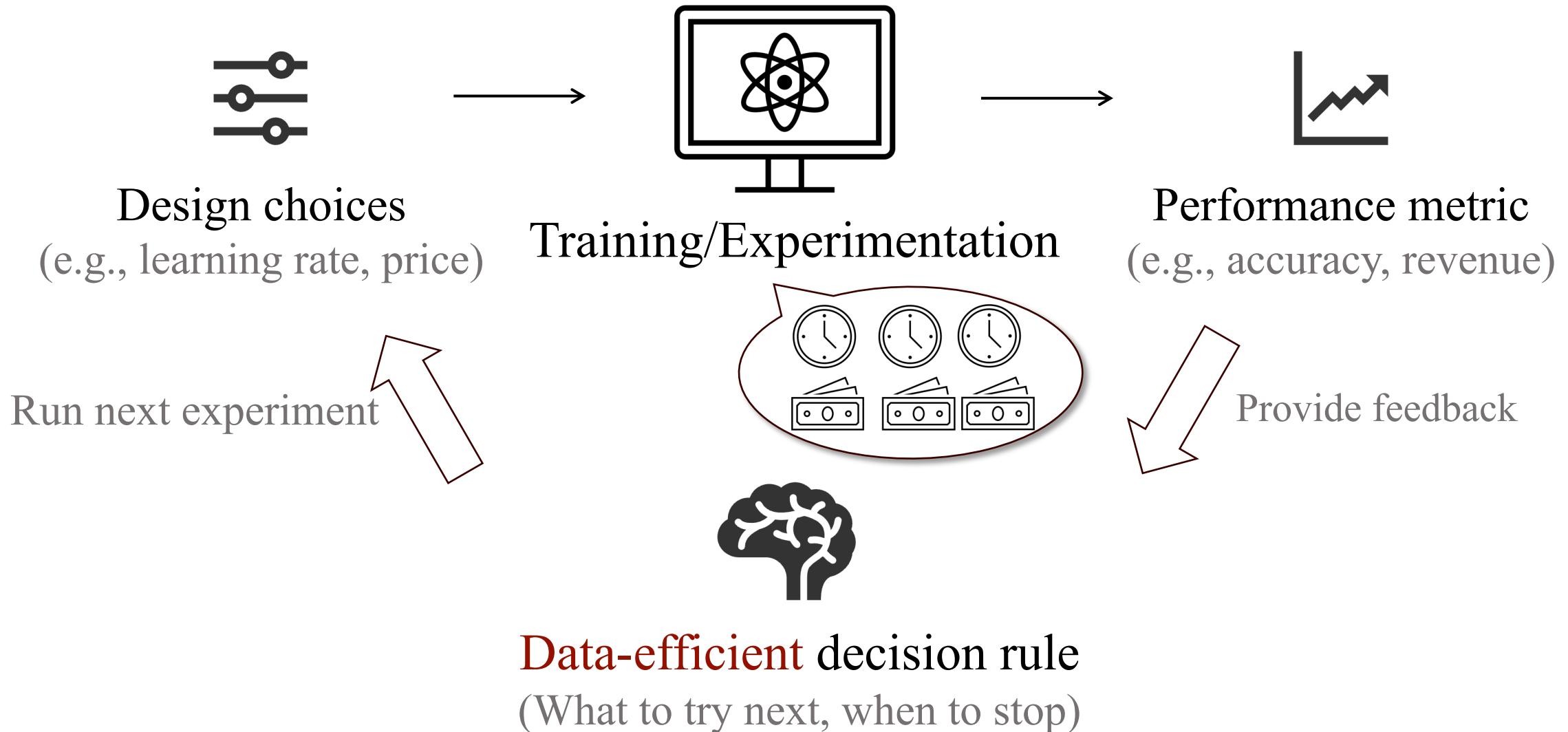


Accuracy

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!

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 ★
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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

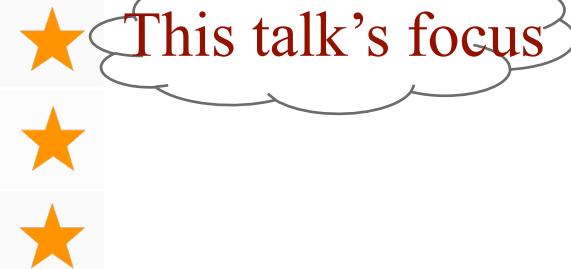
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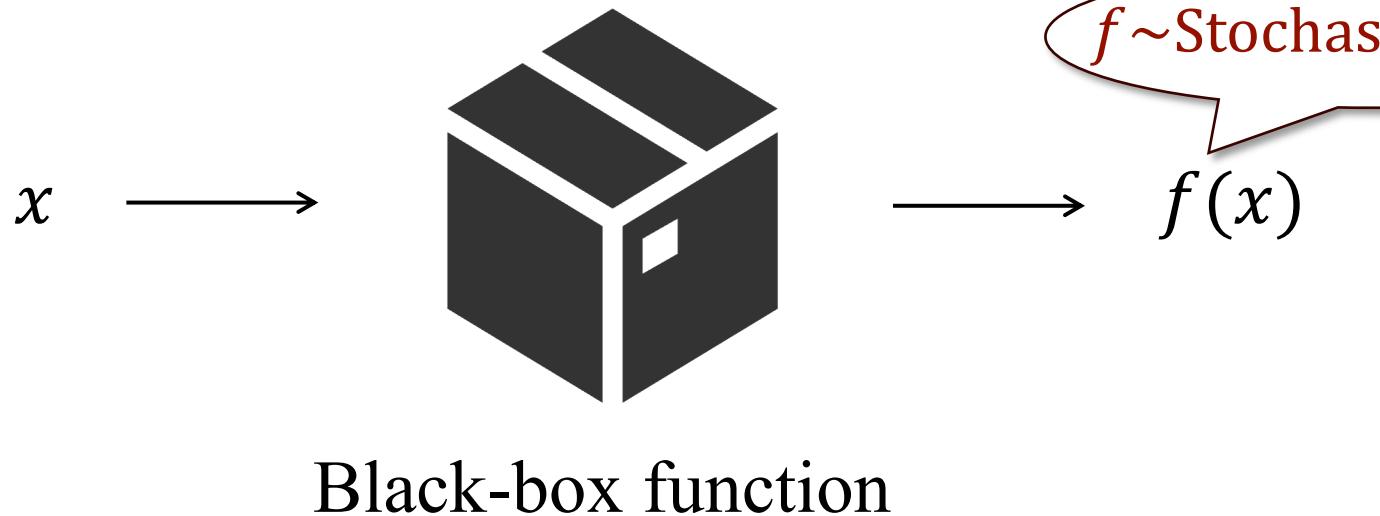


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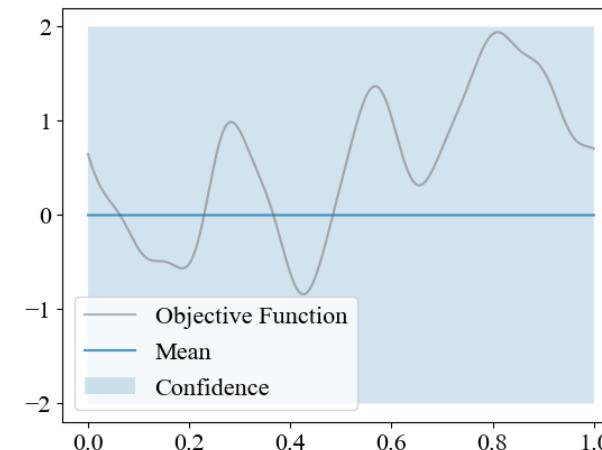
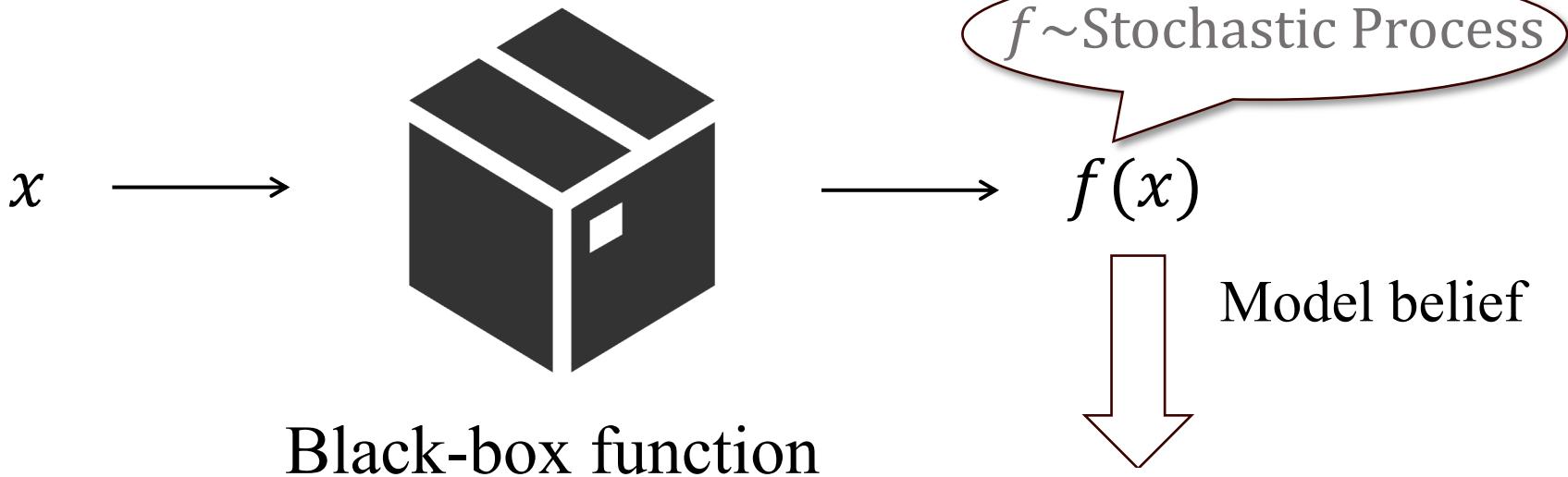
★ New methods under this umbrella

Bayesian Optimization



Bayesian Optimization

Time 0



Probabilistic model
(e.g., Gaussian process)

Bayesian Optimization

Time t

x_1, \dots, x_t

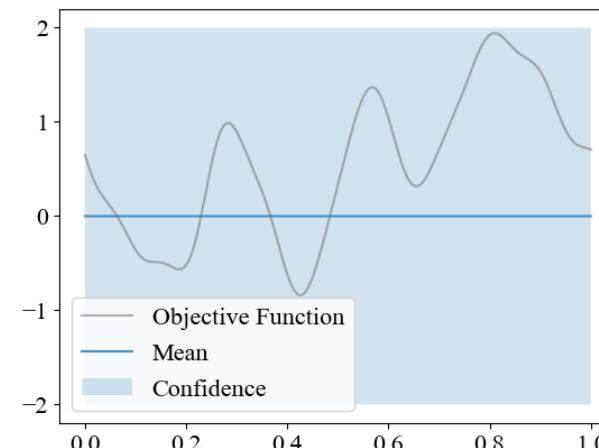


Black-box function

$f \sim \text{Stochastic Process}$

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

Model belief



Probabilistic model
(e.g., Gaussian process)

Bayesian Optimization

Time t

x_1, \dots, x_t \longrightarrow

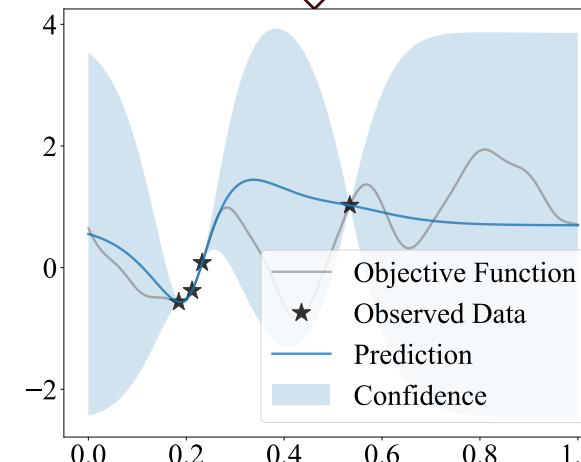


Black-box function

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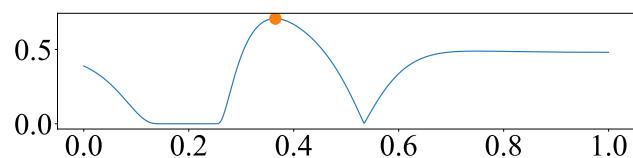
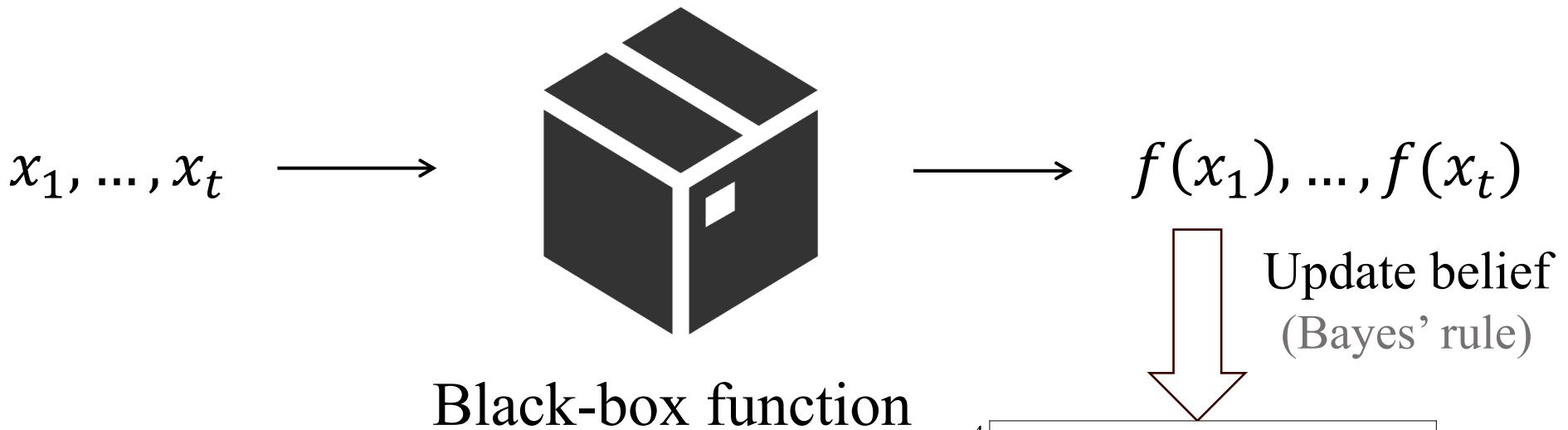
Update belief
(Bayes' rule)



Probabilistic model
(e.g., Gaussian process)

