

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

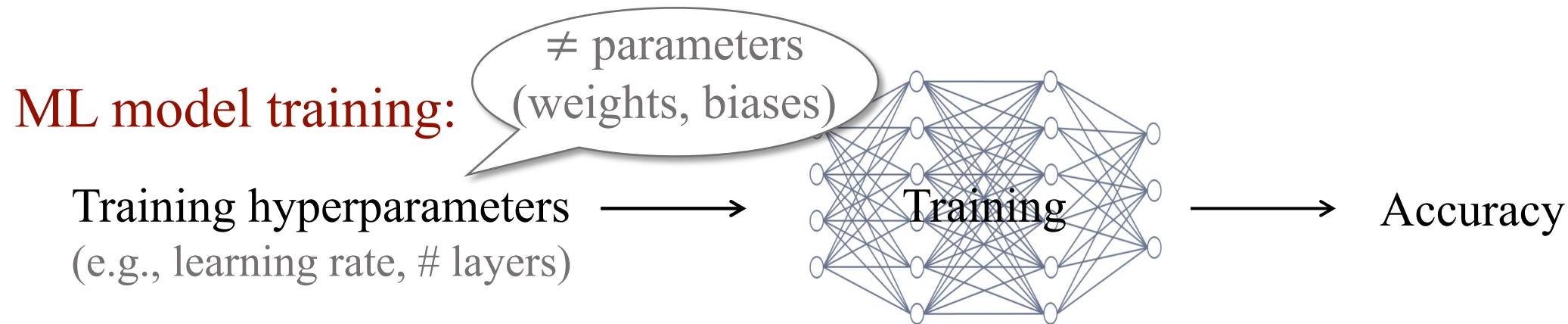
ML model training:

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

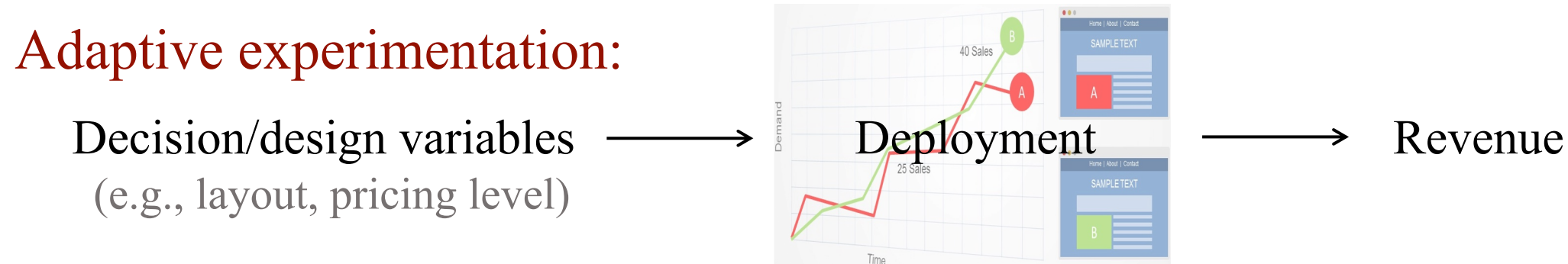
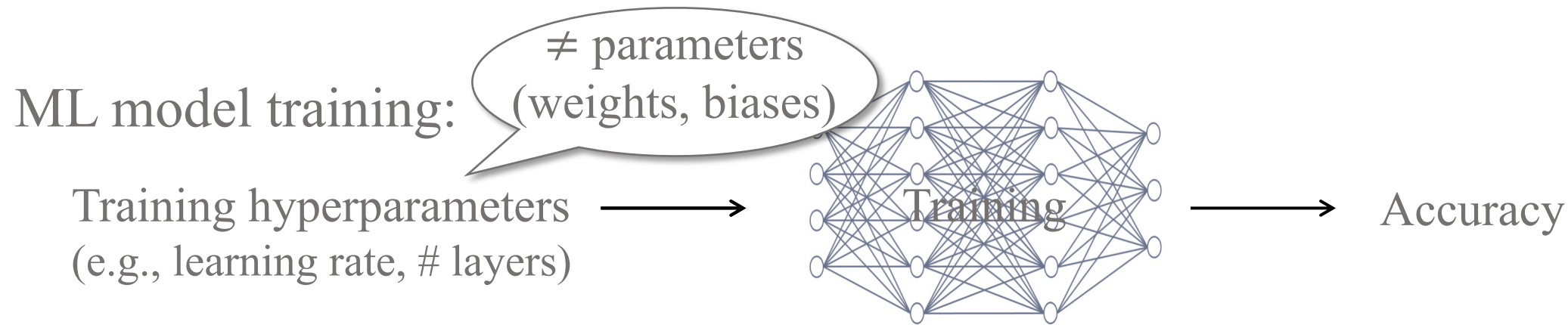


Accuracy

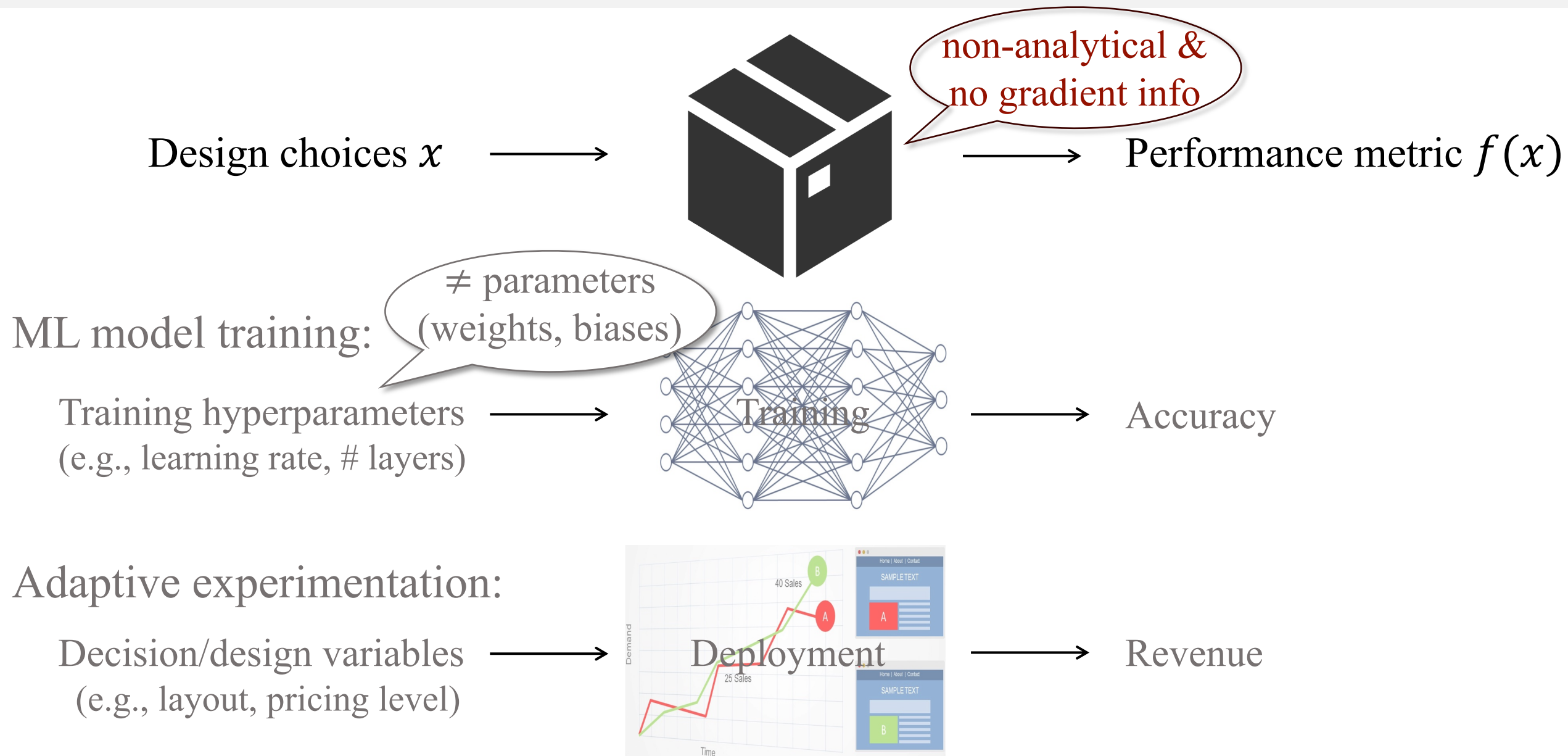
Motivation: World of Optimization under Uncertainty



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Black-box optimization:

(gradient-based methods not applicable)

Input x →



non-analytical &
no gradient info

→ Observed outcome $f(x)$

ML model training:

≠ 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 →

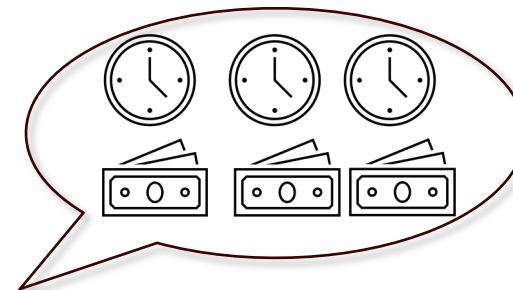


expensive-to-evaluate

→ Observed outcome $f(x)$

ML model training:

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

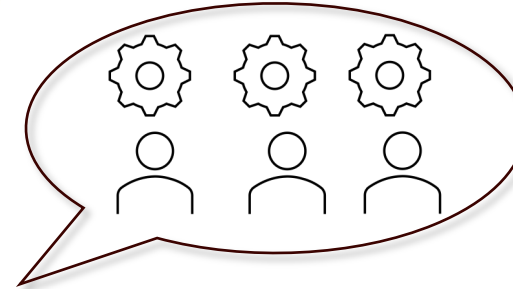
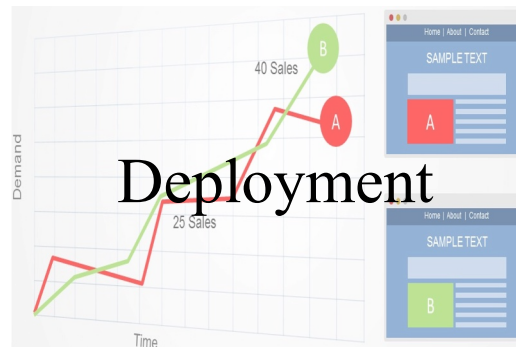


Training time
Compute credits

→ Accuracy

Adaptive experimentation:

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



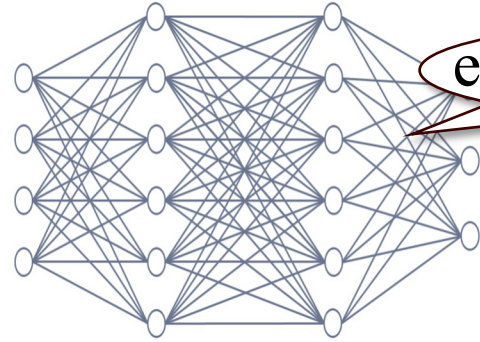
Operational cost
User experience

→ Revenue

Naïve (Non-Adaptive) Approach: Grid Search

ML model training:

Training hyperparameters



expensive-to-evaluate

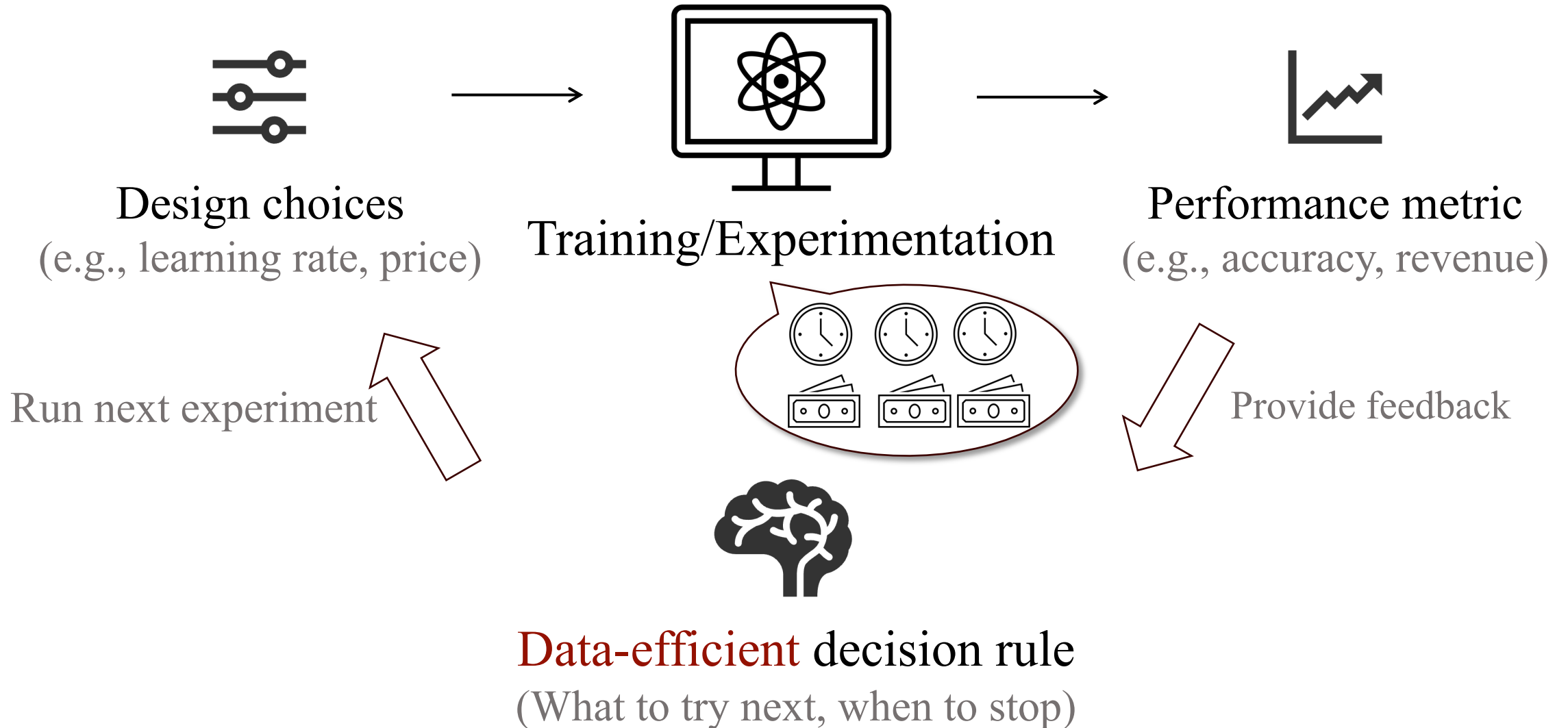


Accuracy

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:

- Grid search
- Random search
- Manual tuning

Data-driven approaches:

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

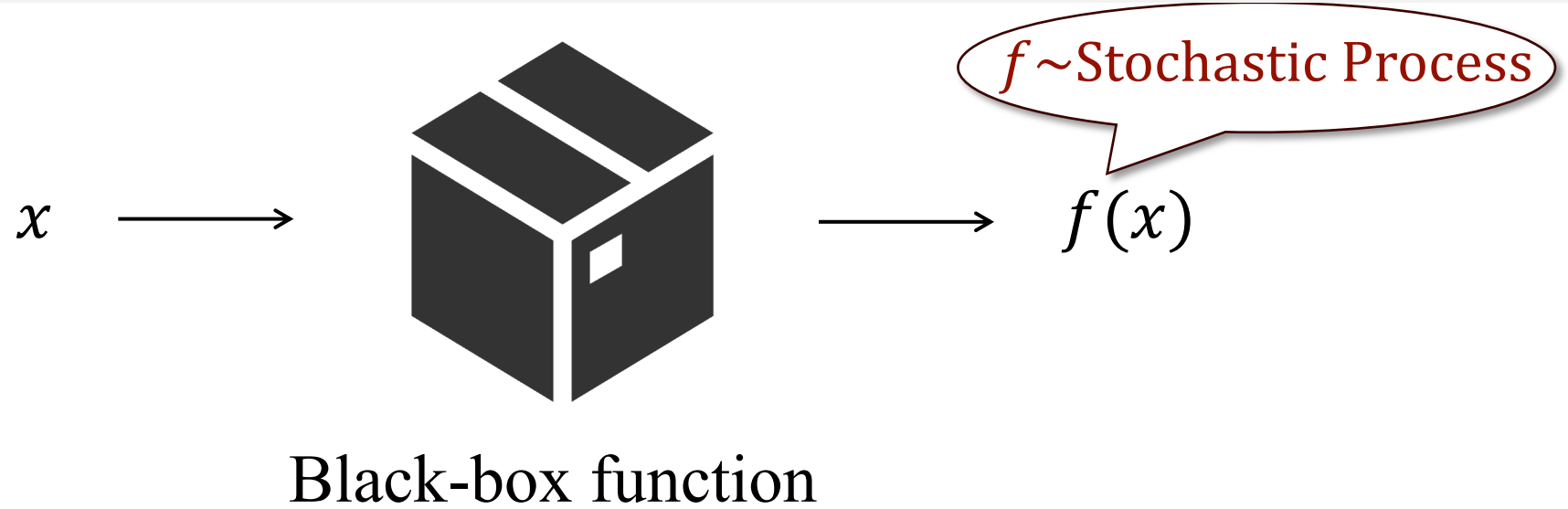
This talk's focus

💡 Contributions of new methods proposed in my work:

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

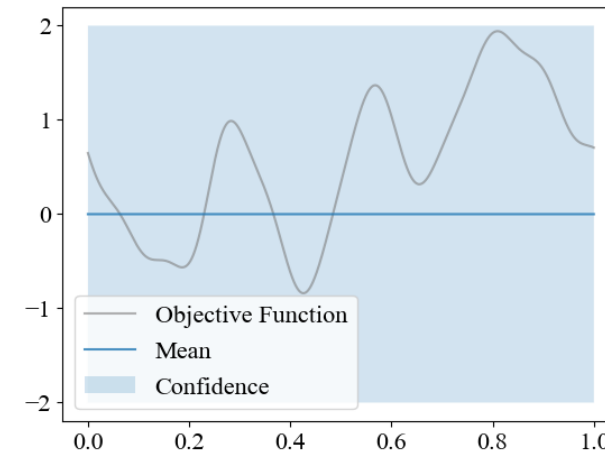
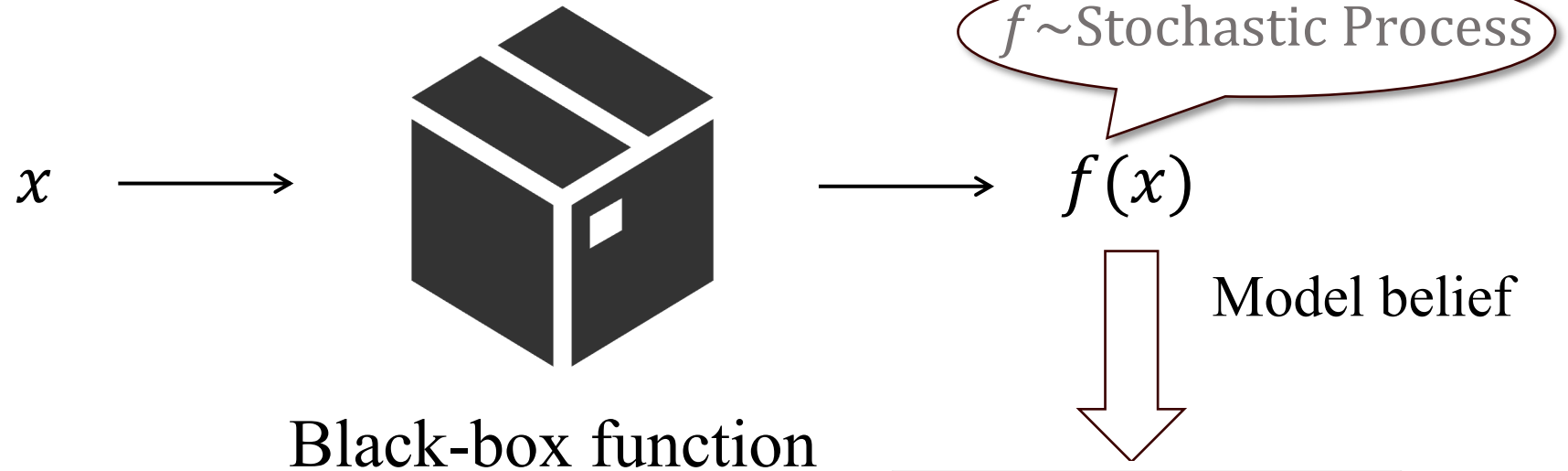
★ New methods under this umbrella

Bayesian Optimization



Bayesian Optimization

Time 0



Probabilistic model
(e.g., Gaussian process)

Bayesian Optimization

Time t

x_1, \dots, x_t



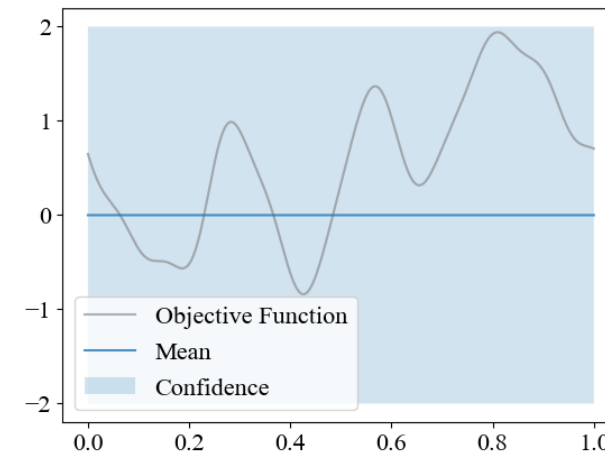
Black-box function



$f \sim \text{Stochastic Process}$

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

Model belief



Probabilistic model
(e.g., Gaussian process)

Bayesian Optimization

Time t

x_1, \dots, x_t

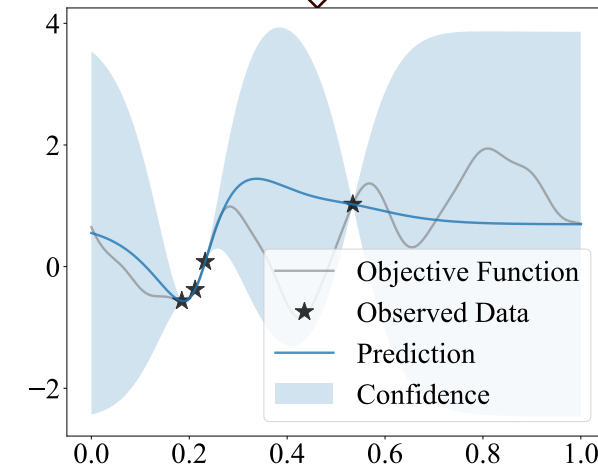


Black-box function

$f \sim \text{Stochastic Process}$

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

Update belief
(Bayes' rule)

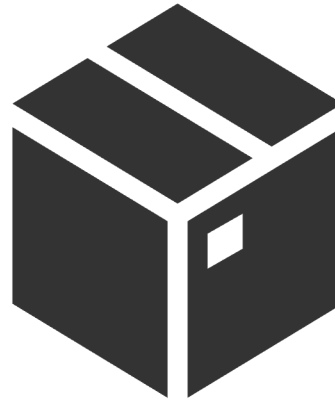
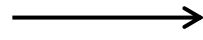


Probabilistic model
(e.g., Gaussian process)

Bayesian Optimization

Time t

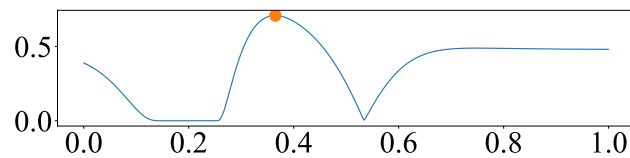
x_1, \dots, x_t



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

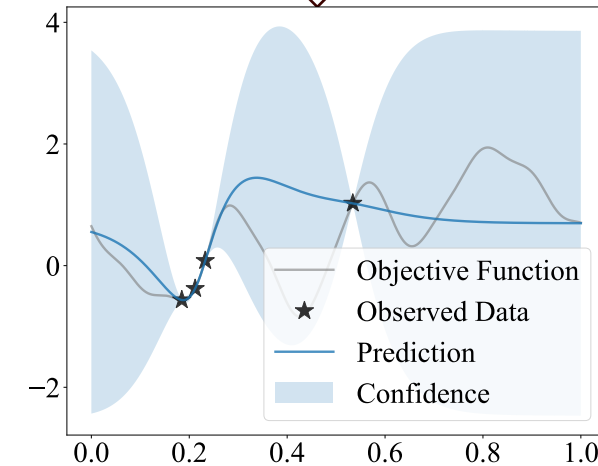
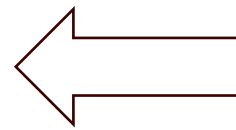
Black-box function