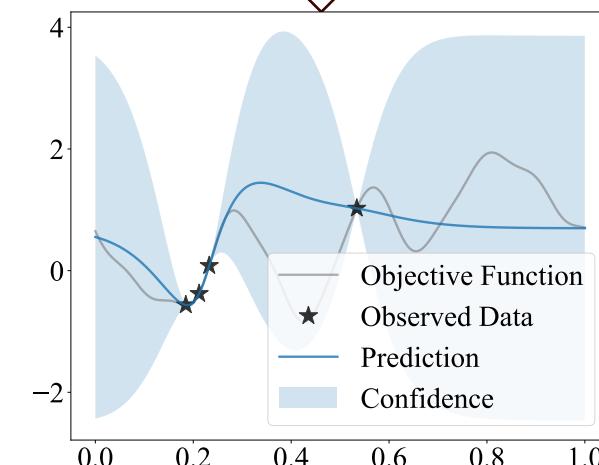
Bayesian Optimization

Time t



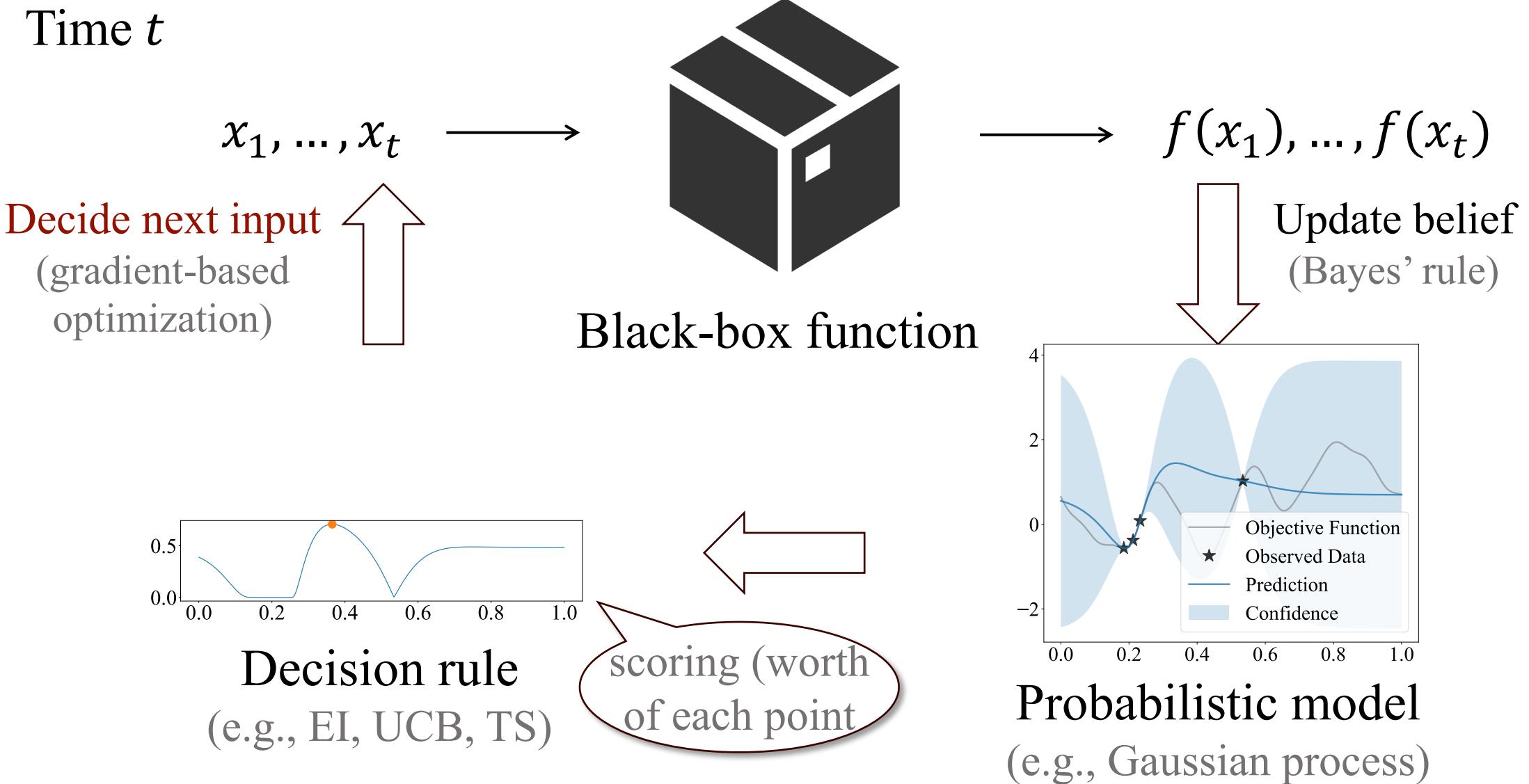
Decision rule
(e.g., EI, UCB, TS)

scoring (worth
of each point)

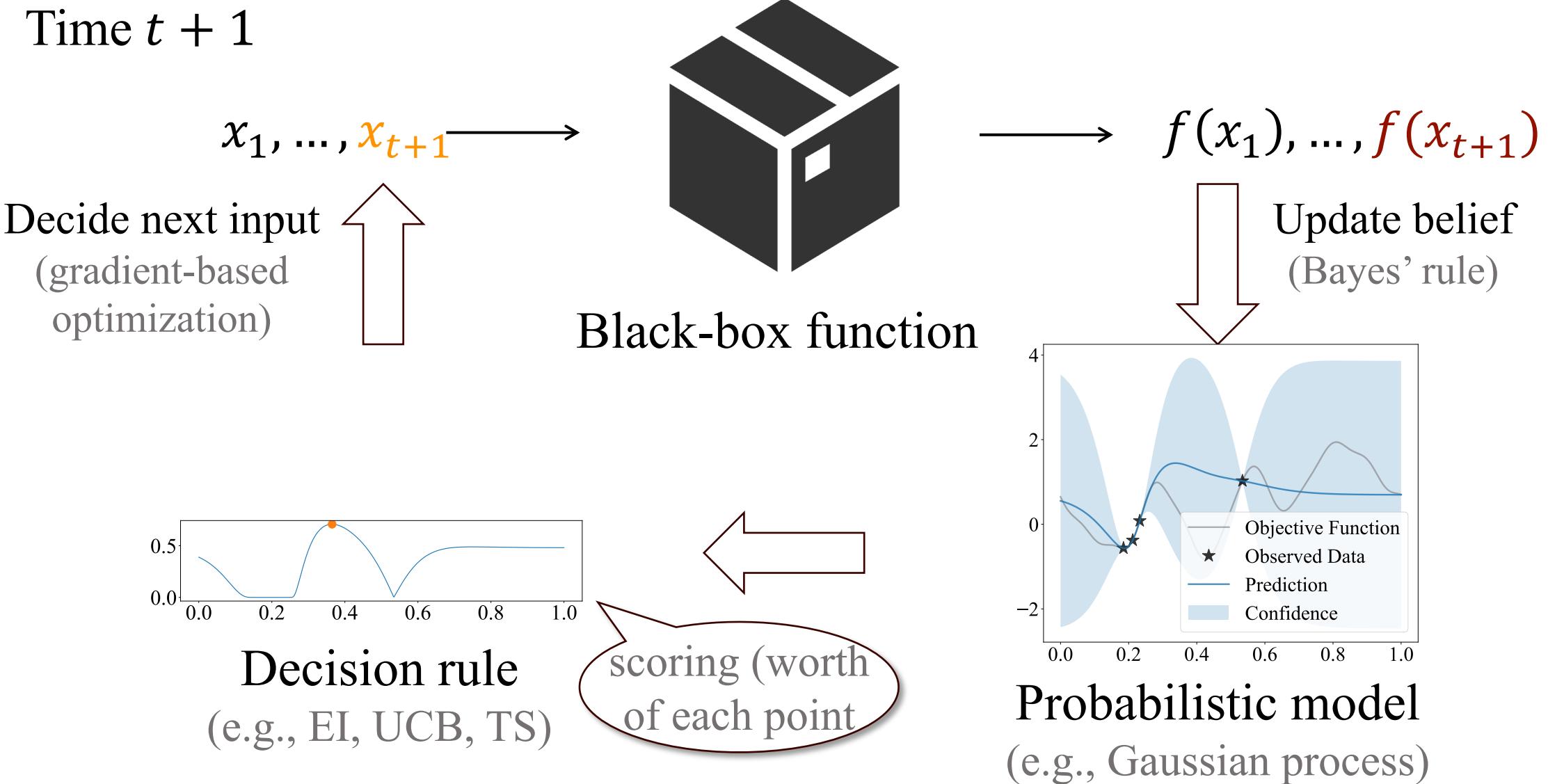


Probabilistic model
(e.g., Gaussian process)

Bayesian Optimization



Bayesian Optimization



Bayesian Optimization

Time $t + 1$

Decide next input
(gradient-based
optimization)

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

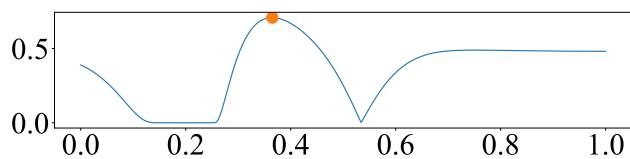


$f(x_1), \dots, f(x_{t+1})$

Update belief
(Bayes' rule)

Black-box function

My focus



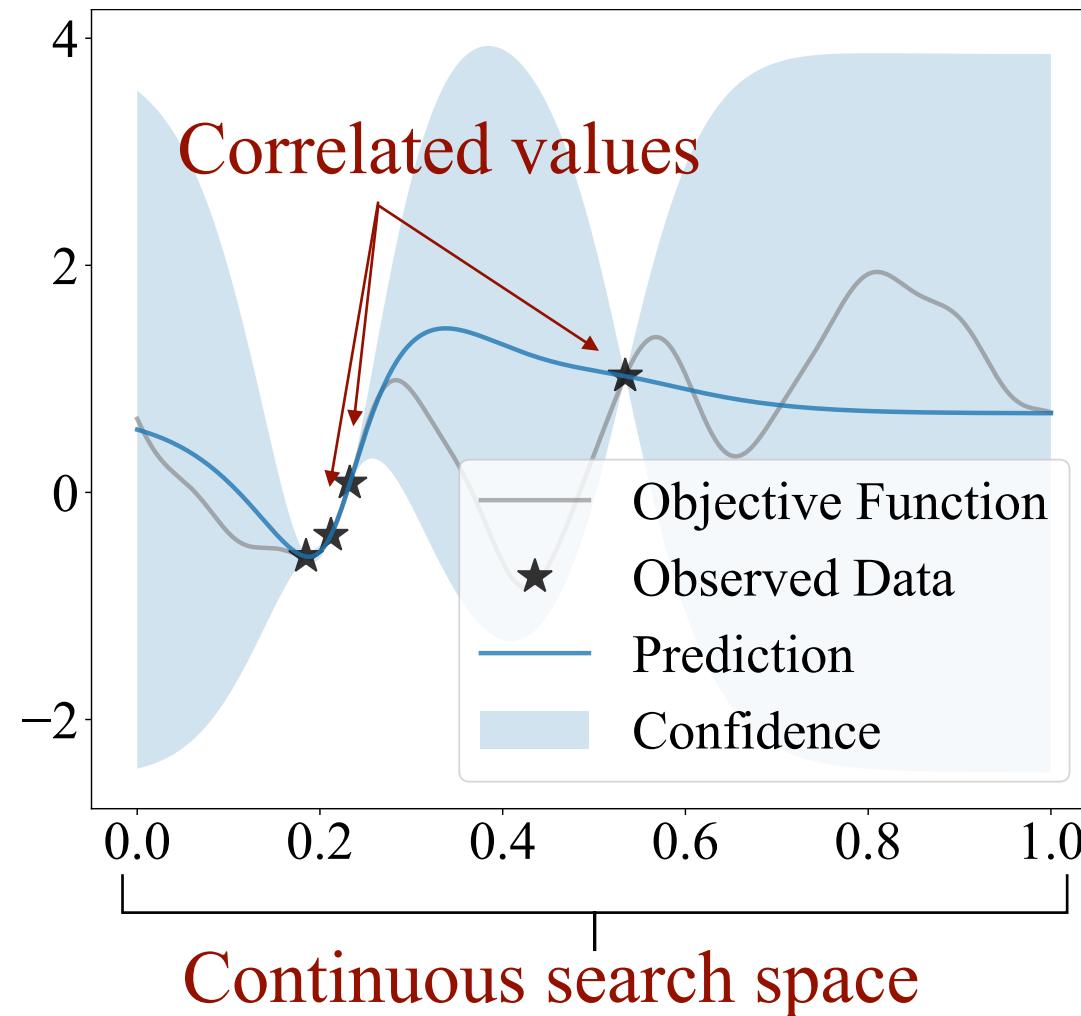
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Probabilistic model
(e.g., Gaussian process)

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”

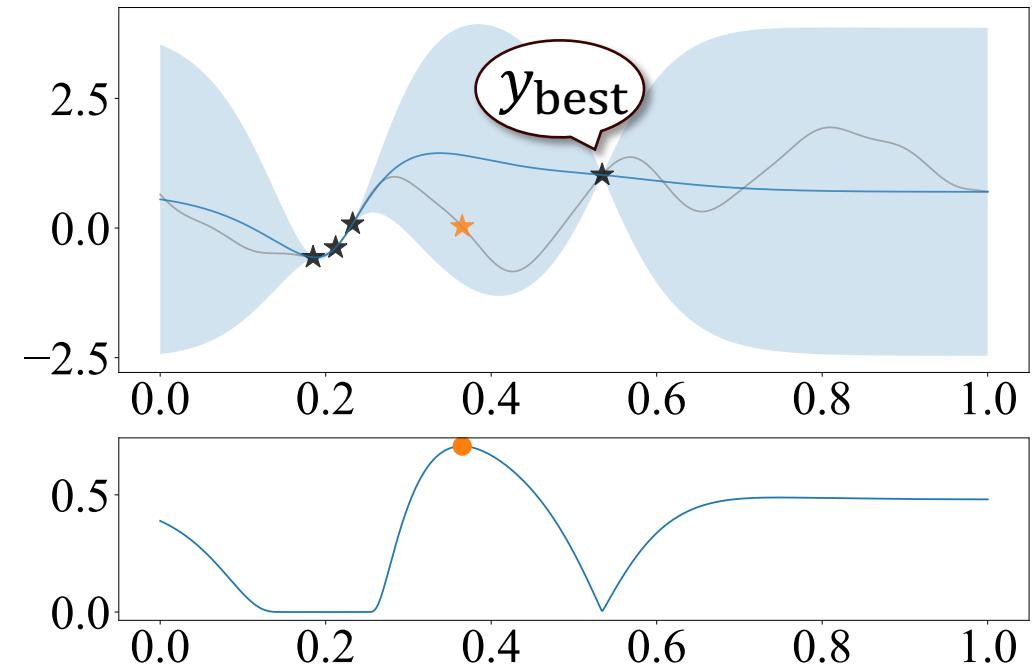
current best observed

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

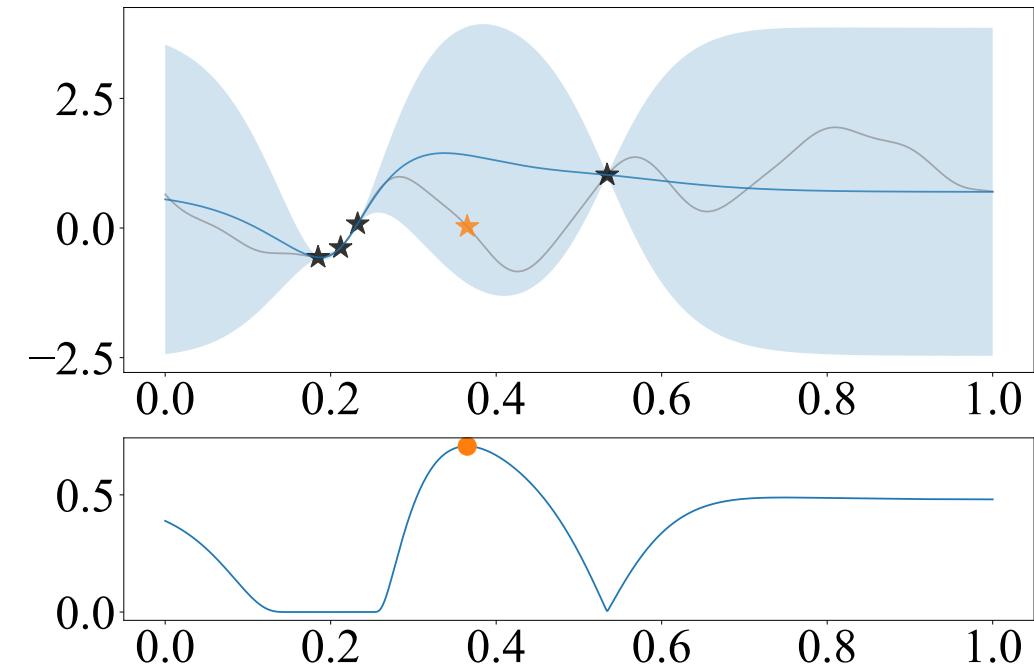
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current best observed
data D
“improvement”

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

posterior distribution

One-step approximation to MDP

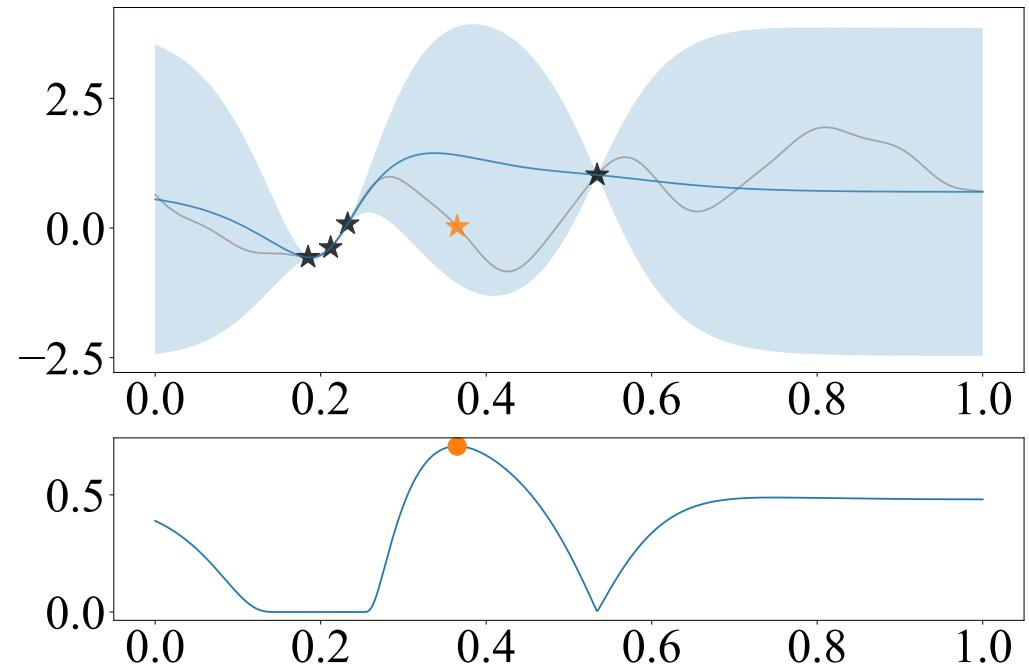


Expected improvement $EI(x)$

Improvement-based
design principle

Existing Design Principles

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

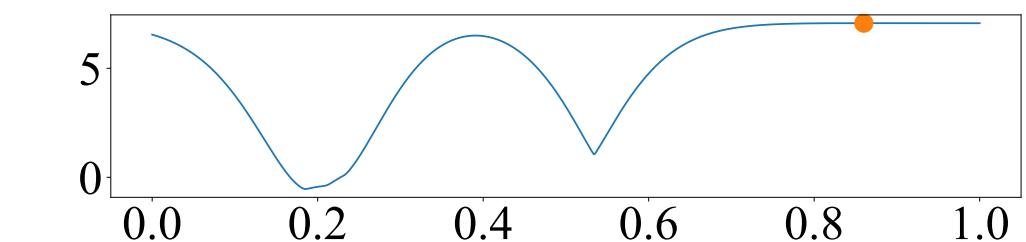
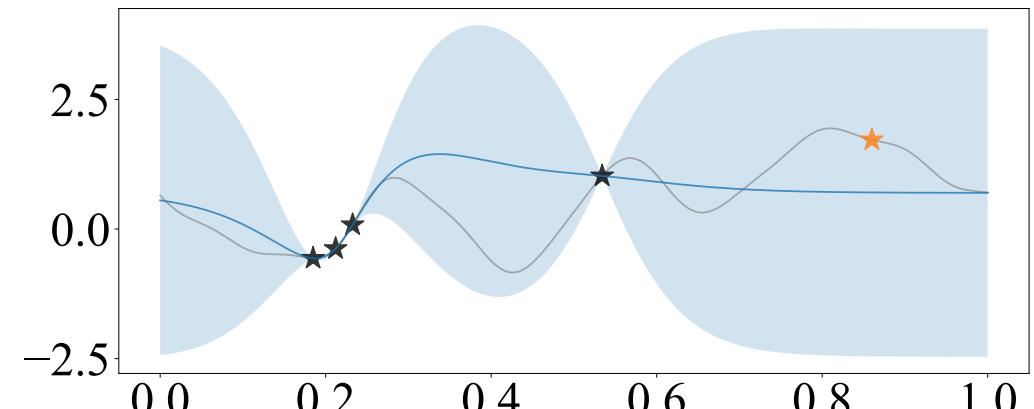


Expected improvement $EI(x)$

Improvement-based
design principle

New Design Principle: Gittins Index

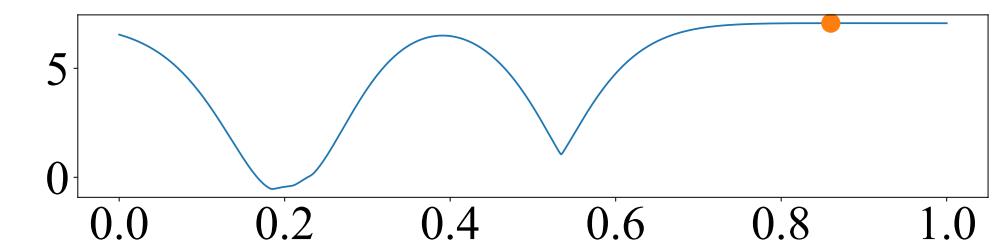
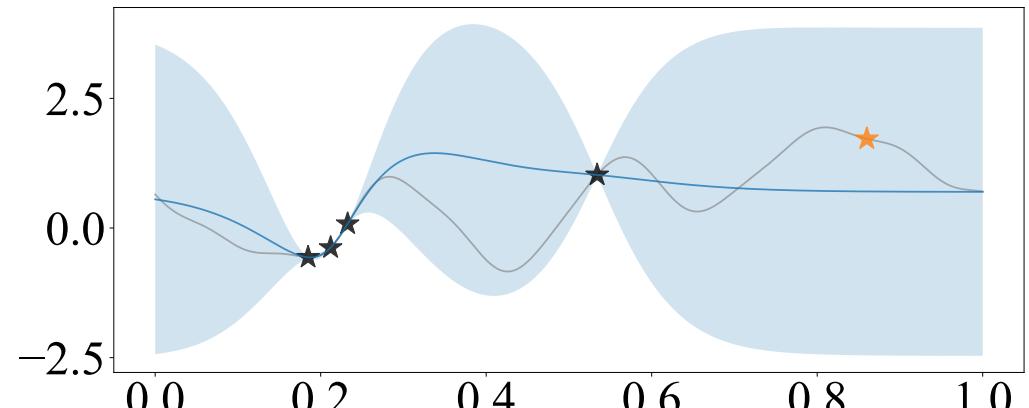
- Improvement-based (e.g., EI)
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- **Gittins Index**



Gittins index $GI(x)$

New Design Principle: Gittins Index

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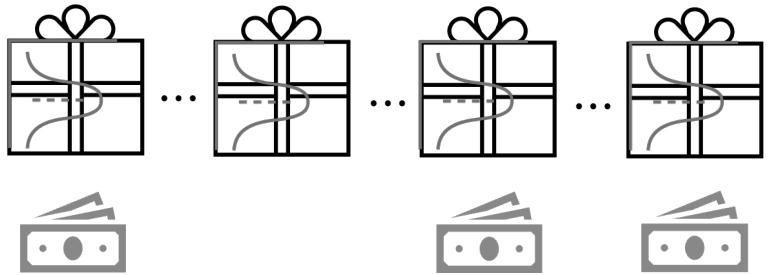


Gittins index $GI(x)$

? Why another principle?

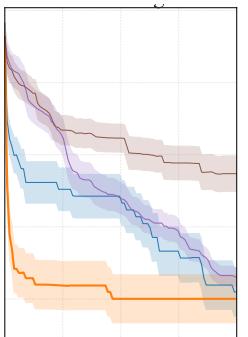
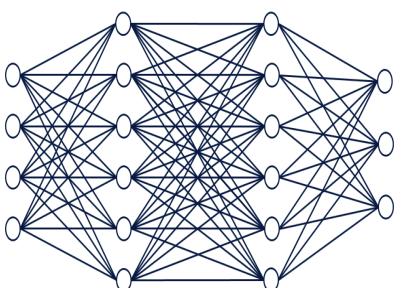
Our Contribution: Gittins Index Principle

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

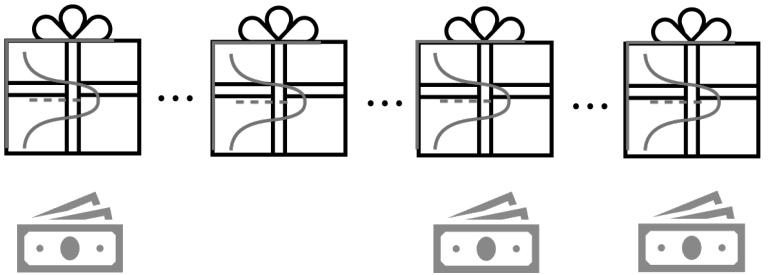
Future potential

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

Application to **efficient LLM**

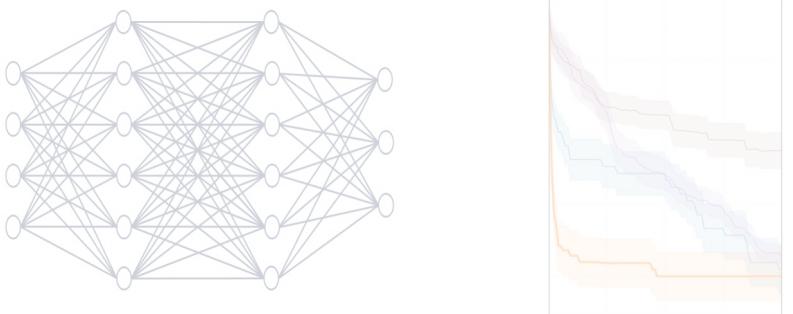
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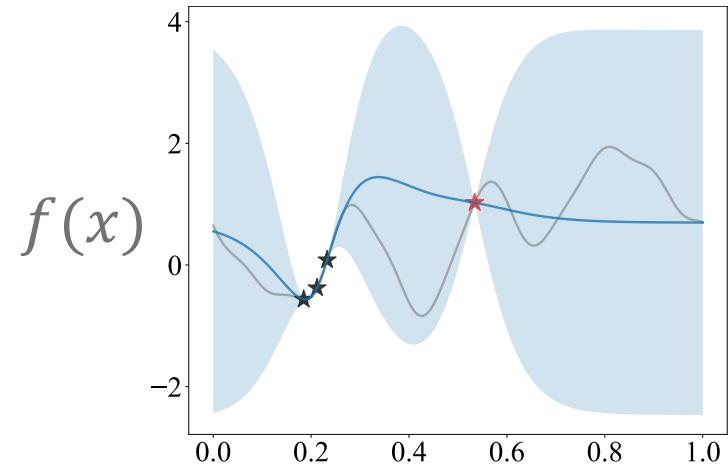


Unified framework for cost-aware selection and stopping



Application to efficient LLM

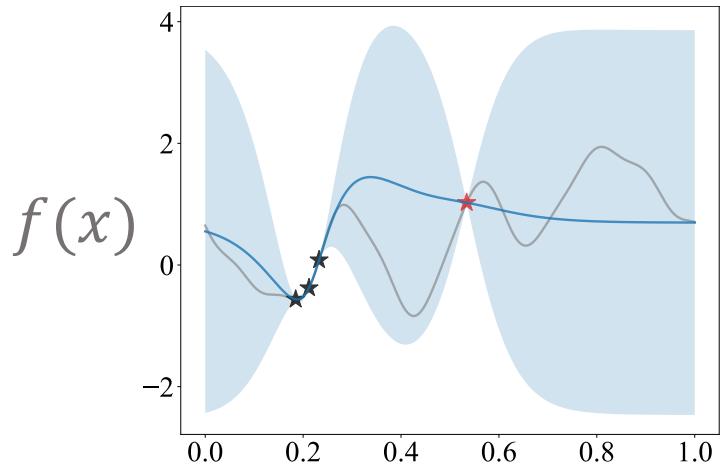
Bayesian Optimization



Continuous search space

Correlated function values

Bayesian Optimization



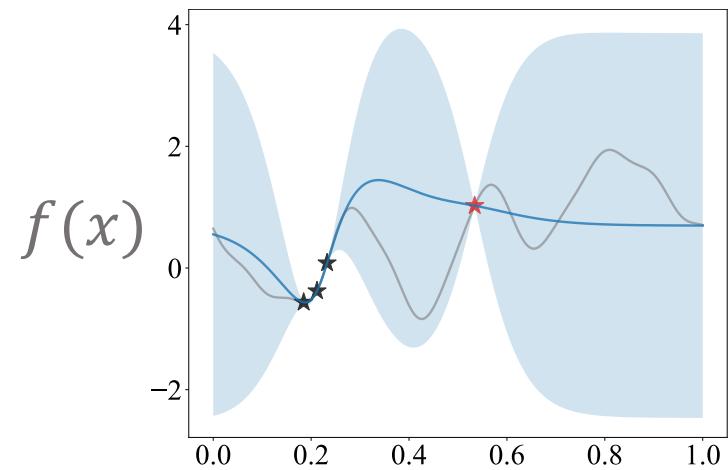
Continuous search space \Rightarrow

Discrete

Correlated function values \Rightarrow

Independent

Bayesian Optimization



Continuous search space

Correlated function values

Pandora's Box

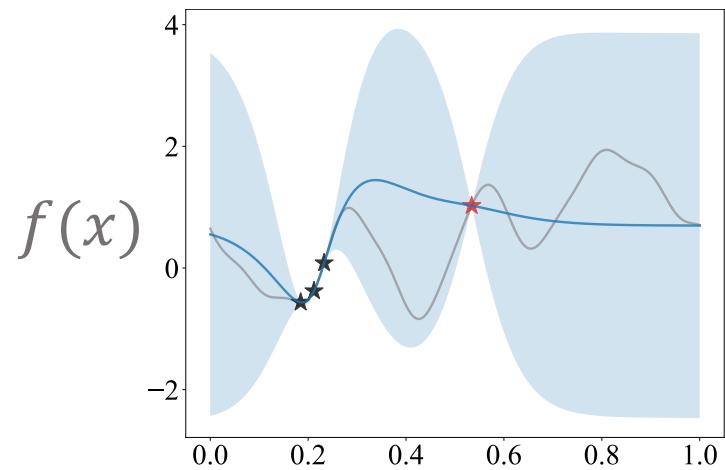
[Weitzman'79]