Update belief
(Bayes' rule)



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

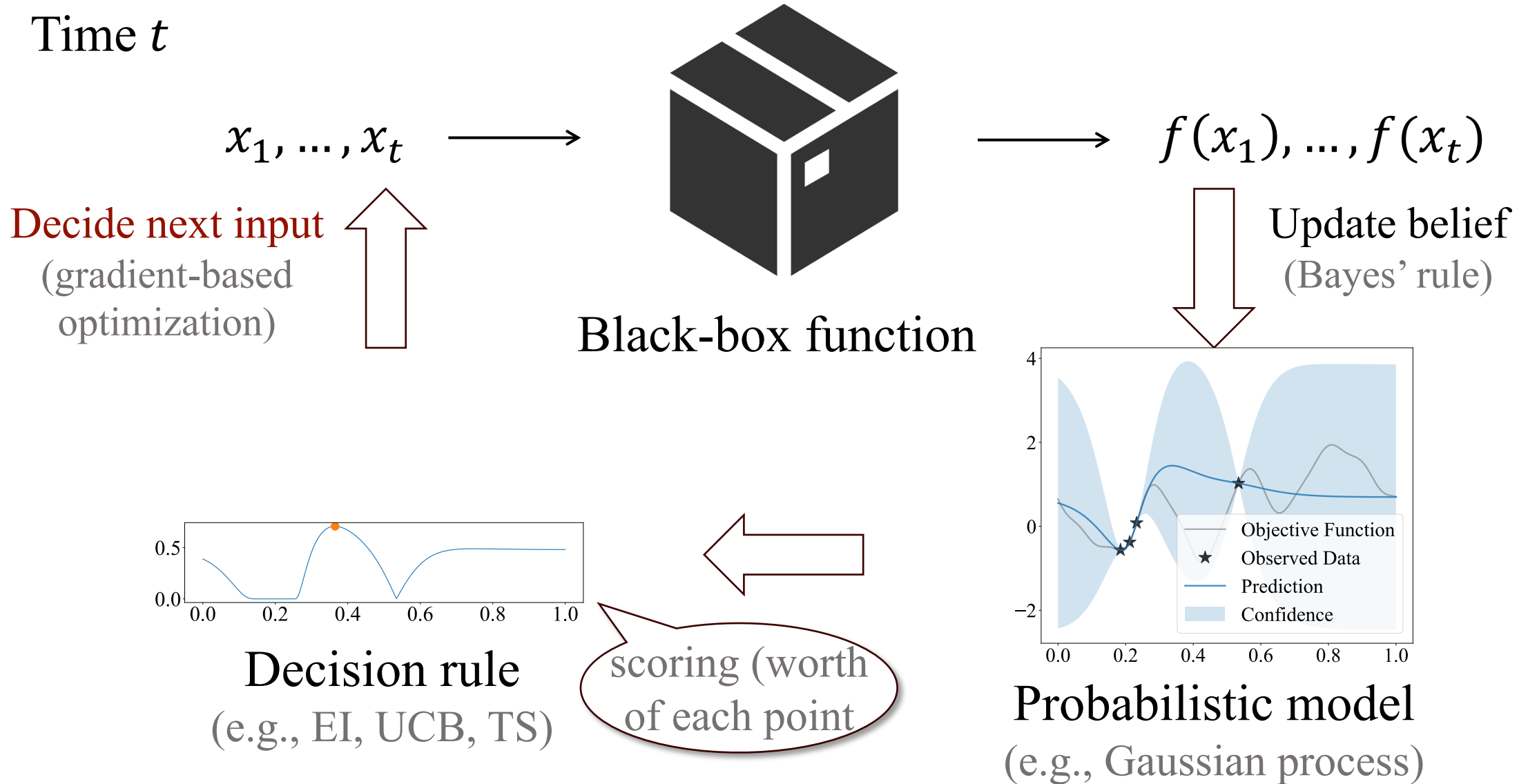
scoring (worth
of each point)



Probabilistic model
(e.g., Gaussian process)

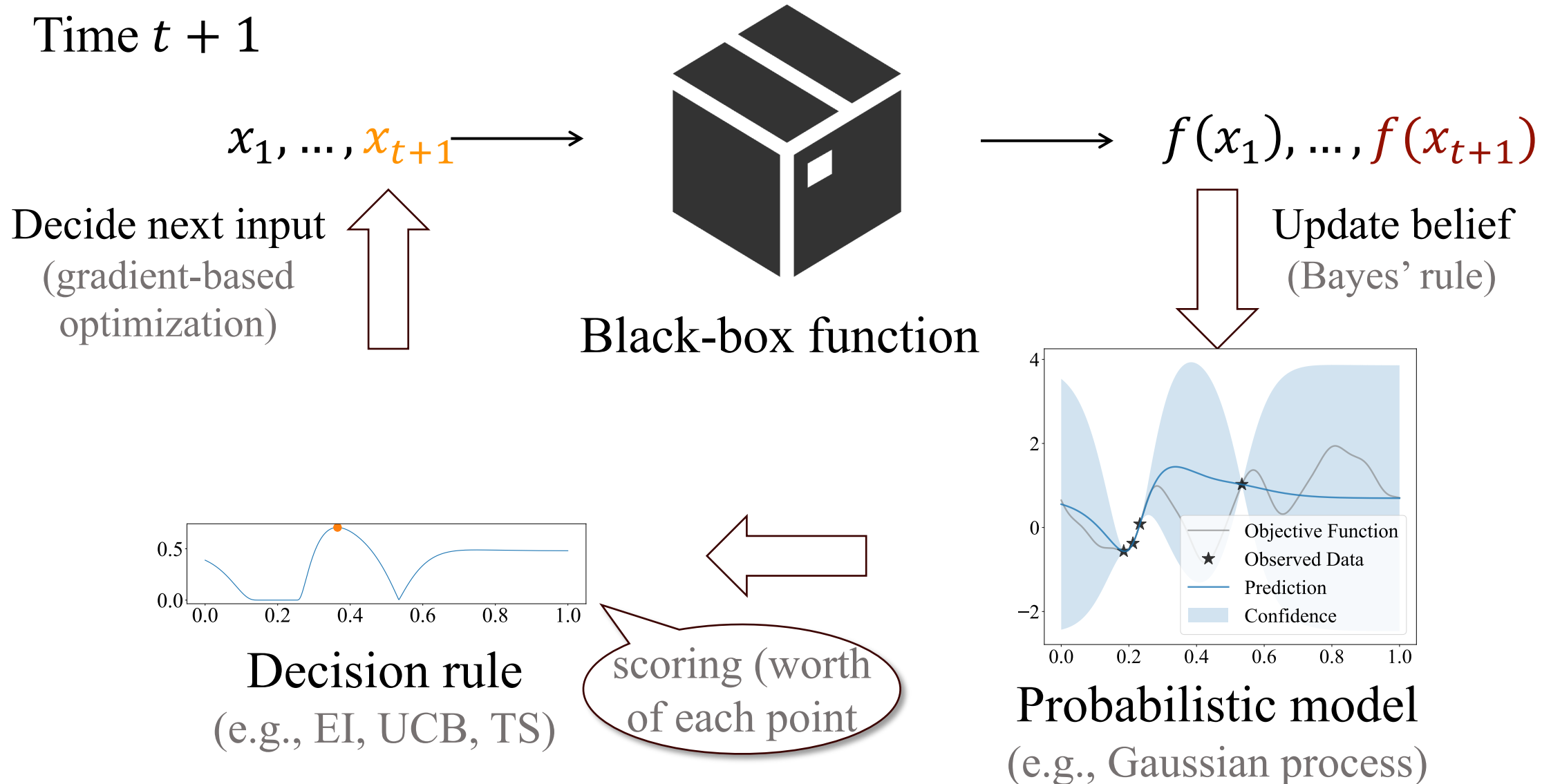
Bayesian Optimization

Time t



Bayesian Optimization

Time $t + 1$



Bayesian Optimization

Time $t + 1$

x_1, \dots, x_{t+1}



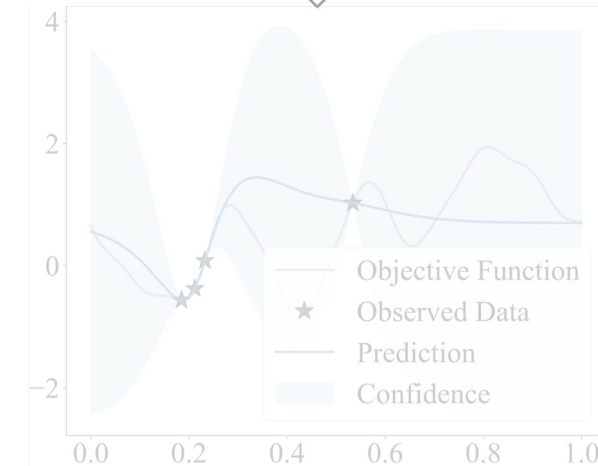
$f(x_1), \dots, f(x_{t+1})$

Decide next input
(gradient-based
optimization)



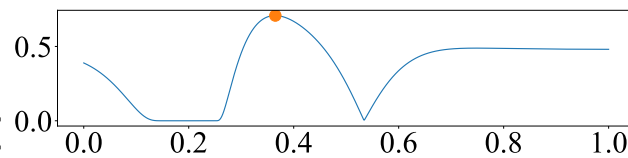
Black-box function

Update belief
(Bayes' rule)



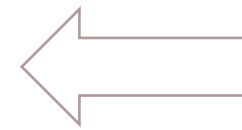
Probabilistic model
(e.g., Gaussian process)

My focus

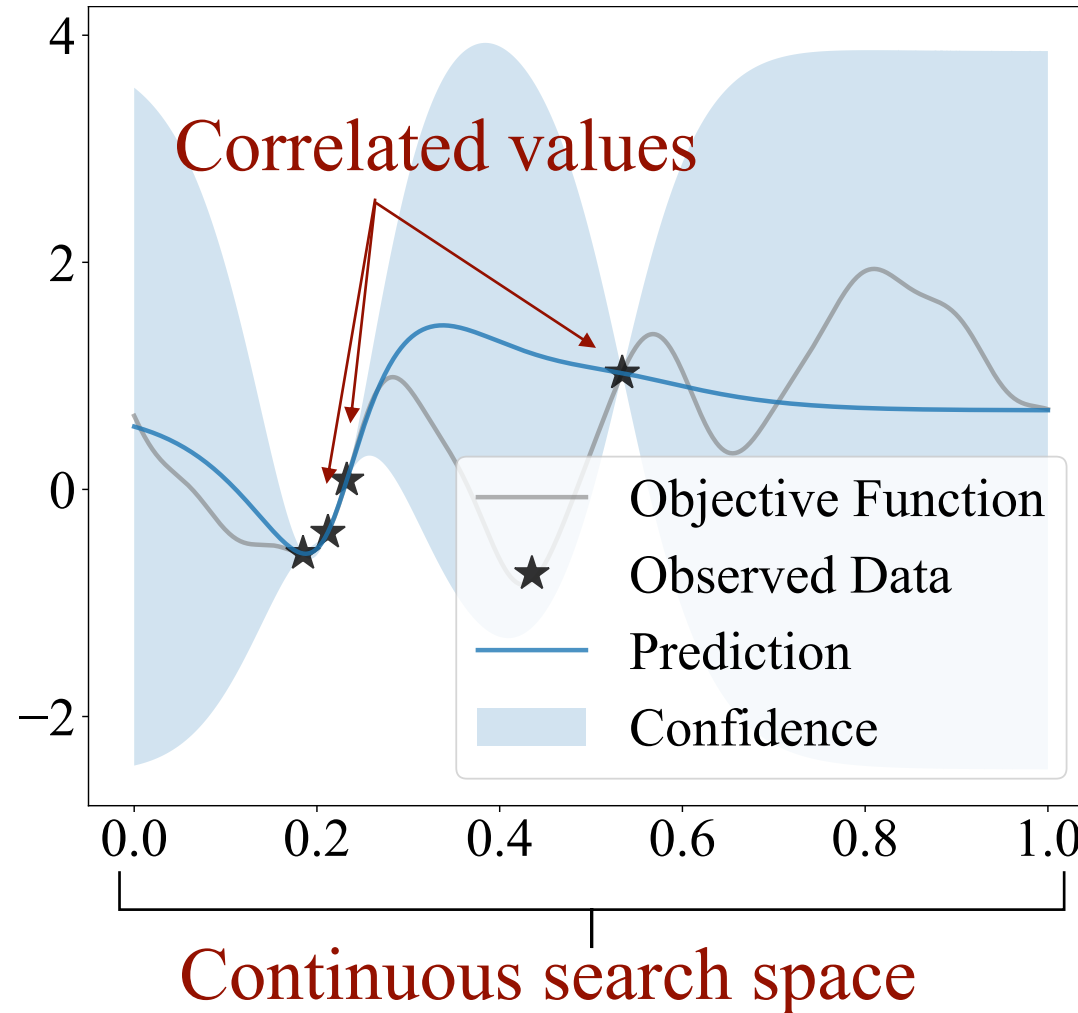


Decision rule
(e.g., EI, UCB, TS)

scoring (worth
of each point)