Discrete

Independent

Bayesian Optimization

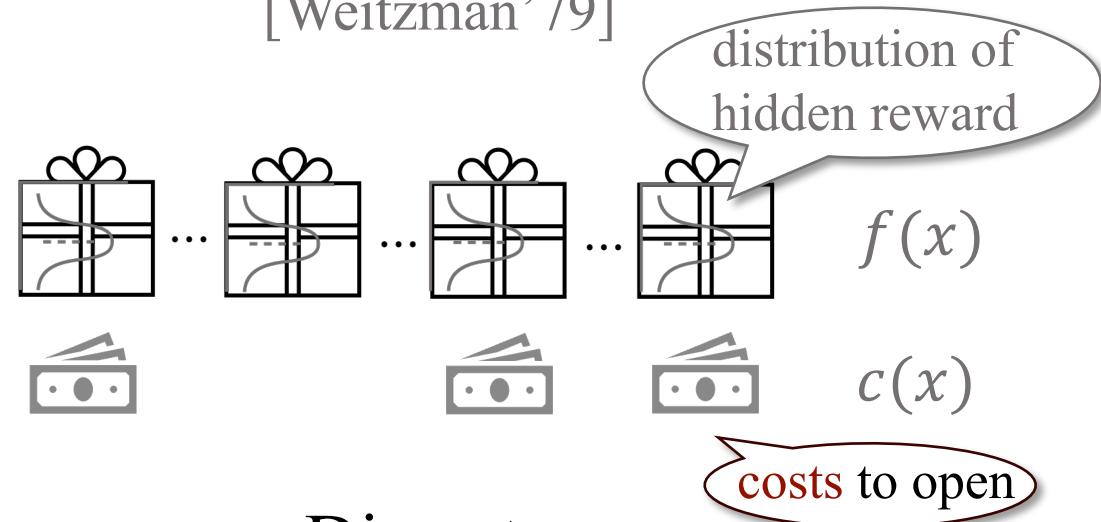


Continuous search space

Correlated function values

Pandora's Box

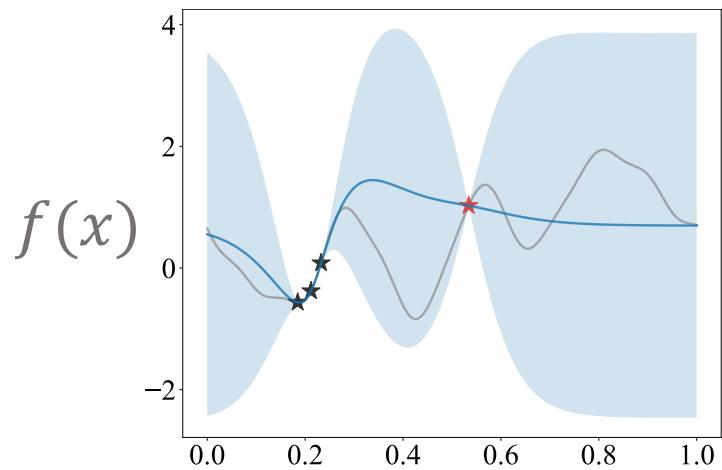
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Discrete

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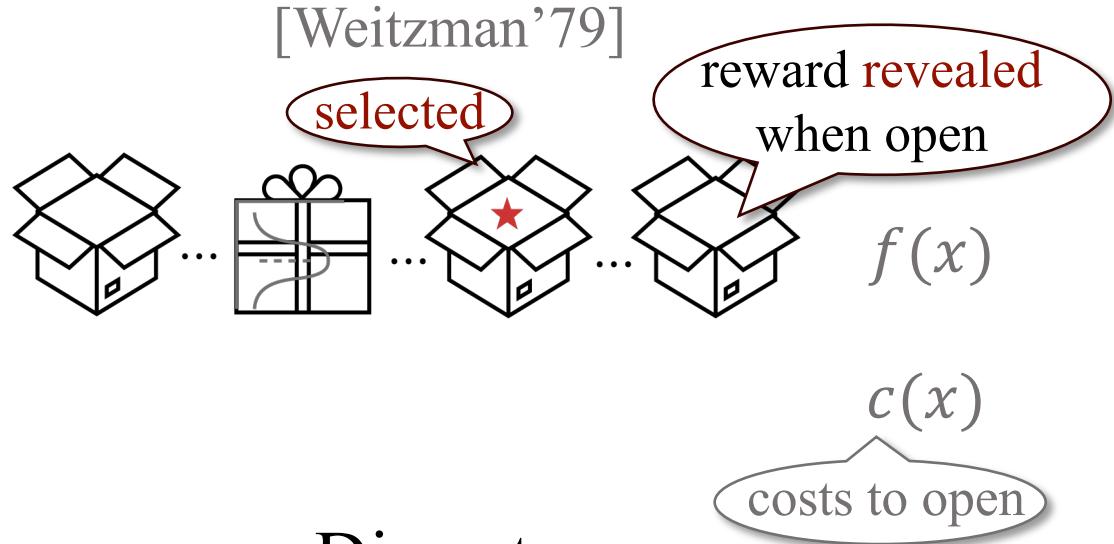
Bayesian Optimization



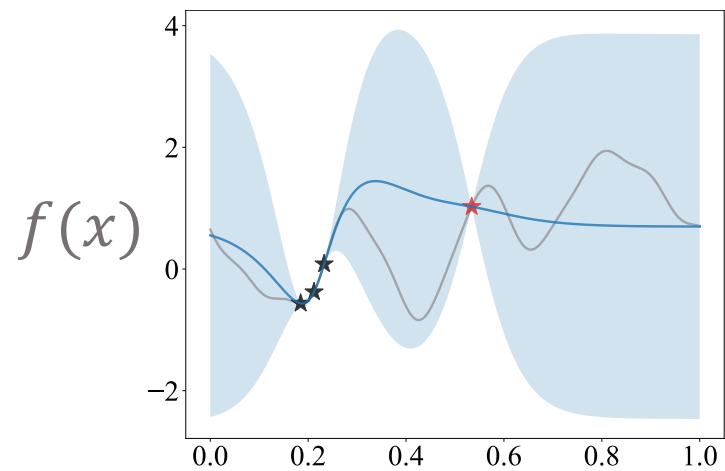
Continuous search space

Correlated function values

Pandora's Box



Bayesian Optimization

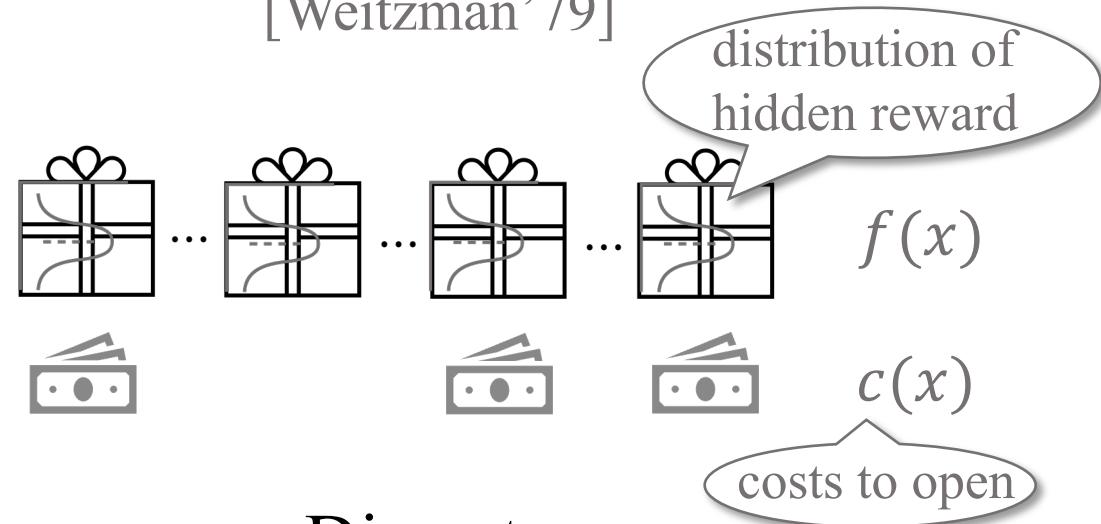


Continuous search space

Correlated function values

Pandora's Box

[Weitzman'79]

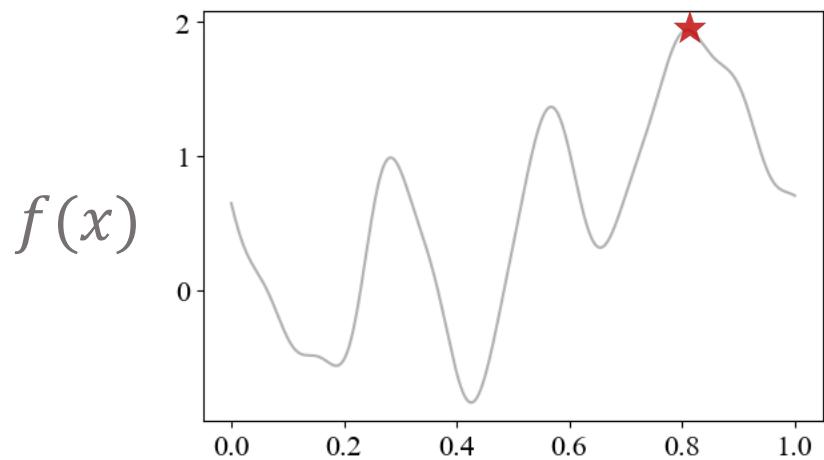


Discrete

Independent

Optimal policy: Gittins index

Bayesian Optimization

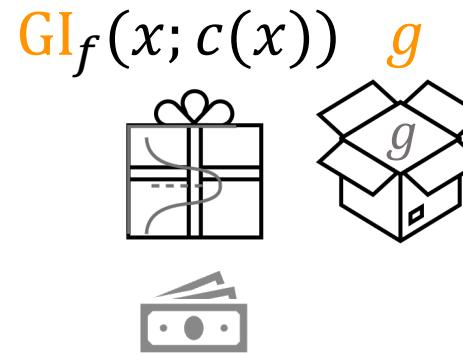


Continuous

Correlated

Pandora's Box

[Weitzman'79]



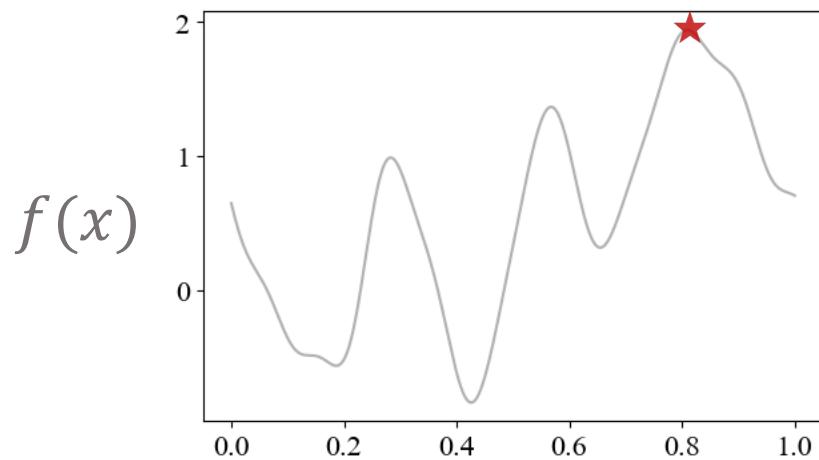
Step 1: Assign each box a Gittins index

Discrete

Independent

Optimal policy: Gittins index

Bayesian Optimization

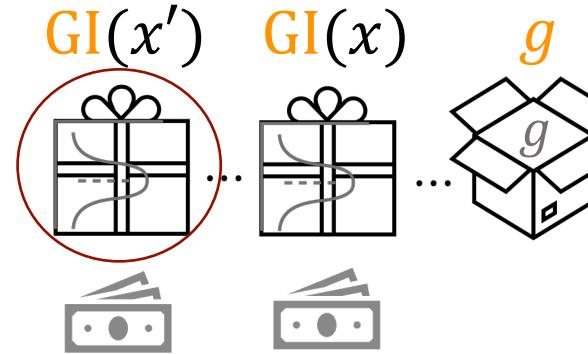


Continuous

Correlated

Pandora's Box

[Weitzman'79]



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

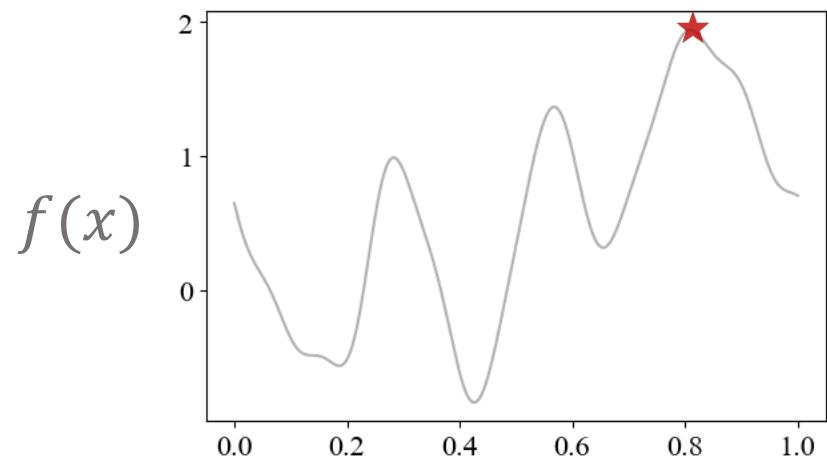
- *Closed*: open it
- *Opened*: select & stop

Discrete

Independent

Optimal policy: **Gittins index**

Bayesian Optimization

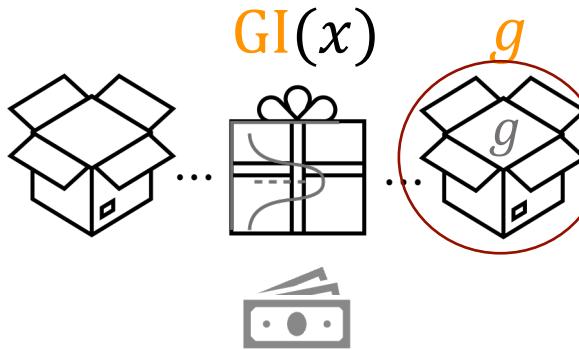


Continuous

Correlated

Pandora's Box

[Weitzman'79]



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

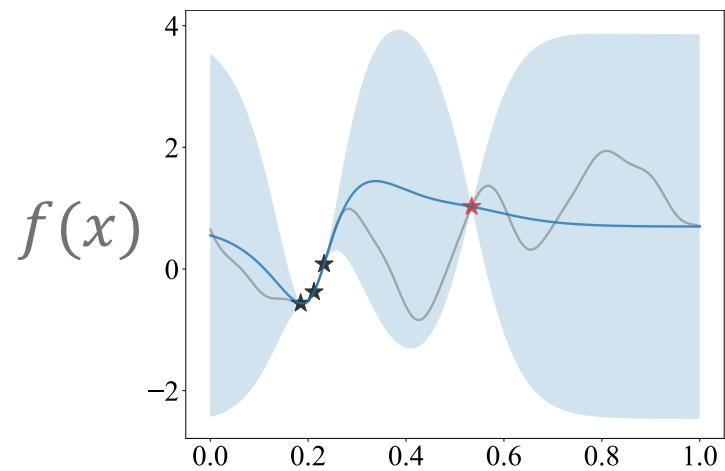
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Discrete

Independent

Optimal policy: **Gittins index**

Bayesian Optimization

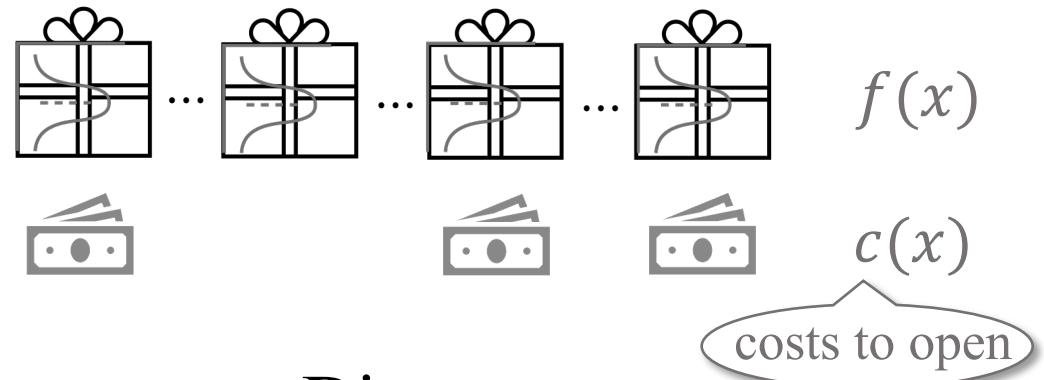


Continuous search space

Correlated function values

Pandora's Box

[Weitzman'79]



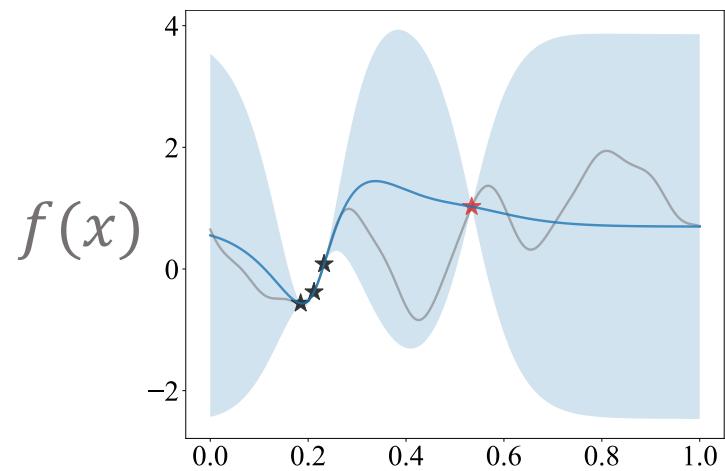
Discrete

Independent

How to translate?

Optimal policy: Gittins index

Bayesian Optimization

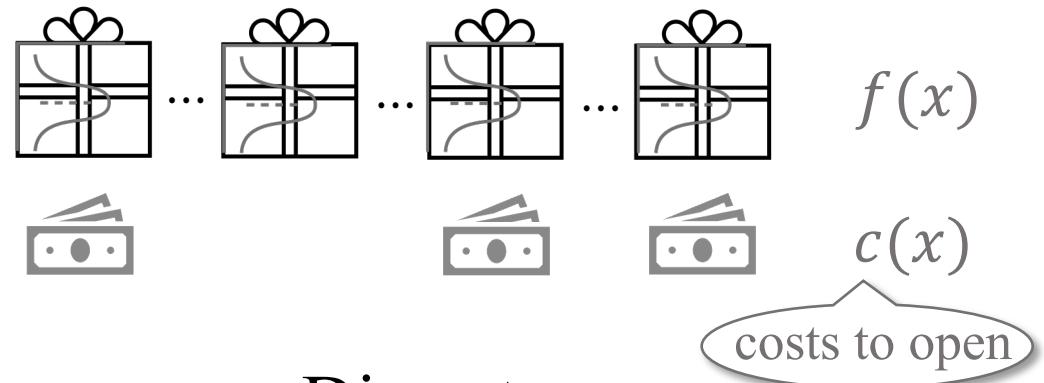


Continuous search space

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Pandora's Box

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Discrete

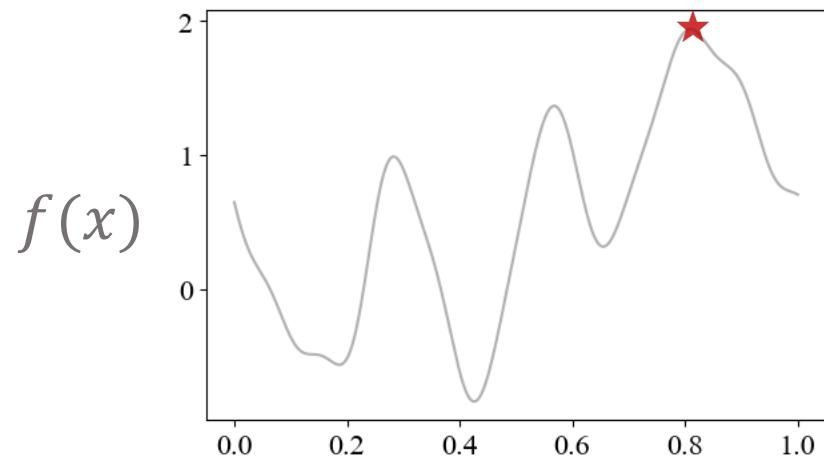
Independent

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

incorporate posterior
take continuum limit

New!

Bayesian Optimization



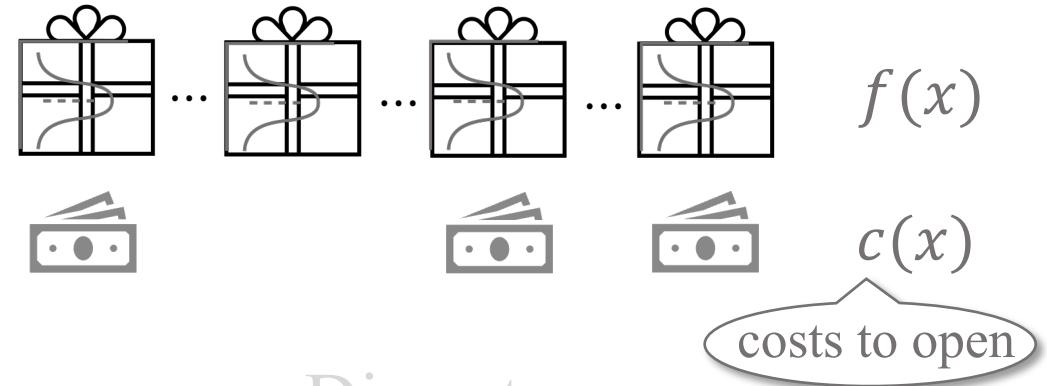
Continuous

Correlated

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

Pandora's Box

[Weitzman'79]



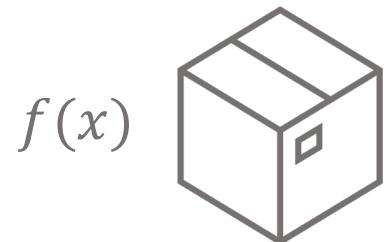
Discrete

Independent

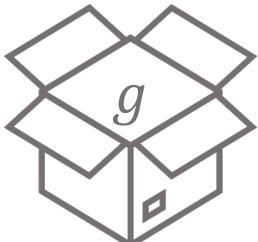
incorporate posterior
take continuum limit
 \Leftarrow Optimal policy: $\text{GI}_f(x; c(x))$

Intuition

Exploration



Exploitation



vs.

Open closed box

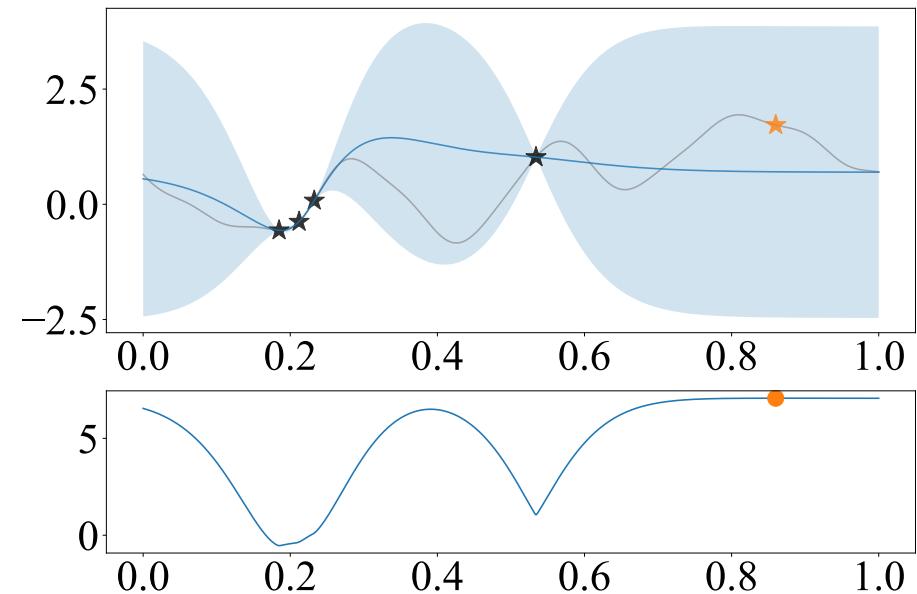
Take opened box

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

$$g$$

Should one open box? Depend on g !

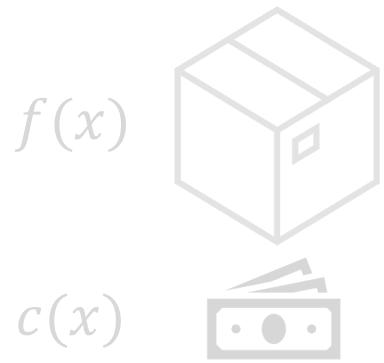
Gittins Index



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

Intuition

Exploration



vs.

Exploitation



Open closed box

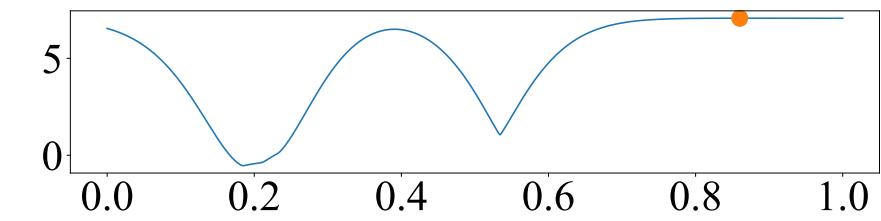
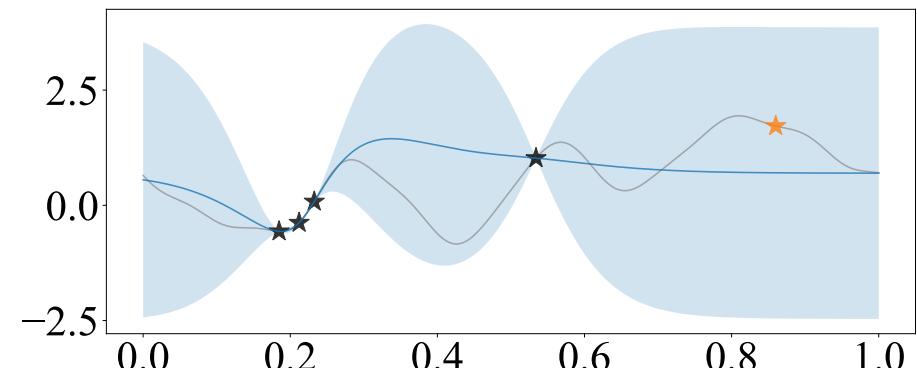
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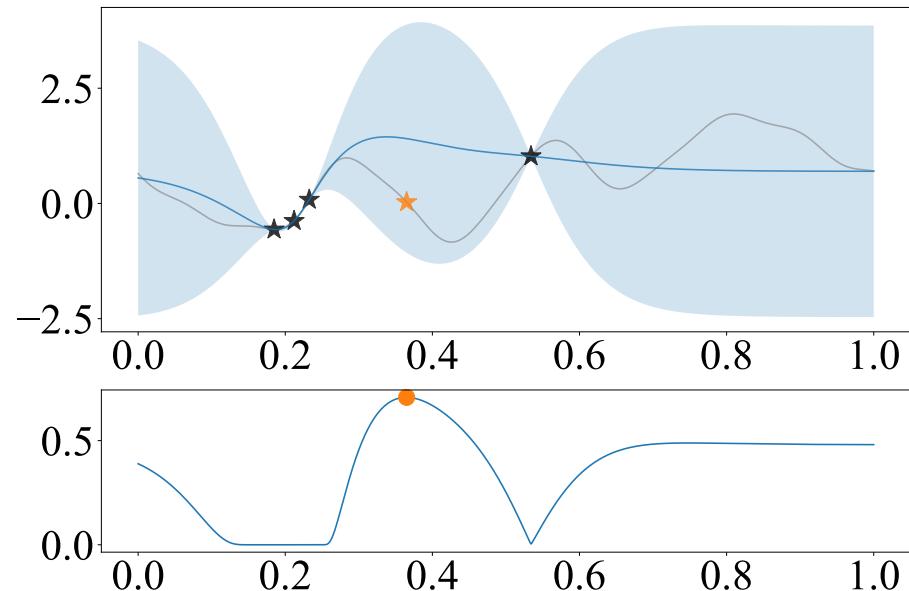
Gittins Index



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

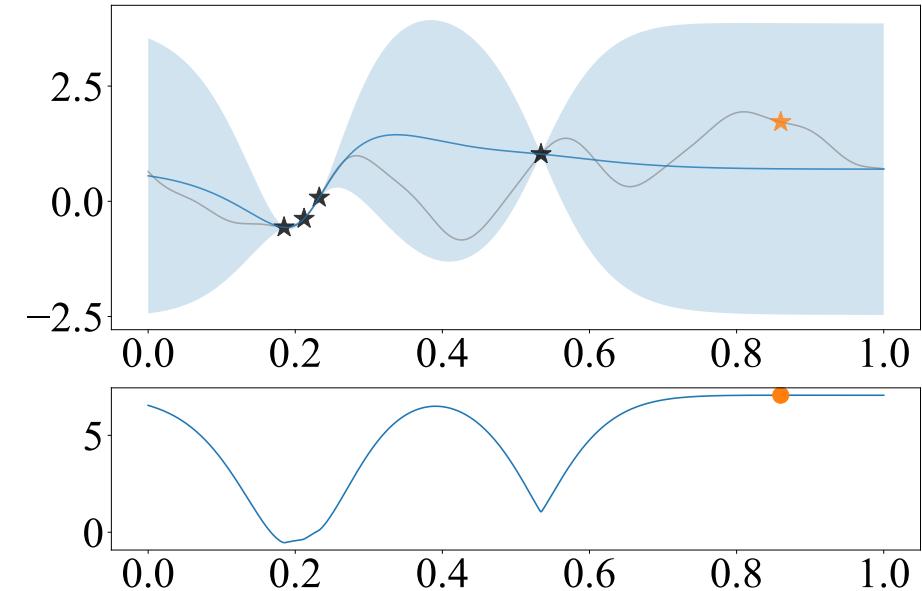
$$\text{EI}_{f|D}(x; g)$$

Expected Improvement



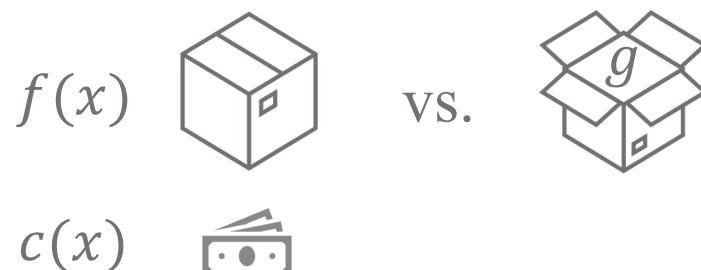
$$\text{EI}_{f|D}(x) := \mathbb{E}[\max(f(x) - y_{\text{best}}, 0) \mid D]$$