Challenges in Decision Rule Design



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

Popular Decision Rule: Expected Improvement

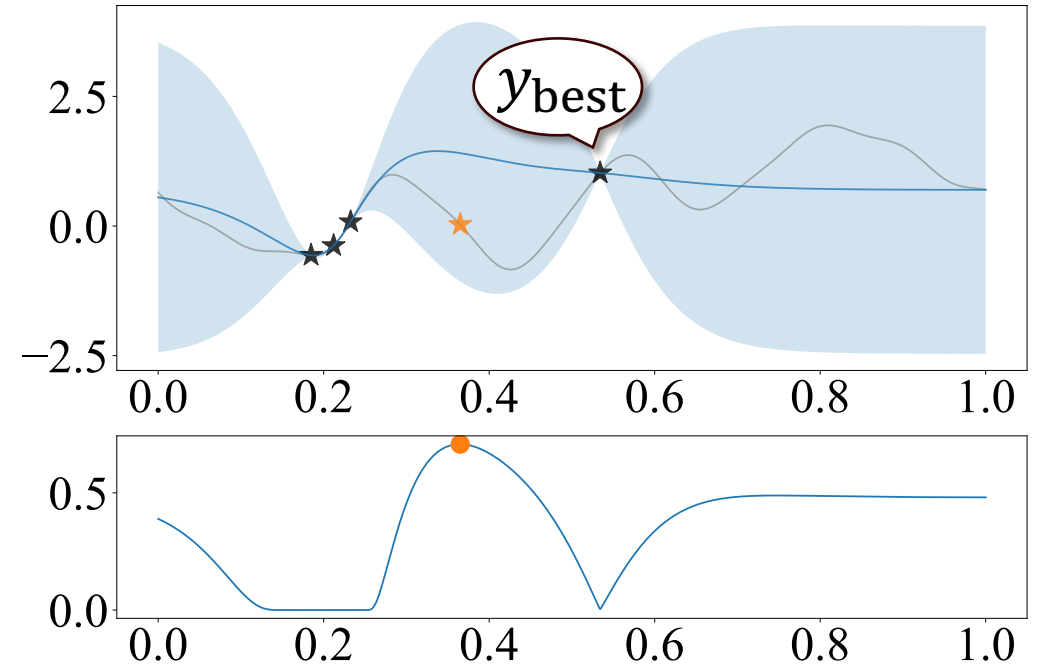
$$\text{EI}(x) = \mathbb{E}[\underbrace{\max(f(x) - y_{\text{best}}, 0)}_{\text{"improvement"}} \mid x_1, \dots, x_t]$$

current best observed data D

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

posterior distribution

One-step approximation to MDP



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

Popular Decision Rule: Expected Improvement

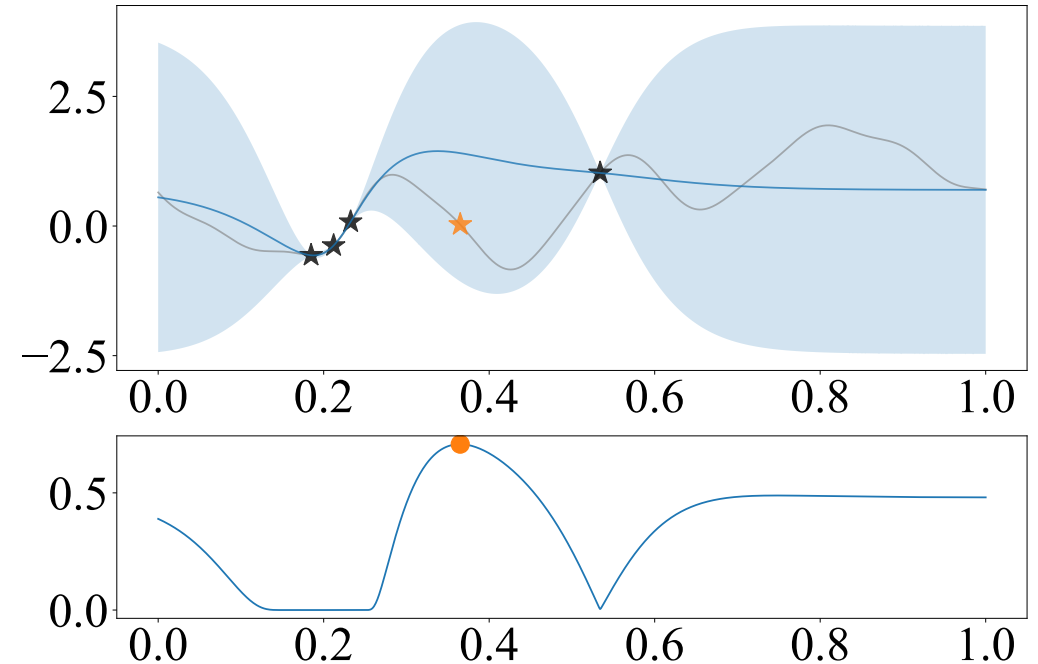
$$\text{EI}(x) = \mathbb{E}[\underbrace{\max(f(x) - y_{\text{best}}, 0)}_{\text{"improvement"}} \mid x_1, \dots, x_t]$$

current best observed data D

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

posterior distribution

One-step approximation to MDP

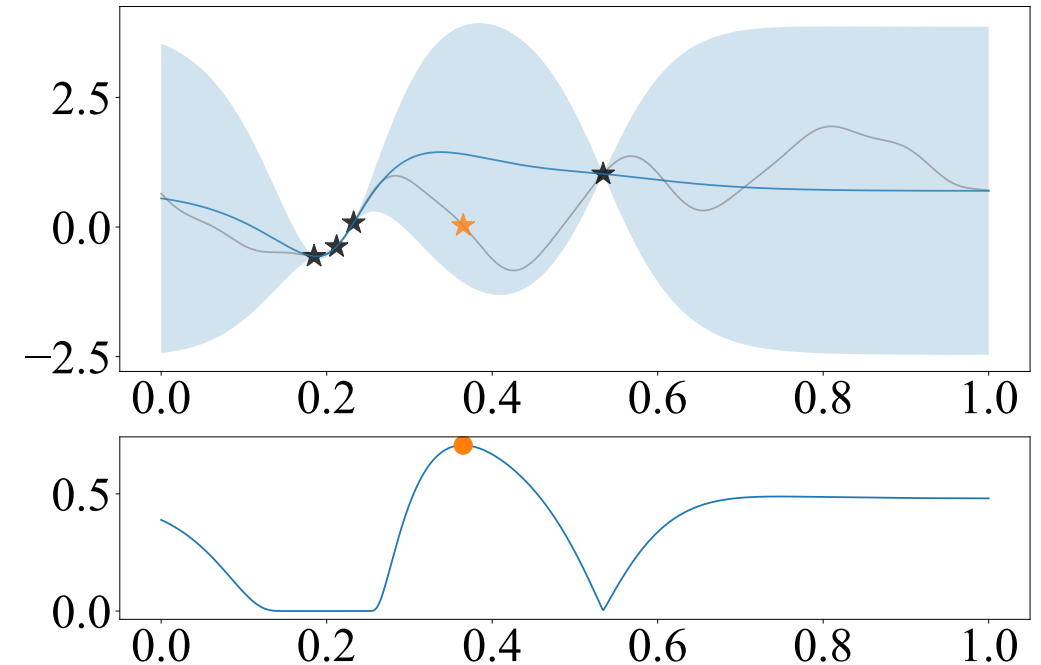


Expected improvement $\text{EI}(x)$

Improvement-based
design principle

Existing Design Principles

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

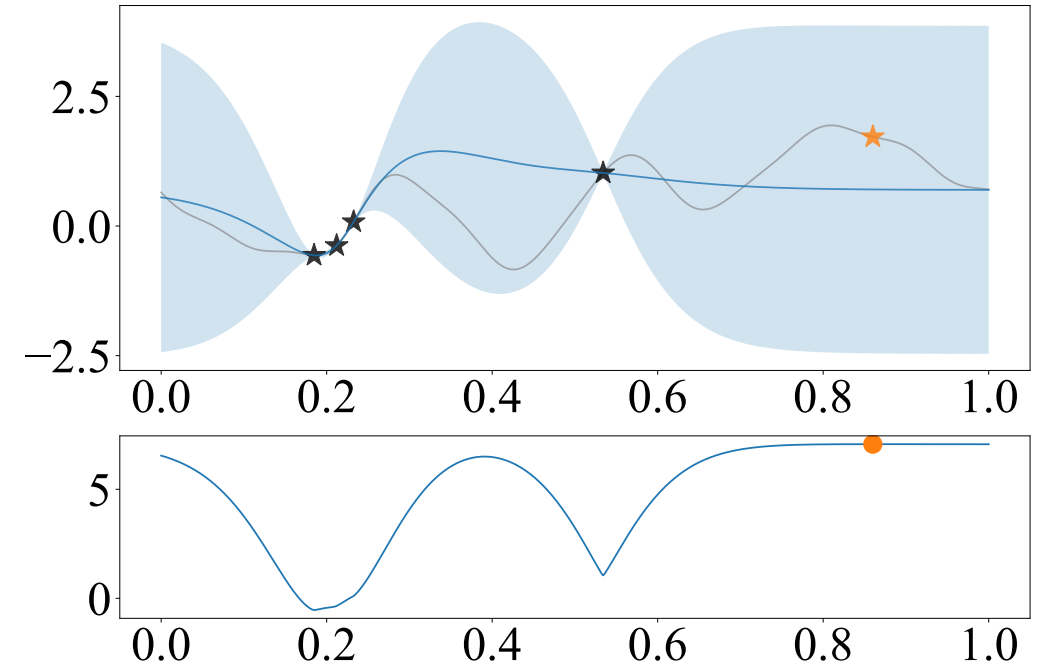


Expected improvement $EI(x)$

Improvement-based
design principle

New Design Principle: Gittins Index

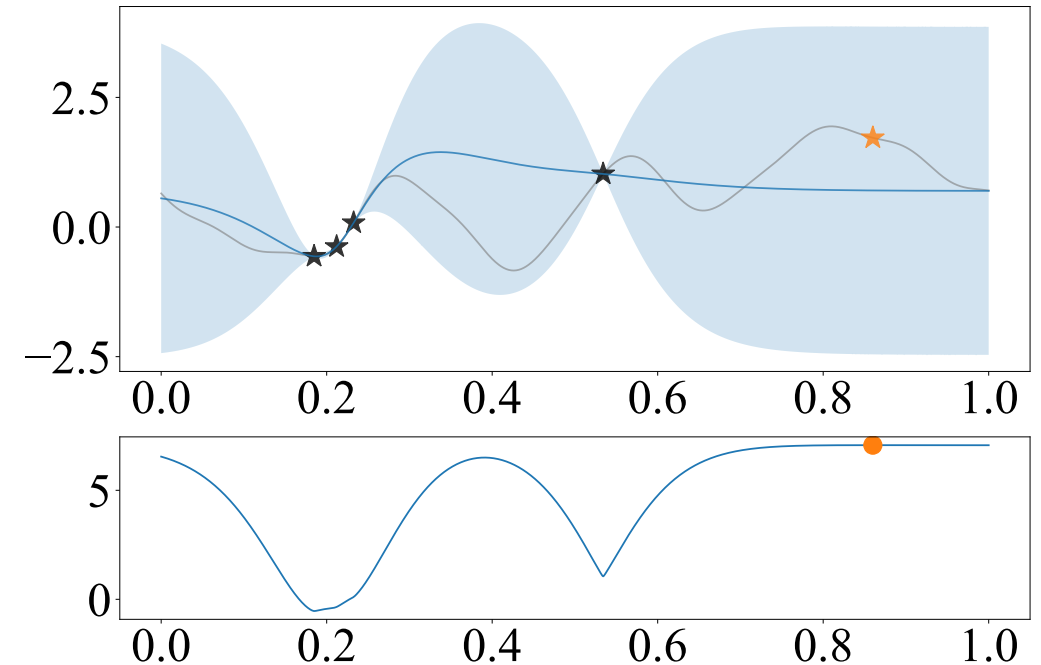
- Improvement-based (e.g., EI)
- Entropy-based
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- Thompson sampling (TS)
- Gittins Index



Gittins index $GI(x)$

New Design Principle: Gittins Index

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

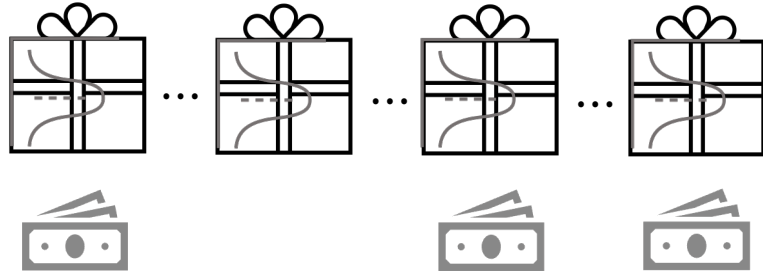


Gittins index $GI(x)$

? Why another principle?

Our Contribution: Gittins Index Principle

Novel connection

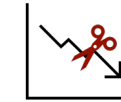


Link to **Pandora's Box** problem
& **Gittins index** theory

Principled decision rules



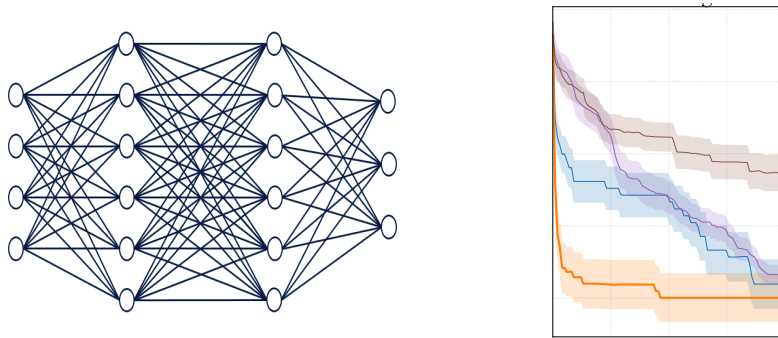
Varying evaluation costs



Adaptive stopping time

Unified framework for
selection and stopping

Competitive empirical performance

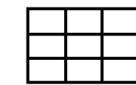


Interests from practitioners (e.g., Meta)

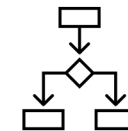
Future potential



Adaptive response sampling



Best-prompt identification

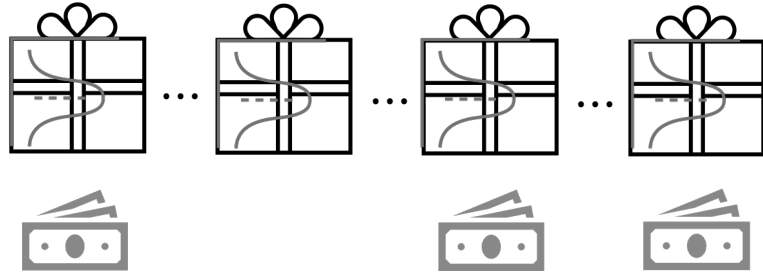


Chain-of-thought selection

Application to **efficient LLM**

Our Contribution: Gittins Index Principle

Novel connection



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

Principled decision rules



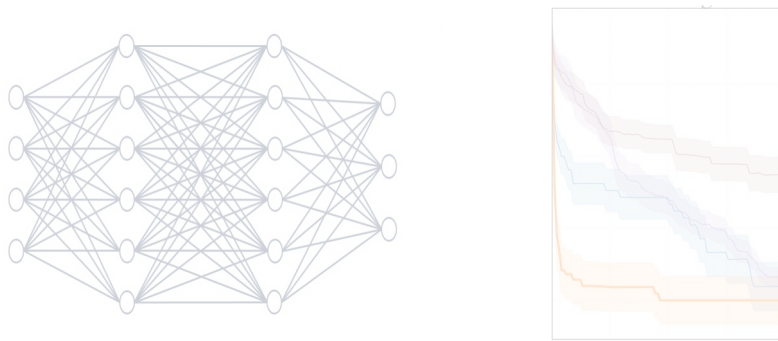
Varying evaluation costs



Adaptive stopping time

Unified framework for cost-aware
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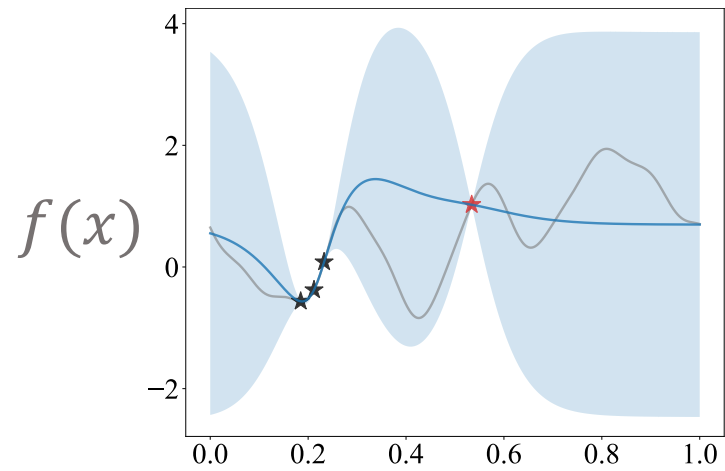


Chain-of-thought selection

Application to efficient LLM

Interests from practitioners (e.g., Meta)

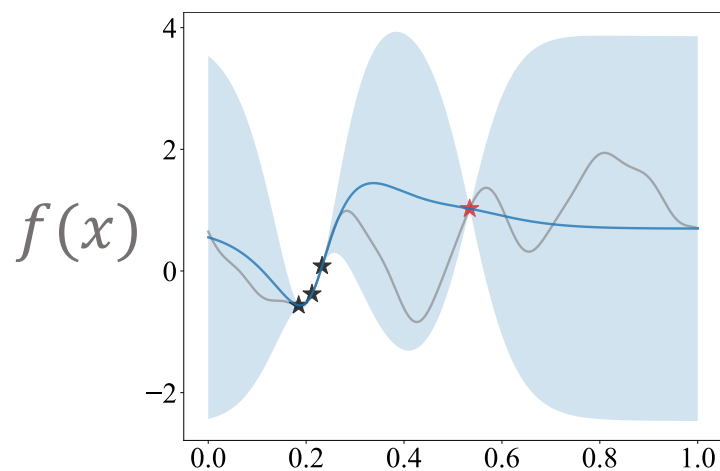
Bayesian Optimization



Continuous search space

Correlated function values

Bayesian Optimization



Continuous search space

\Rightarrow

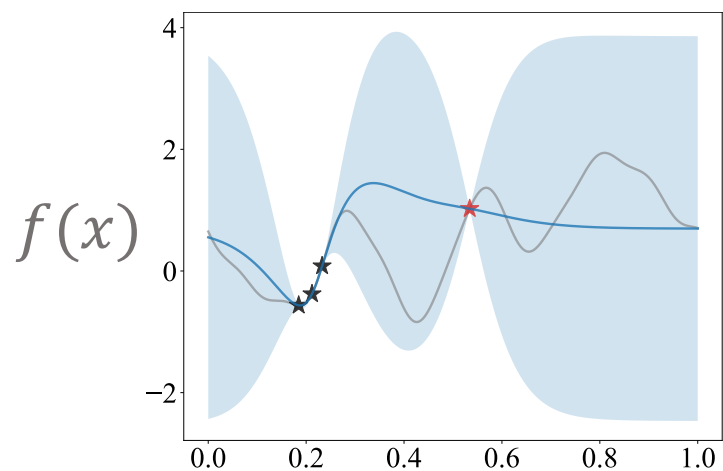
Discrete

Correlated function values

\Rightarrow

Independent

Bayesian Optimization

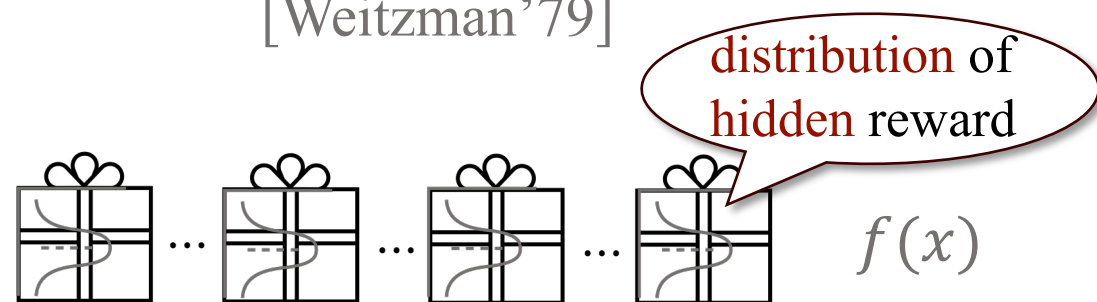


Continuous search space

Correlated function values

Pandora's Box

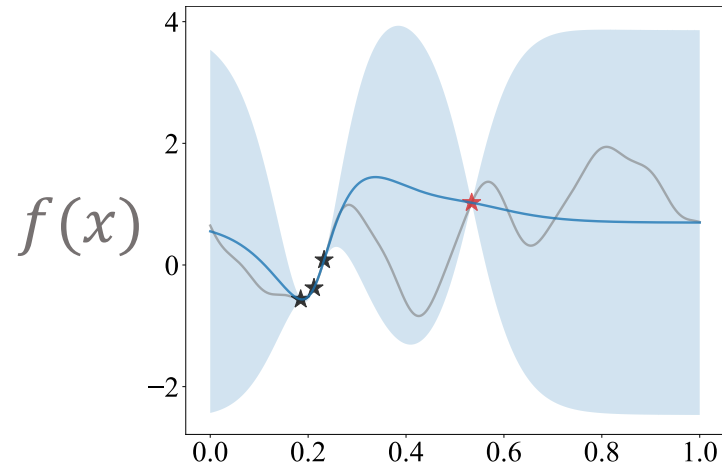
[Weitzman'79]



Discrete

Independent

Bayesian Optimization

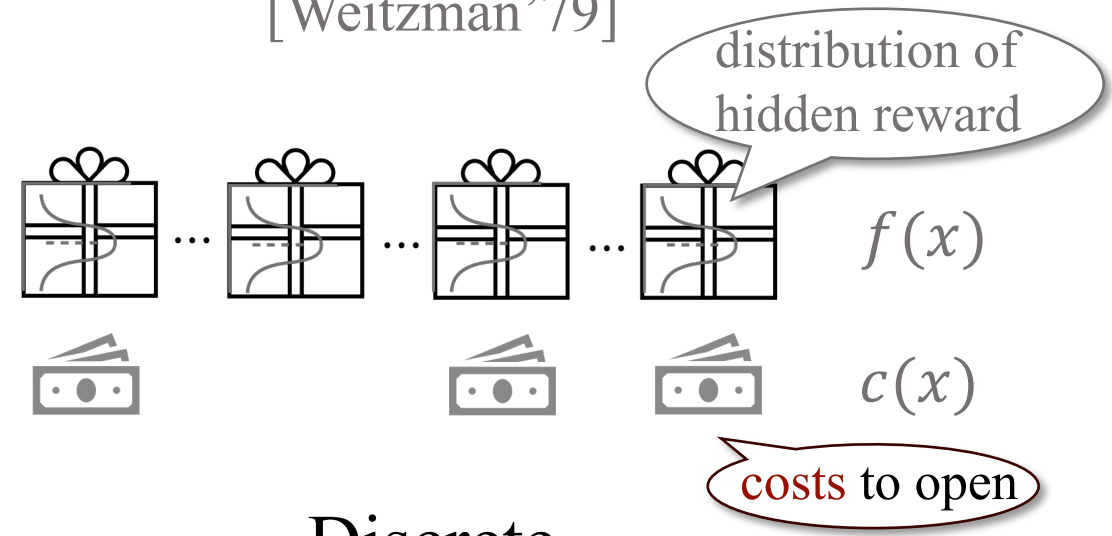


Continuous search space

Correlated function values

Pandora's Box

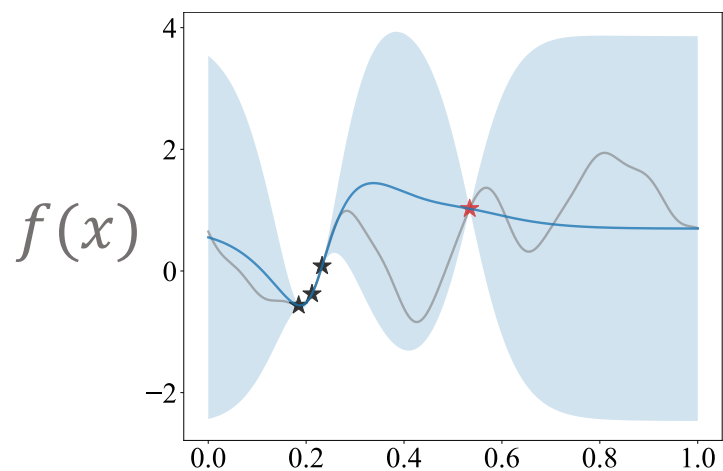
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Discrete