Gittins Index



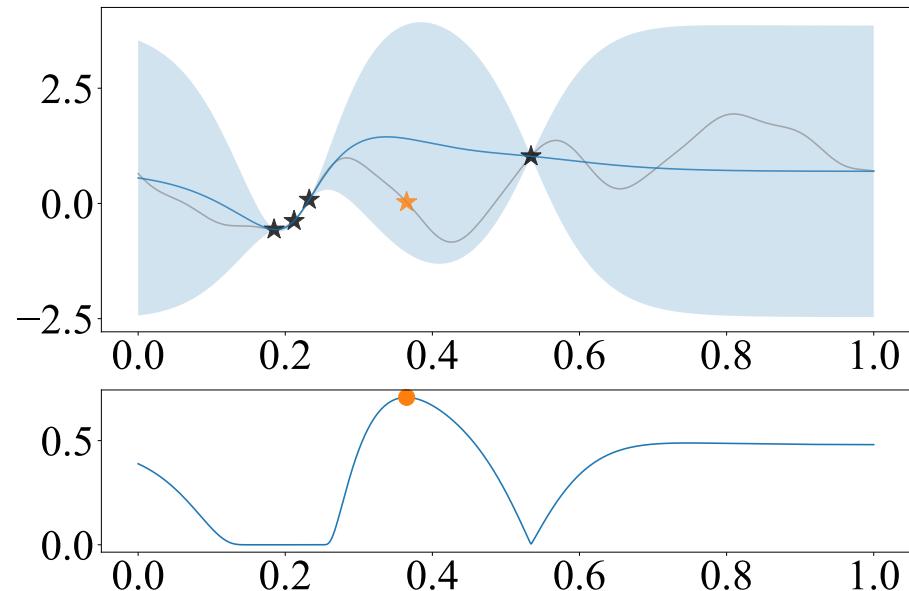
$$\text{GI}_{f|D}(x; c) := \text{solution } g \text{ s.t. } \text{EI}_{f|D}(x; g) = c(x)$$

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



Exploration Exploitation

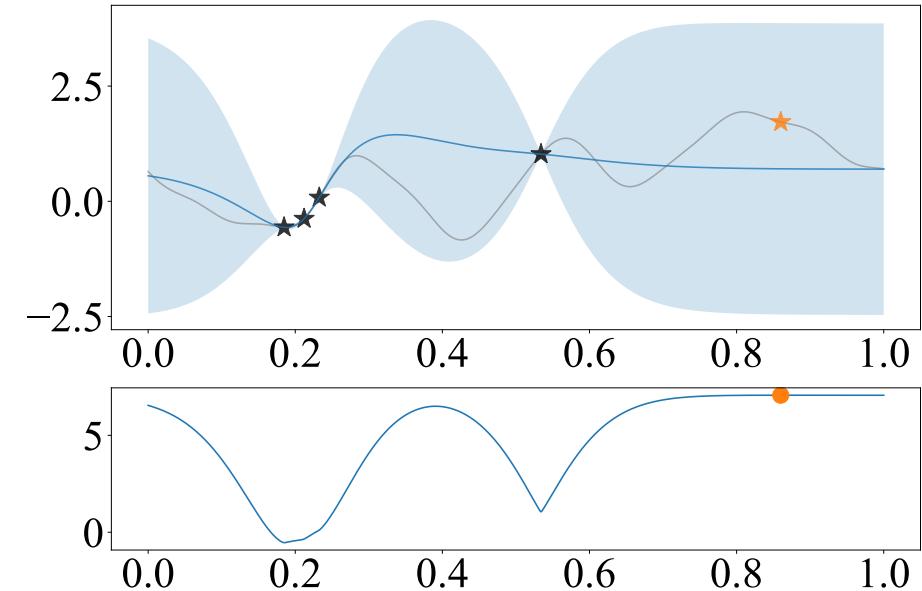
Expected Improvement



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

Temporal simplification to MDP
(One-step)

Gittins Index

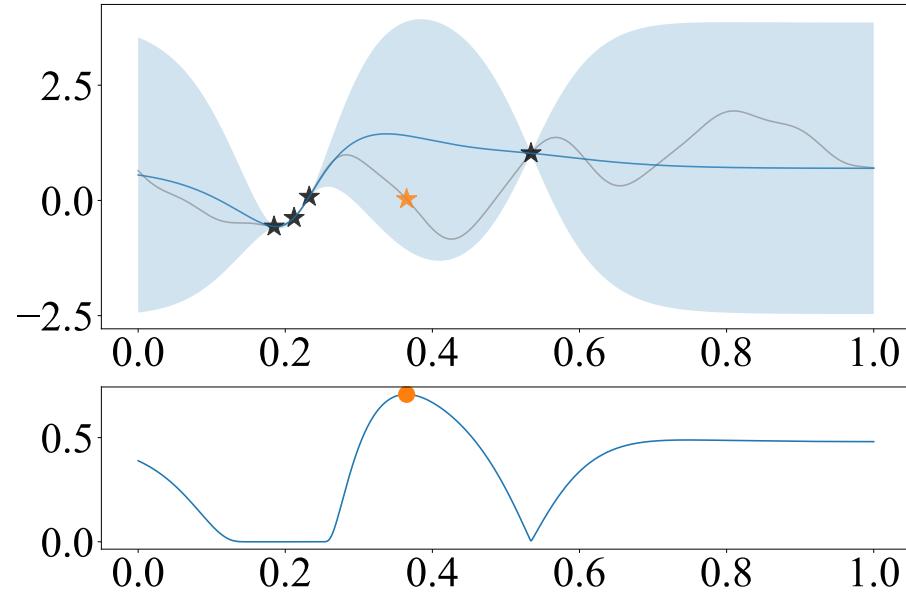


$$GI_{f|D}(x; c) := \text{solution } g \text{ s.t. } EI_{f|D}(x; g) = c(x)$$

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

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

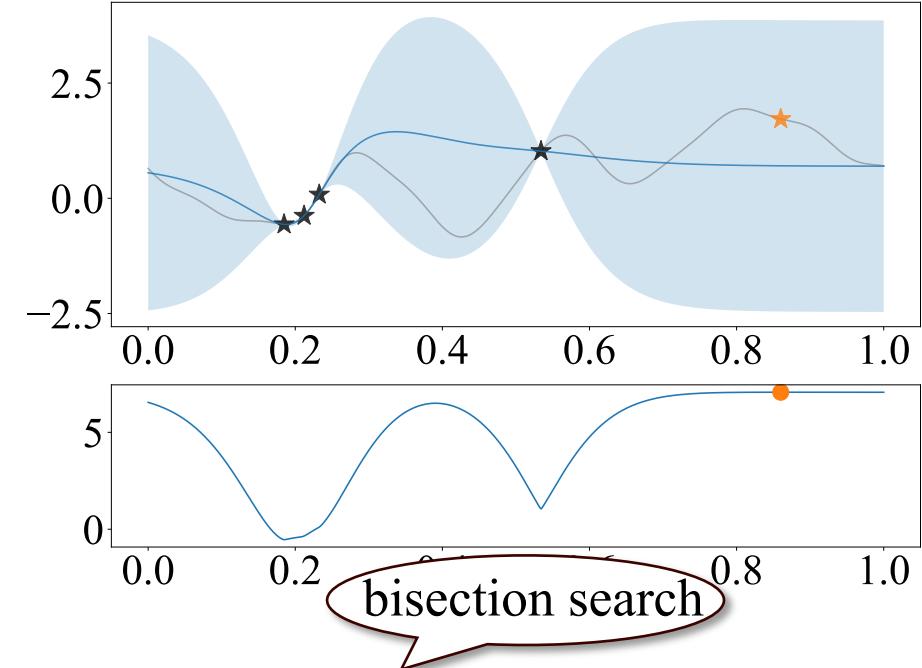


Both are **principled** and **easy-to-compute!**



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

Gittins Index



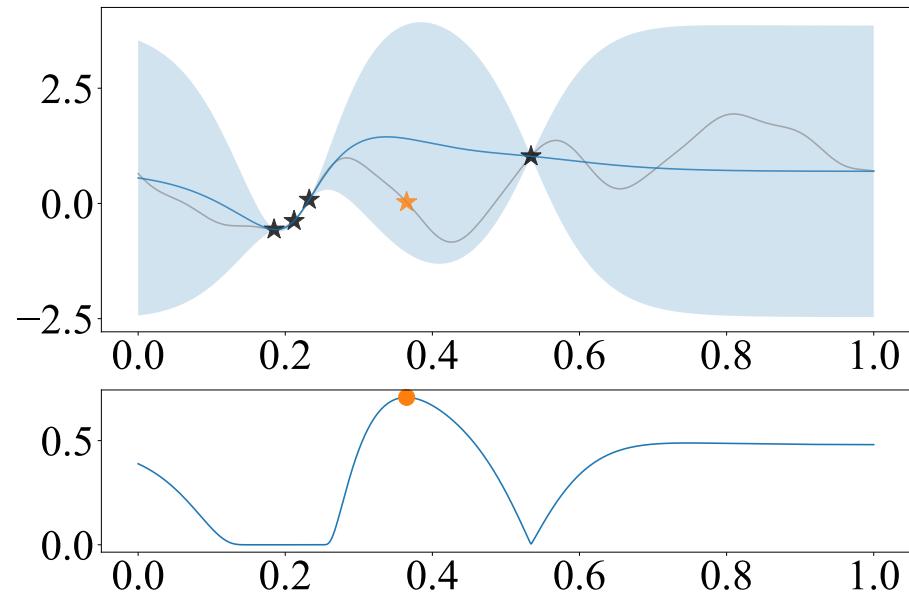
$$\text{GI}_{f|D}(x; c) := \text{solution } g \text{ s.t. } \text{EI}_{f|D}(x; g) = c(x)$$

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

analytical expression

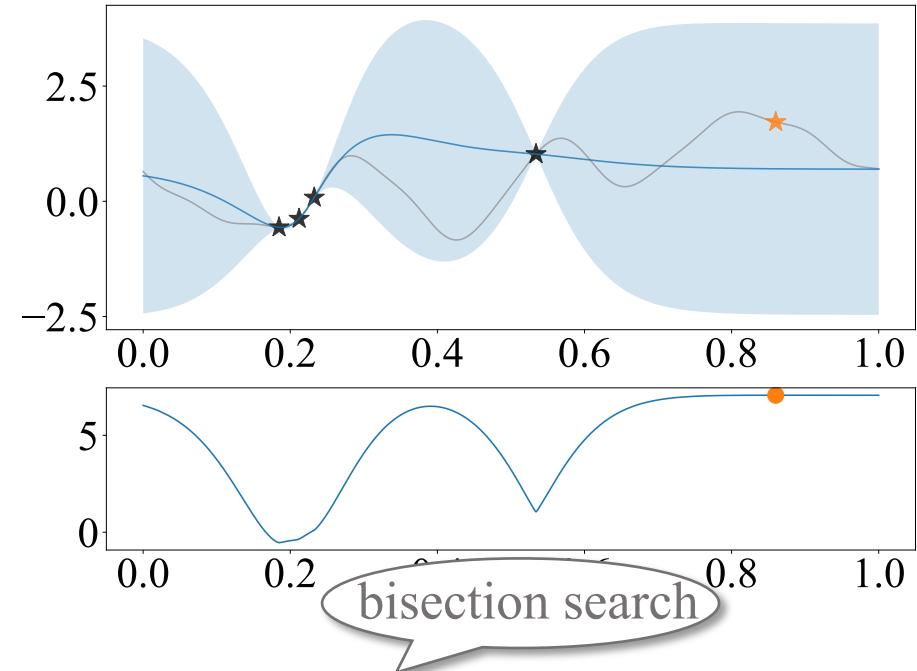
Spatial simplification to MDP

Expected Improvement



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

Gittins Index



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

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

Google DeepMind

FunBO: Discovering new acquisition functions for
Bayesian Optimization with FunSearch

hard to discover GI

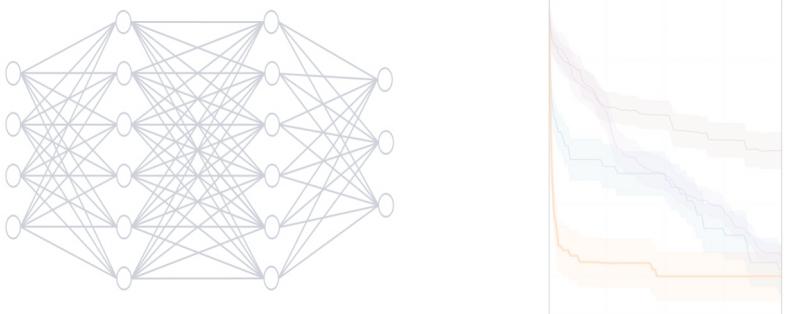
Our Contribution: Gittins Index Principle

Novel connection



Link to Pandora's Box problem
& Gittins index theory

Competitive empirical performance



Interests from practitioners (e.g., Meta)

Principled decision rules

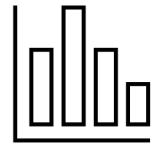
- Varying evaluation costs
- Adaptive stopping time

Unified framework for selection and stopping

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

Application to efficient LLM

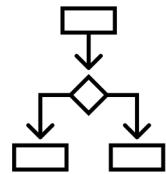
Under-explored Information for Better Decisions



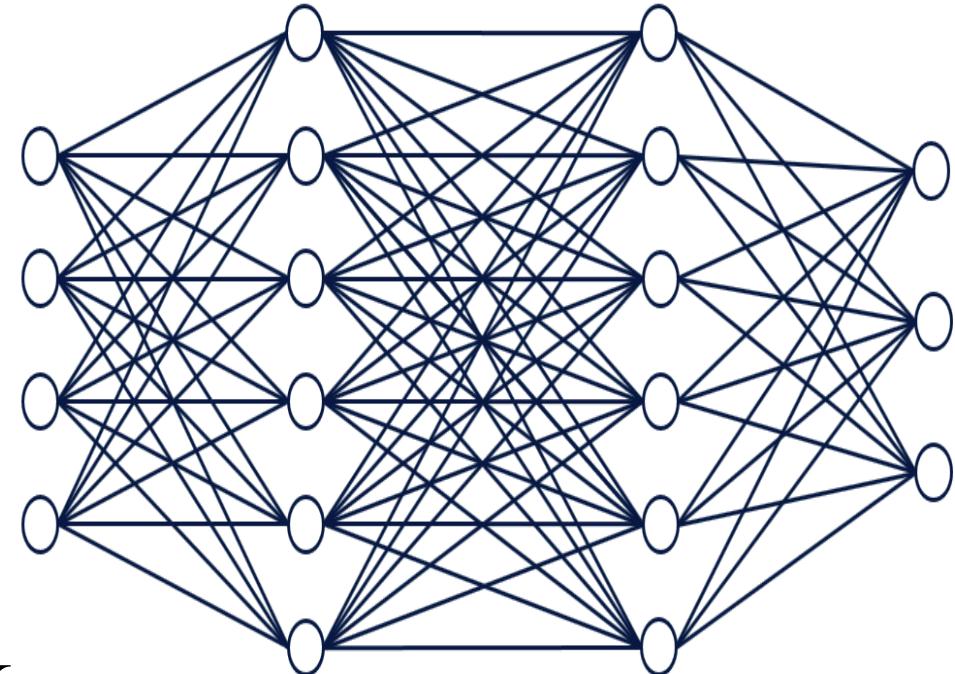
Varying evaluation costs



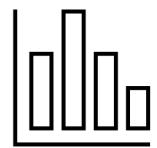
Smart stopping time



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

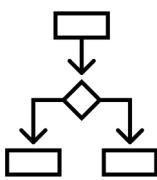
$$\tau: \text{EI}(x_\tau) \leq \theta$$

[Locatelli'97,

Nguyen et al.'17,

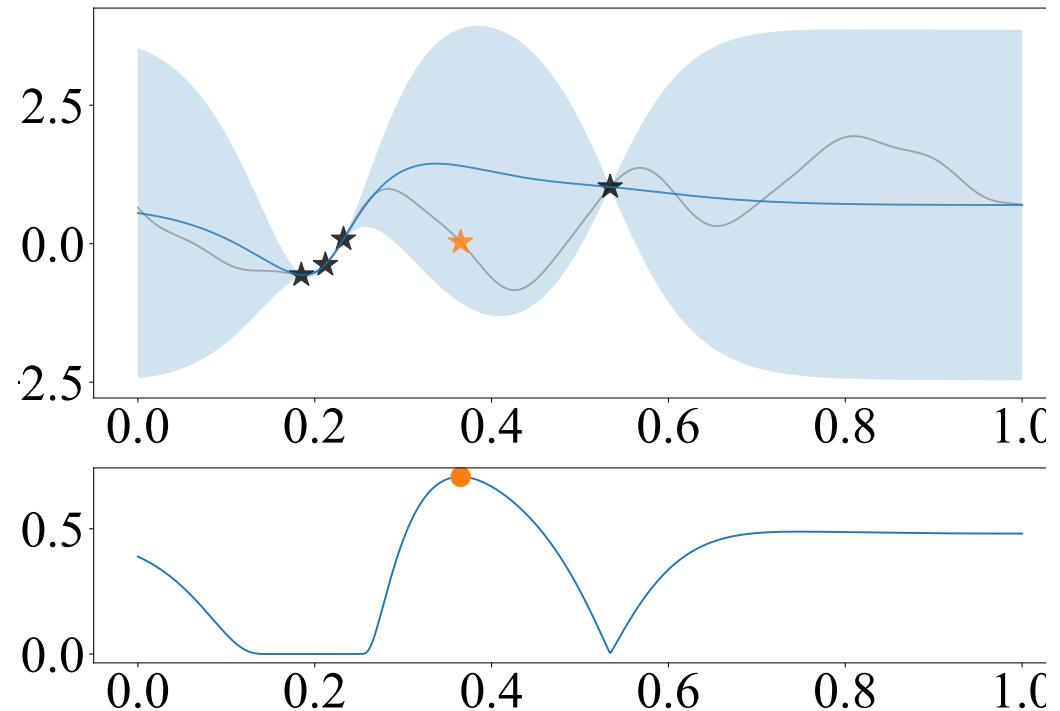
Ishibashi et al.'23]

Which threshold?