Independent

Bayesian Optimization

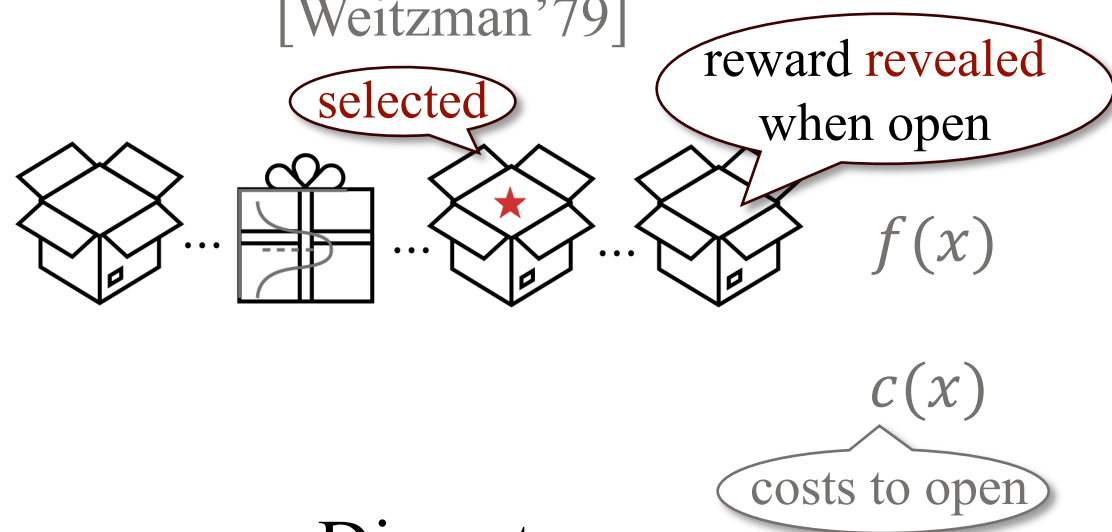


Continuous search space

Correlated function values

Pandora's Box

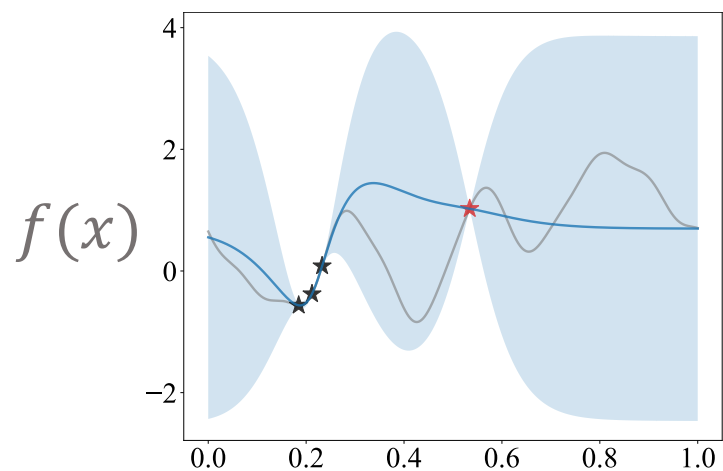
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Discrete

Independent

Bayesian Optimization

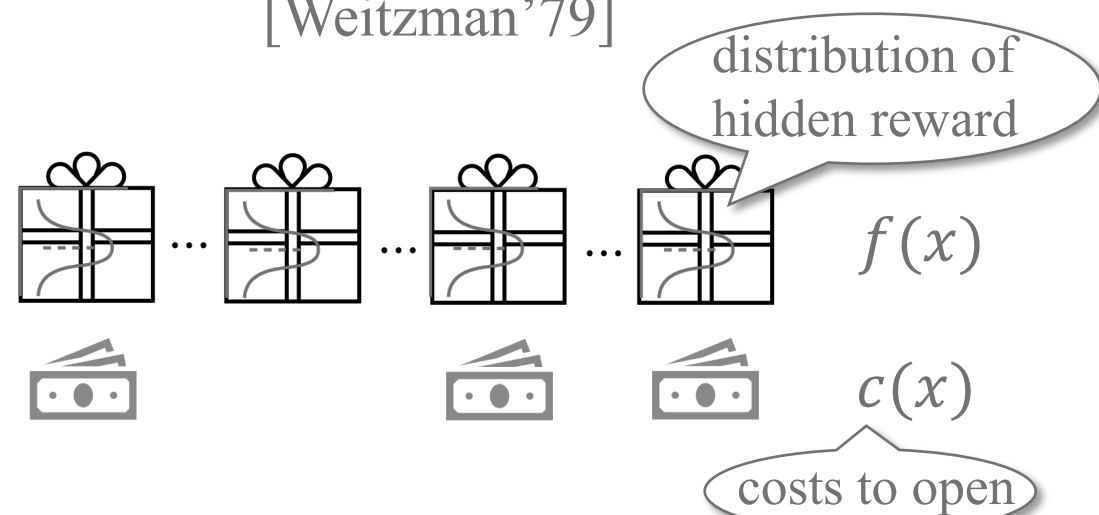


Continuous search space

Correlated function values

Pandora's Box

[Weitzman'79]

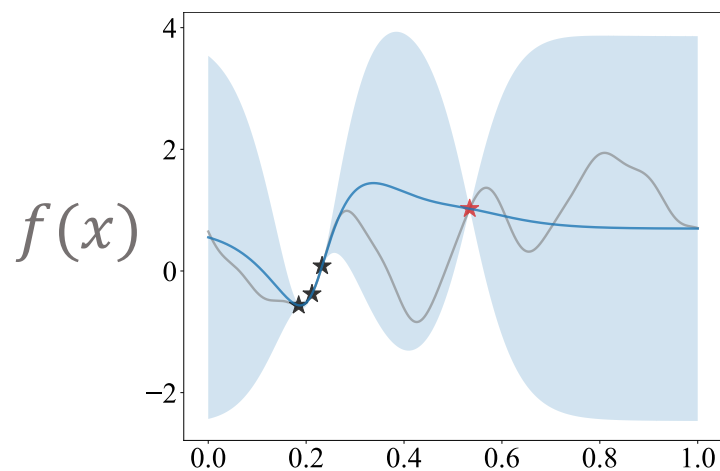


Discrete

Independent

Optimal policy: Gittins index

Bayesian Optimization

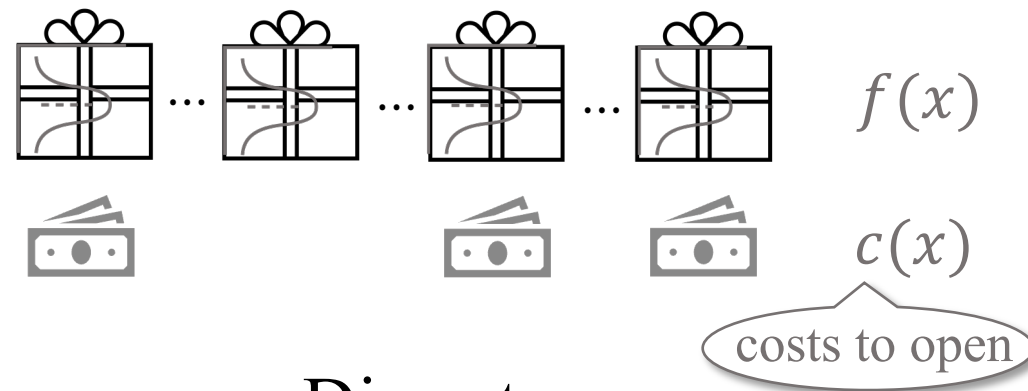


Continuous search space

Correlated function values

Pandora's Box

[Weitzman'79]



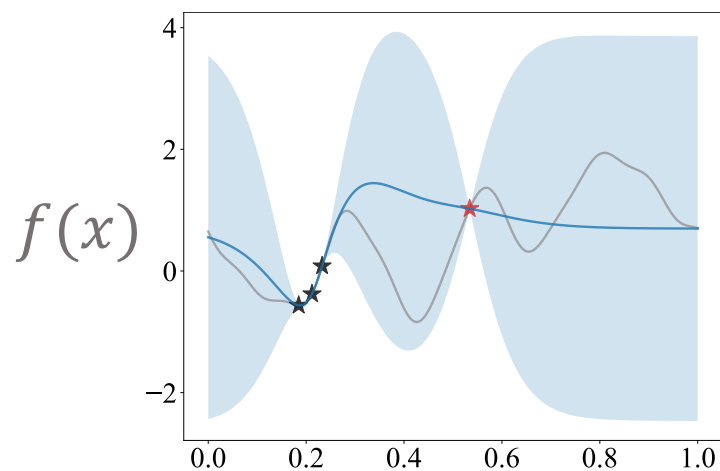
Discrete

Independent

How to translate?

⇐ Optimal policy: **Gittins index**

Bayesian Optimization

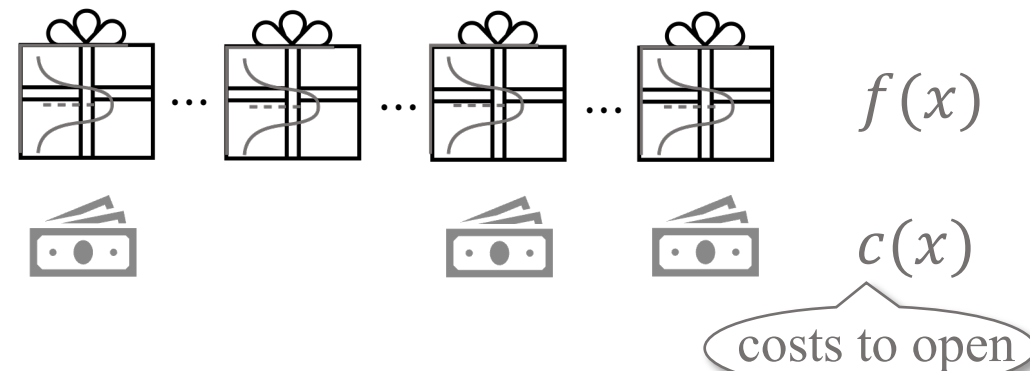


Continuous search space

Correlated function values

Pandora's Box

[Weitzman'79]



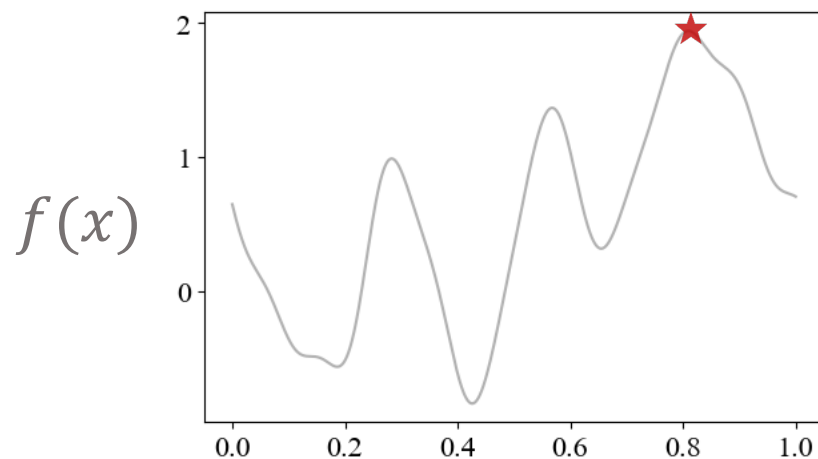
Discrete

Independent

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

incorporate posterior
take continuum limit

Bayesian Optimization

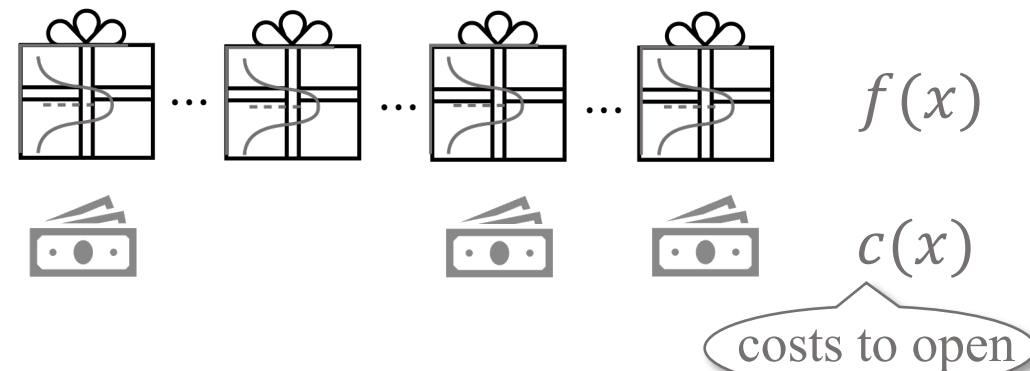


Continuous

Correlated

Pandora's Box

[Weitzman'79]



Discrete

Independent

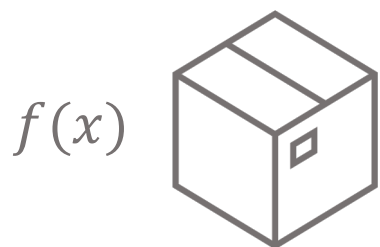
Our policy: $\text{GI}_{f|D}(x; c(x))$ $\xleftarrow[\text{take continuum limit}]{\text{incorporate posterior}}$ Optimal policy: $\text{GI}_f(x; c(x))$

How to compute?

Intuition

Exploration

Exploitation



vs.



Open closed box

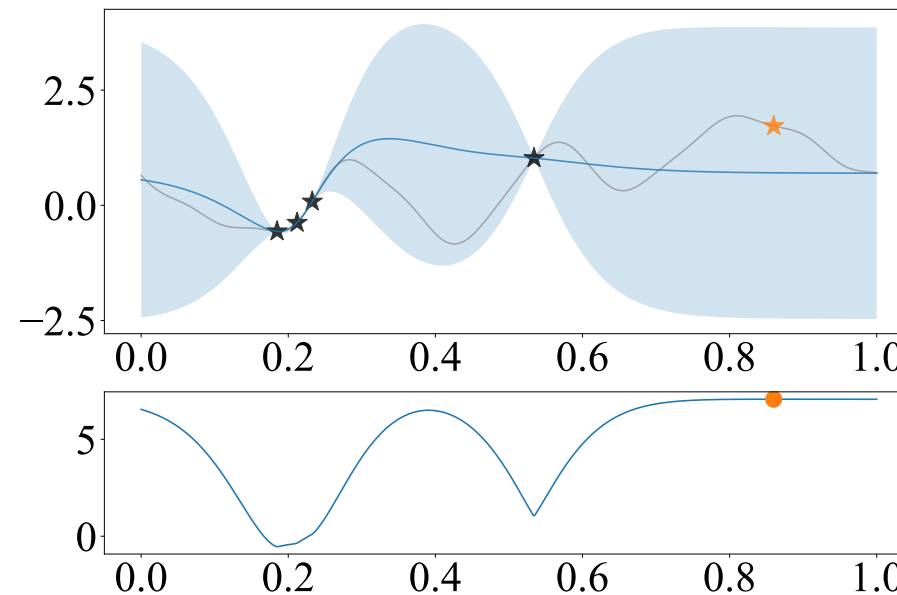
Take opened box

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

g

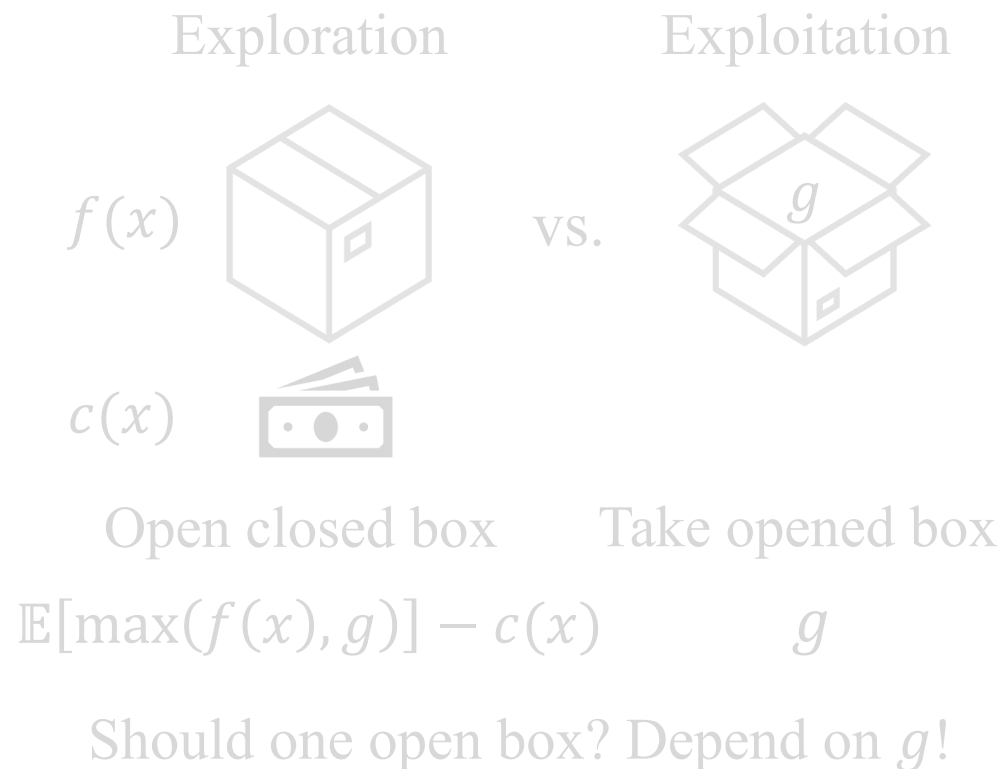
Should one open box? Depend on g !

Gittins Index

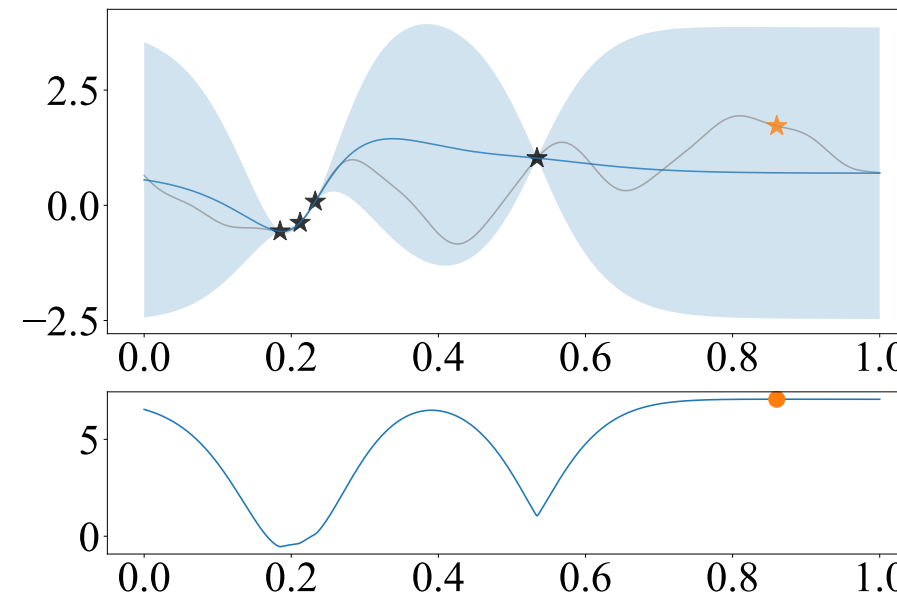


$$\text{GI}_{f|D}(x; c) := \text{solution } g \text{ s.t.} \\ \mathbb{E}[\max(f(x), g) | D] - c(x) = g$$

Intuition

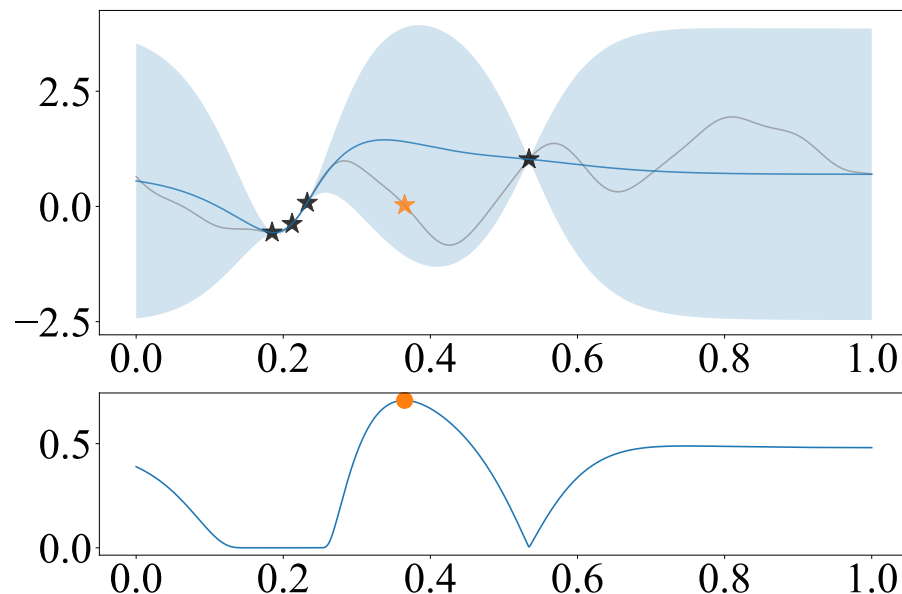


Gittins Index



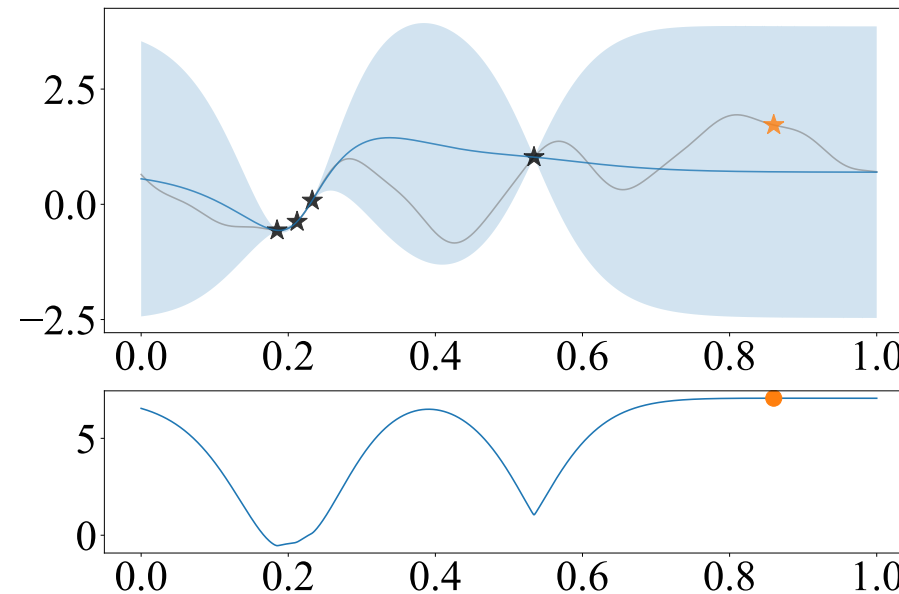
$$\begin{aligned}
 & \text{GI}_{f|D}(x; c) := \text{solution } g \text{ s.t.} \\
 & \mathbb{E}[\max(f(x), g) | D] - c(x) = g \\
 \Leftrightarrow & \mathbb{E}[\max(f(x) - g, g - g) | D] - c(x) = 0 \\
 \Leftrightarrow & \underbrace{\mathbb{E}[\max(f(x) - g, 0) | D]}_{\text{EI}_{f|D}(x; g)} = c(x)
 \end{aligned}$$