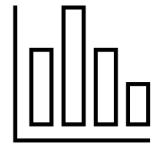
Observable multi-stage feedback

?



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

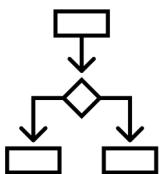
Under-explored Information for Better Decisions



Varying evaluation costs



Smart stopping time

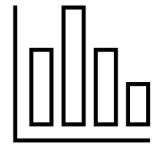


Observable multi-stage feedback



New design principle:
Gittins index

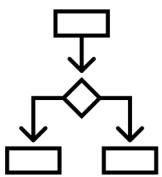
Why Gittins index?



Varying evaluation costs



Smart stopping time

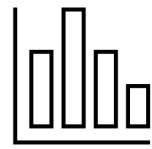


Observable multi-stage feedback

New design principle:
Gittins index

Optimal in related sequential
decision problems

Why Gittins index?



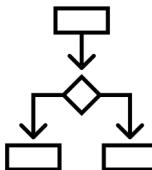
Varying evaluation costs

Features in **Pandora's box**



Smart stopping time

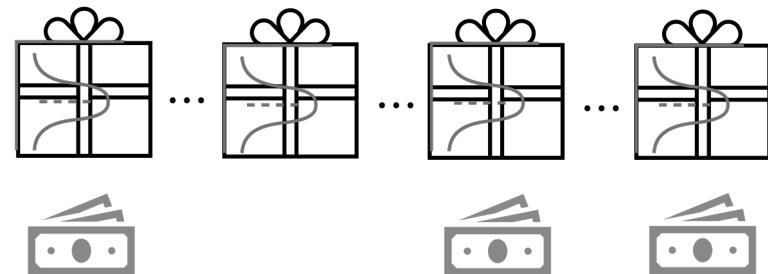
Features in **Pandora's box**



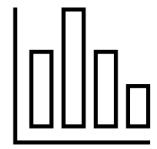
Observable multi-stage feedback

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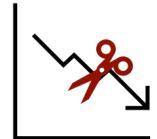


Why Gittins index?



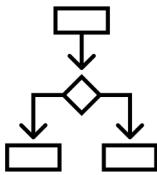
Varying evaluation costs

Features in Pandora's box



Smart stopping time

Features in Pandora's box

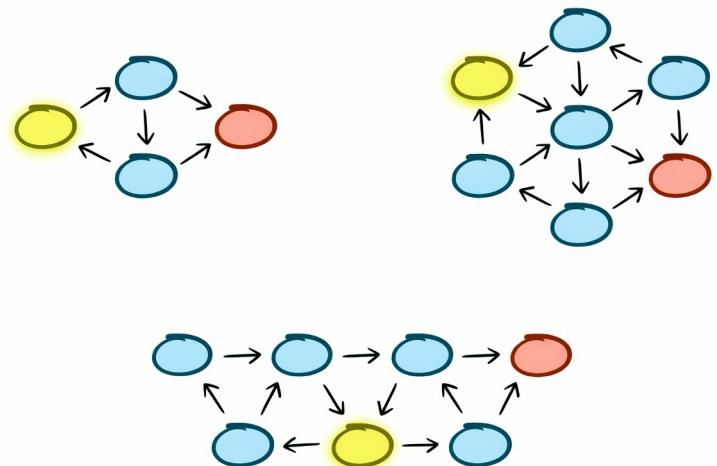


Observable multi-stage feedback

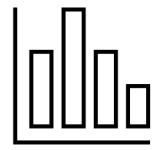
Features in Markov chain selection

New design principle:
Gittins index

Optimal in related sequential
decision problems

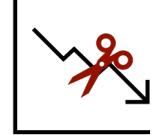


Why Gittins index?



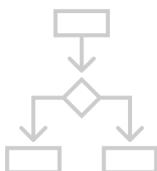
Varying evaluation costs

Features in **Pandora's box**



Smart stopping time

Features in **Pandora's box**



Observable multi-stage feedback

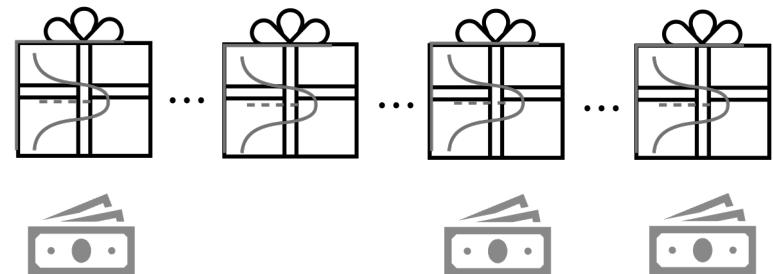
Features in Markov chain selection



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

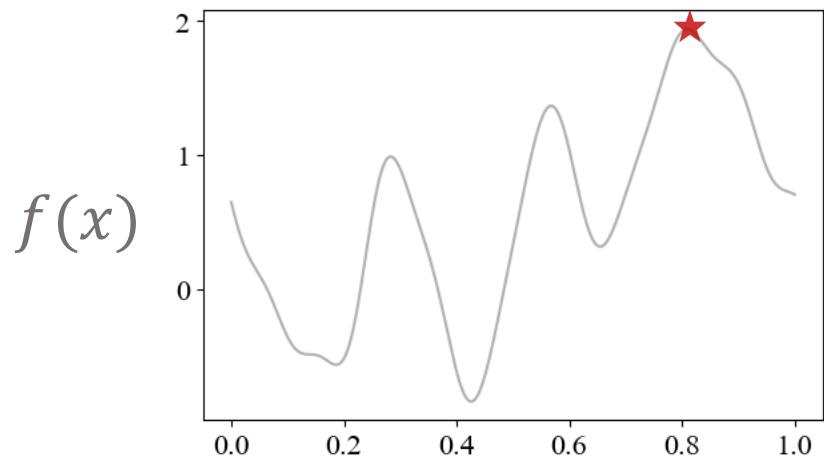
New design principle:
Gittins index

Optimal in related sequential
decision problems



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

Bayesian Optimization



Continuous

Correlated

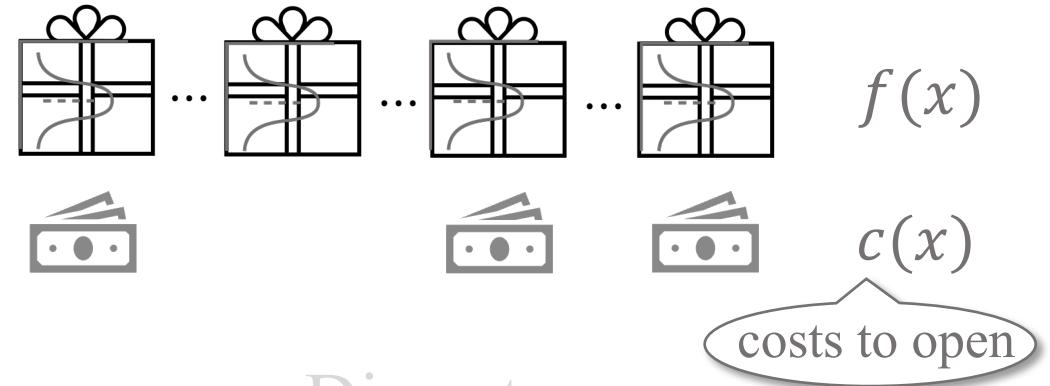
Cost-unaware

Fixed-iteration

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

Pandora's Box

[Weitzman'79]



Discrete

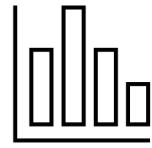
Independent

Cost-aware

Flexible-stopping

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

Expected Improvement vs Gittins Index



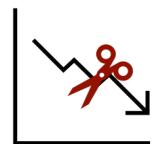
Varying evaluation costs

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

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:

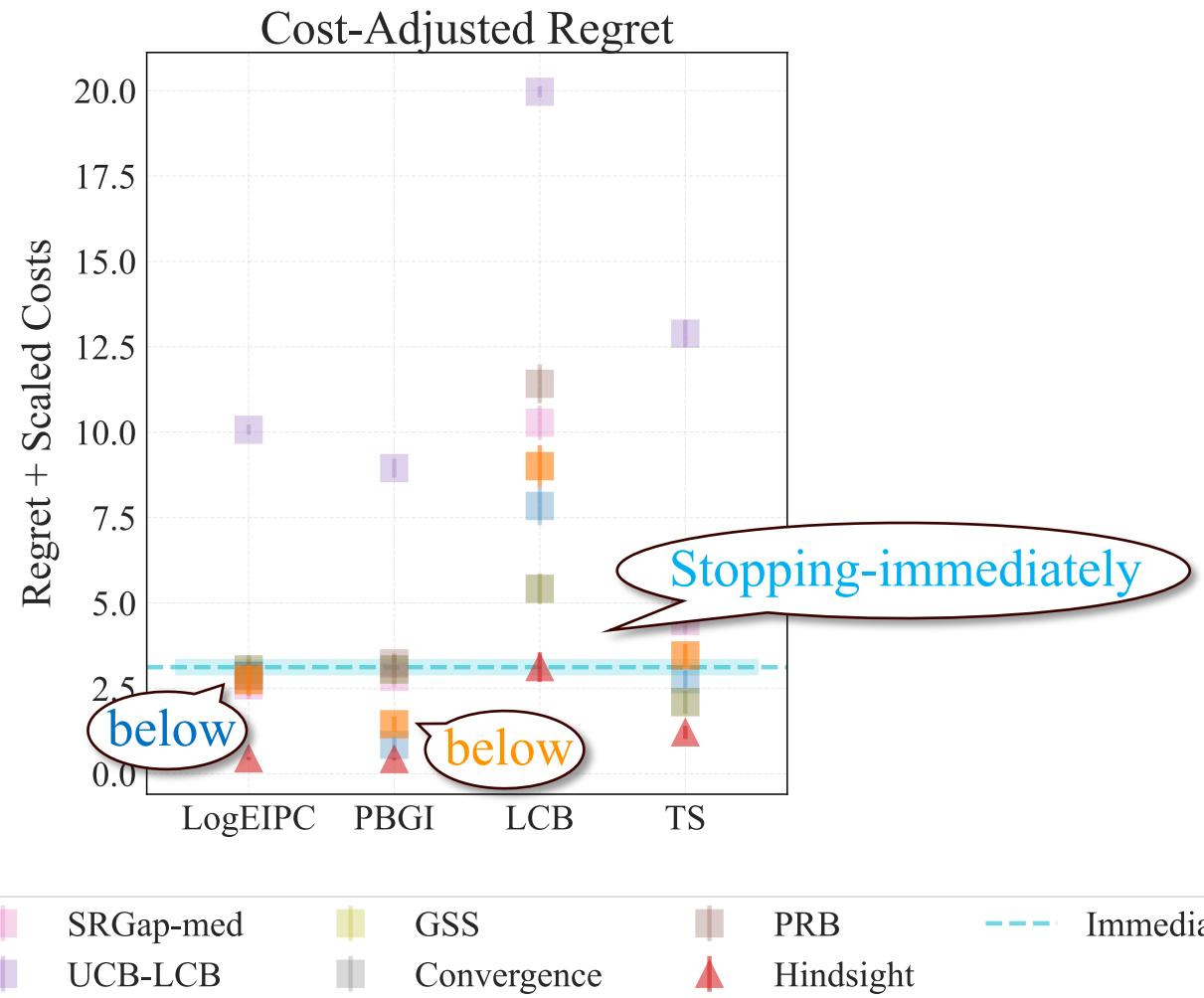
- Matches the **best achievable performance in the worst case** (evaluations are all very costly).
- Avoids **over-spending** — a property many cost-unaware stopping rules lack.

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



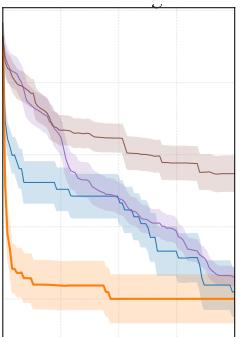
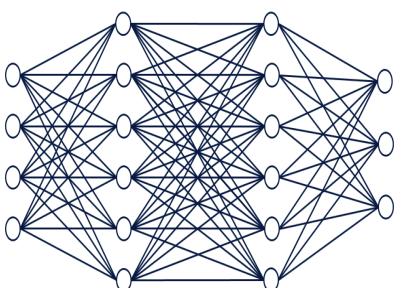
Link to Pandora's Box problem
& Gittins index theory

Principled decision rules

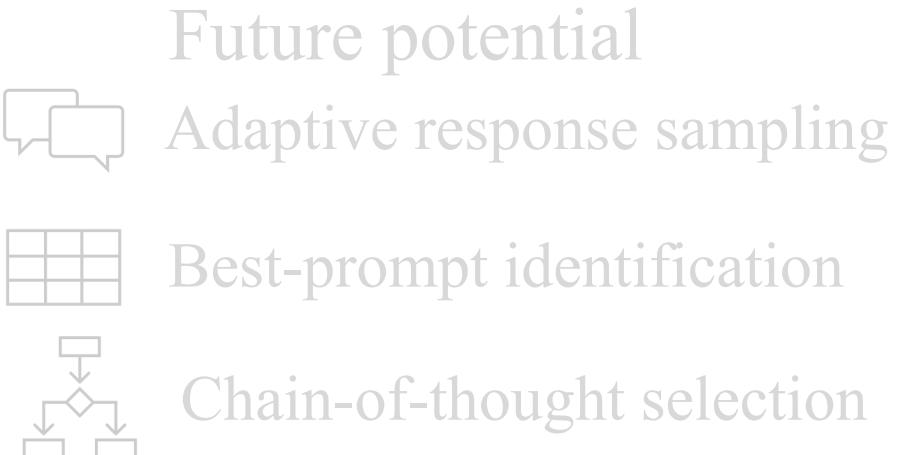


Unified framework for
selection and stopping

Competitive empirical performance

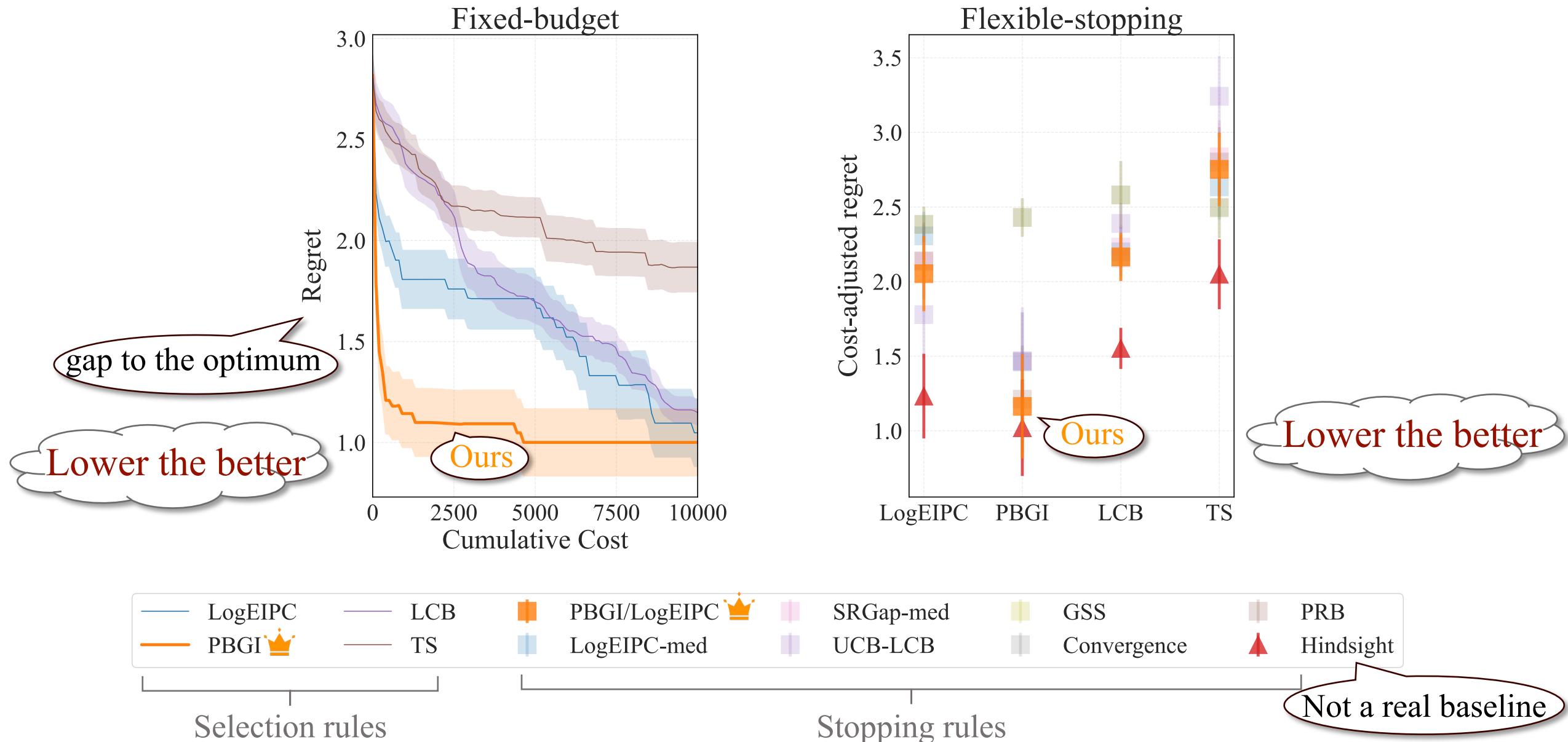


Interests from practitioners (e.g., Meta)



Application to efficient LLM

Gittins Index vs Baselines on AutoML Benchmark



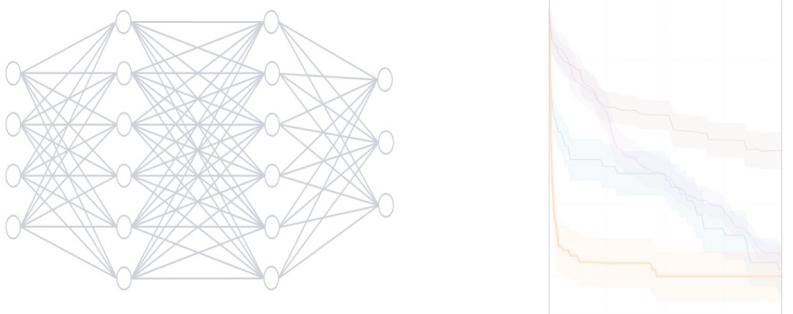
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Link to Pandora's Box problem
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Competitive empirical performance



Interests from practitioners (e.g., Meta)

Principled decision rules

- Varying evaluation costs
- Adaptive stopping time

Unified framework for cost-aware selection and stopping

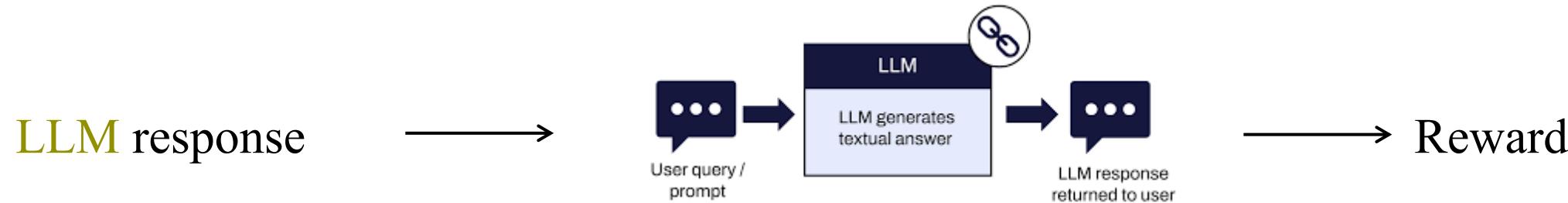
Future potential

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

Application to efficient LLM

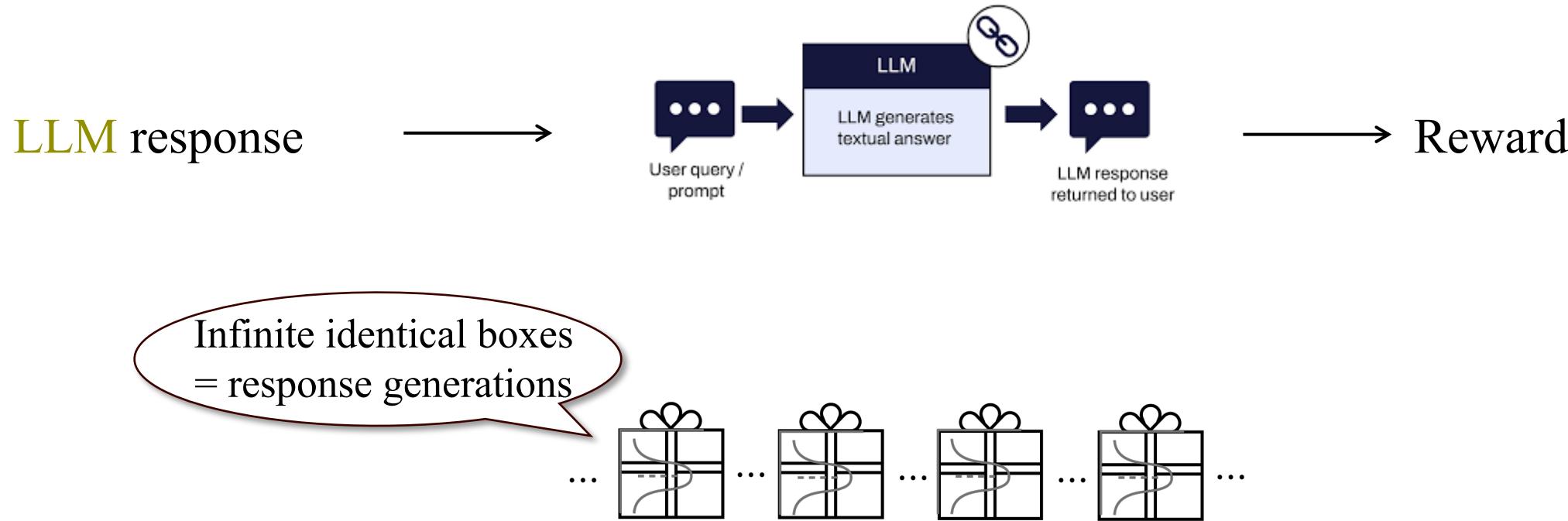
Adaptive Response Sampling in LLM Inference

LLM inference time alignment (optimization):



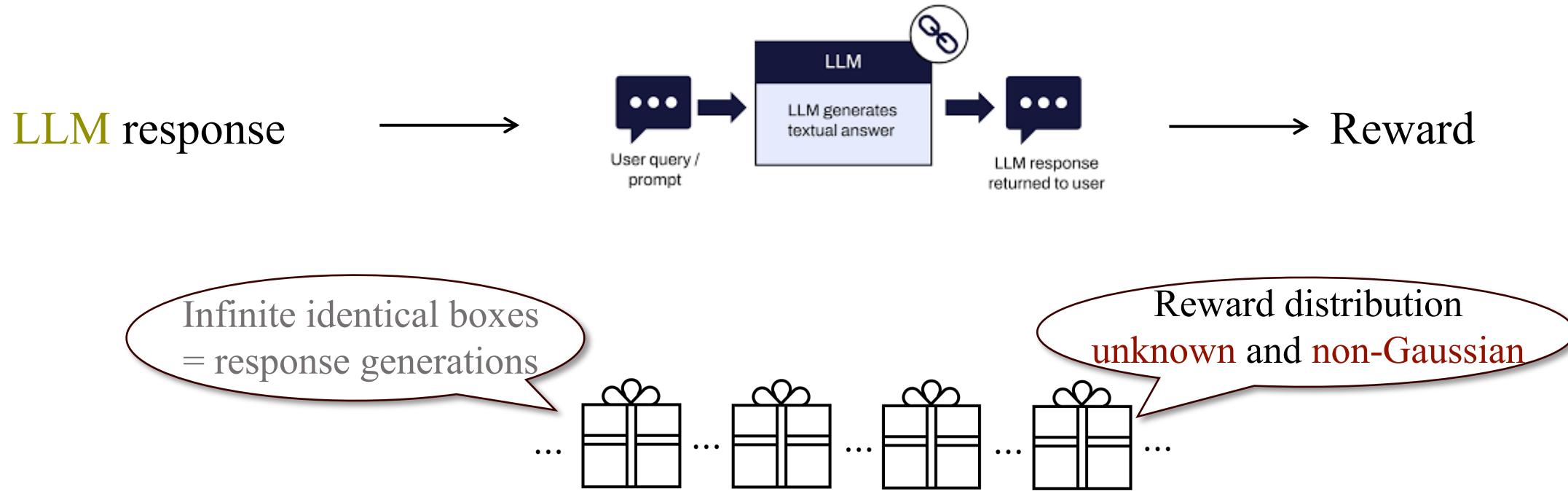
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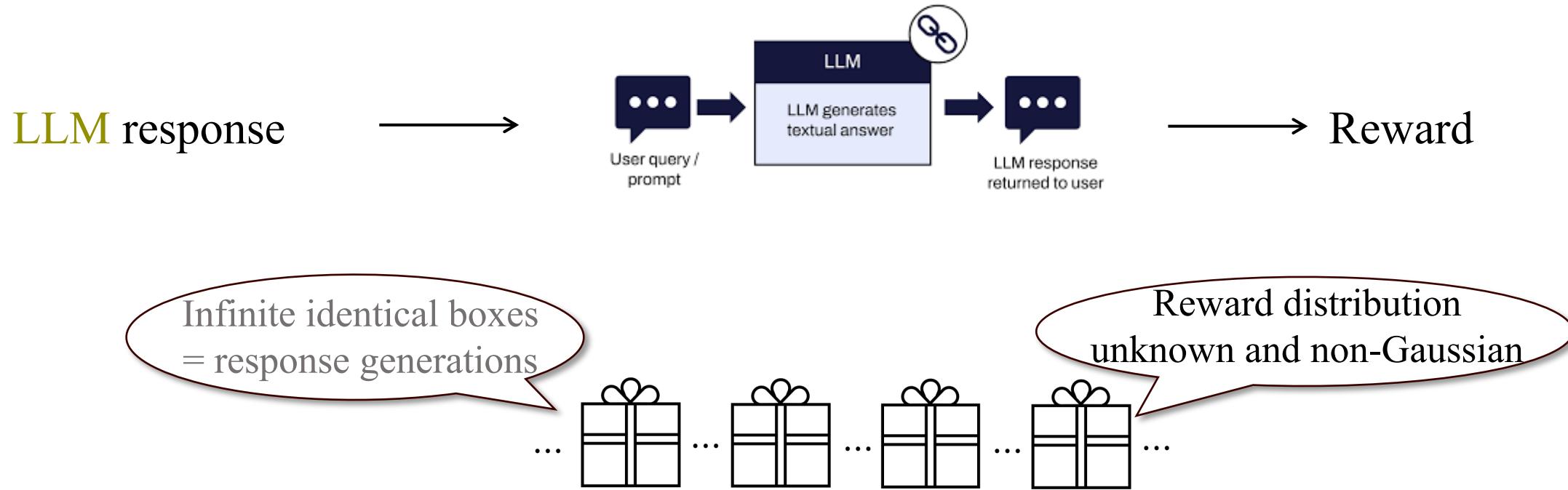
Adaptive stopping vs. fixed budget (best-of- N)
(Kalayci et al. 2025)

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

LLM multi-prompt evaluation:

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Claude 3.5 Sonnet	★★★★★	★★★★★	★★★★★		★★★★★
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

LLM multi-prompt evaluation:

Prompt template
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Claude 3.5 Sonnet	★★★★★	★★★★★	★★★★★		★★★★★
Gemini 1.5 Pro	★★★★★	★★★	?	★★★	★★★★★
deepseek	?	?	★★★	?	★★★
Llama 3.1-70B	?	?	★★★	?	★★★
Mistral Large	?	?	★★★	?	★

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...

Matrix completion
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Best-prompt Identification in LLM 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
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Prompt/ Question	Q1	Q2	Q3	...	Predicted avg performance
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...

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	?	?	★★★	?	★

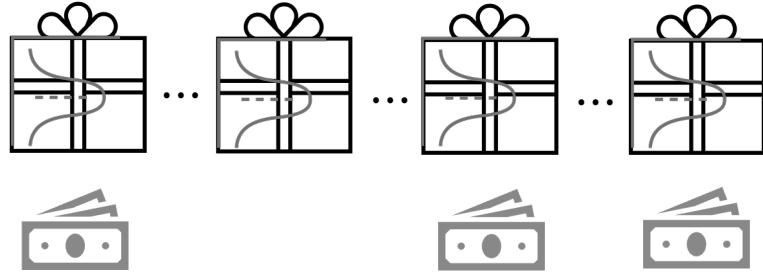
Average performance
of (LLM, prompt) pairs

Boxes = entries



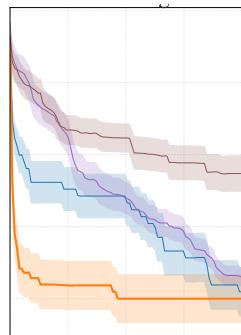
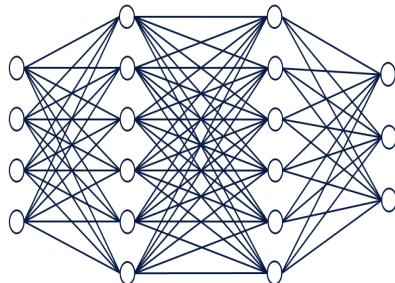
Applicable to tensors

Novel connection



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

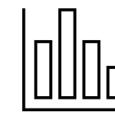
Competitive empirical performance



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

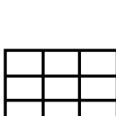


Adaptive stopping time

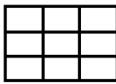
Unified framework for selection and stopping



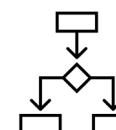
Future potential



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.