Expected Improvement



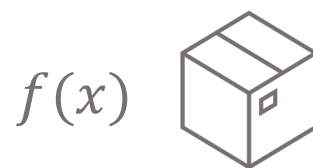
$$\text{EI}_{f|D}(x) := \mathbb{E}[\max(f(x) - y_{\text{best}}, 0) \mid D]$$

Gittins Index



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

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



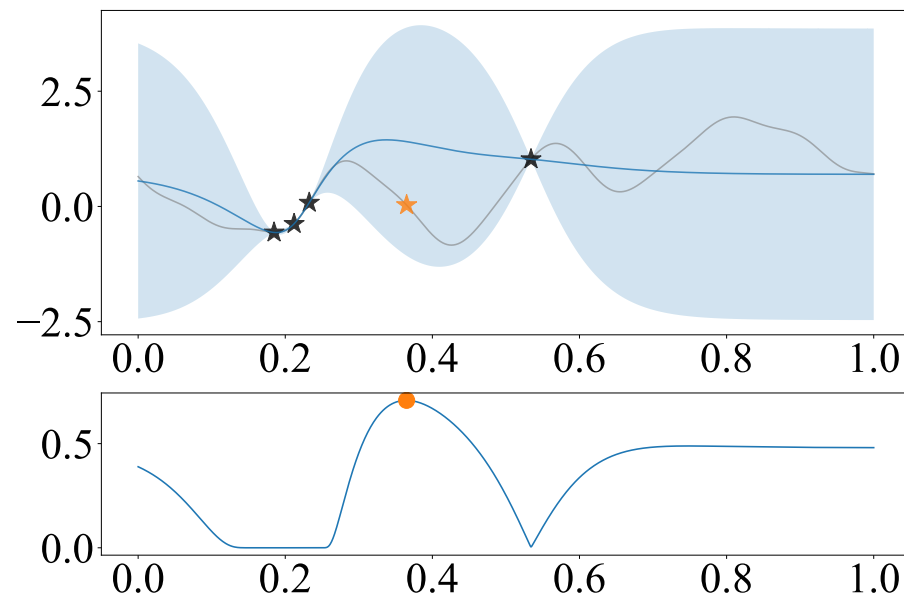
vs.



Exploration

Exploitation

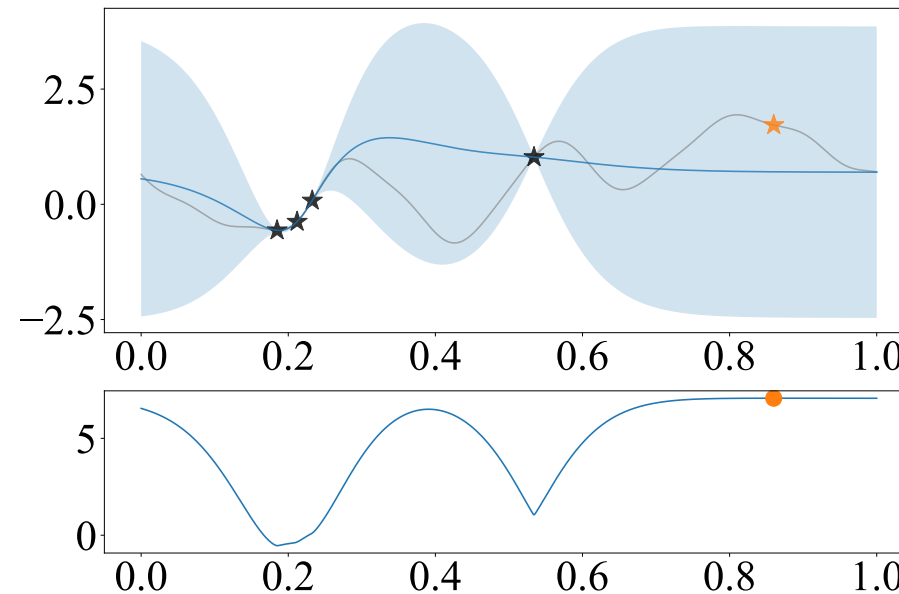
Expected Improvement



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

Temporal simplification to MDP
(One-step)

Gittins Index

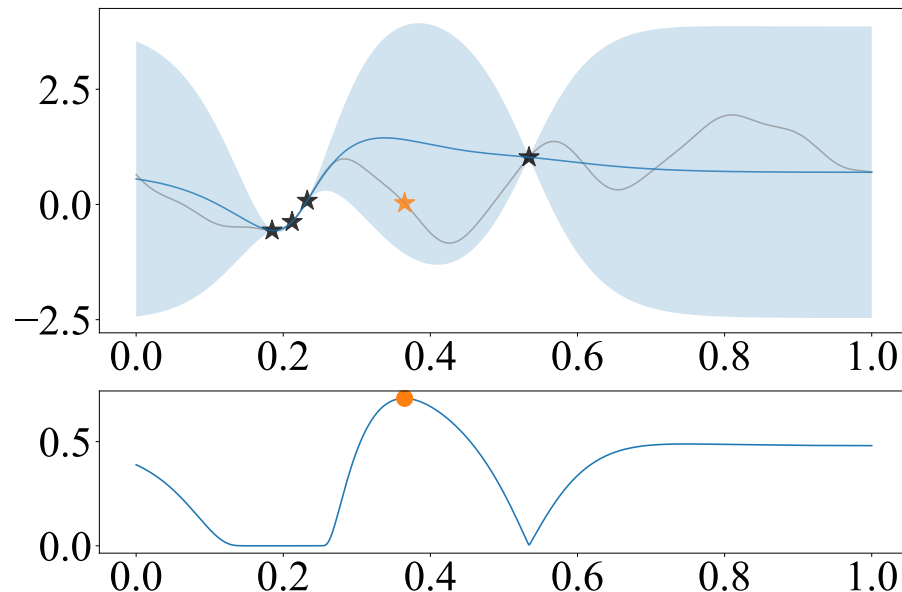


$$\text{GI}_{f|D}(x; c) := \text{solution } g \text{ s.t. } \text{EI}_{f|D}(x; g) = c(x)$$

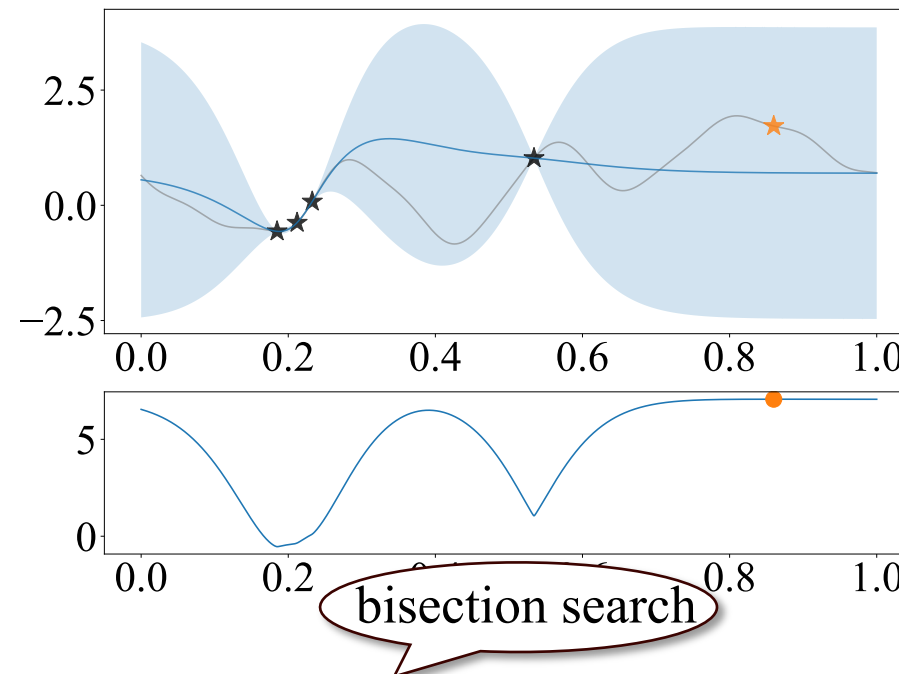
where $\text{EI}_{f|D}(x; g) := \mathbb{E}[\max(f(x) - g, 0) \mid D]$

Spatial simplification to MDP

Expected Improvement



Gittins Index



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

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

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

analytical expression

Temporal simplification to MDP

Spatial simplification to MDP

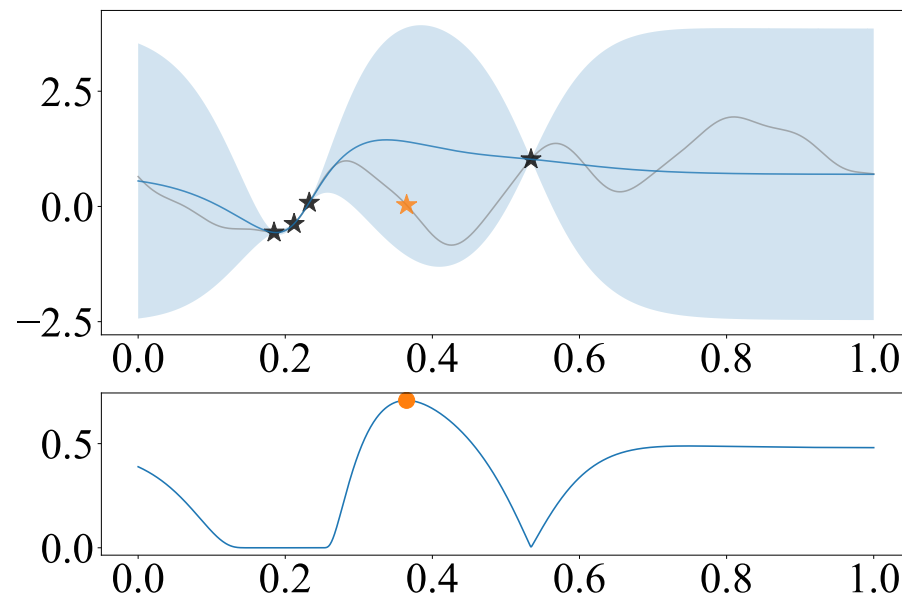


Both are **principled** and **easy-to-compute**!



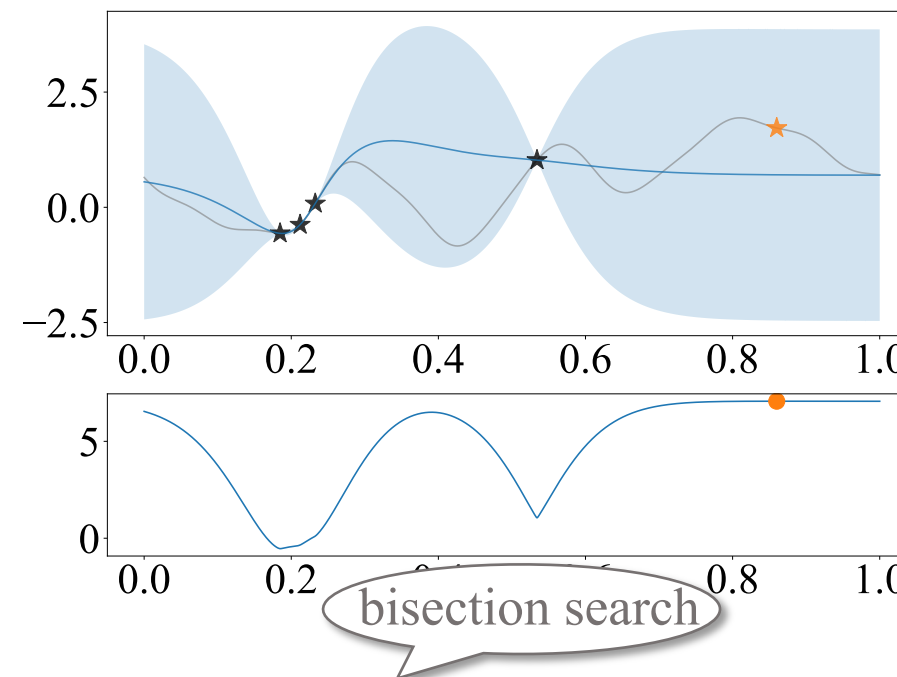
"Cost-aware Bayesian Optimization via the Pandora's Box Gittins Index." NeurIPS'24.

Expected Improvement



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

Gittins Index



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Google DeepMind

FunBO: Discovering new acquisition functions for
Bayesian Optimization with FunSearch

hard to discover GI

Our Contribution: Gittins Index Principle

Novel connection

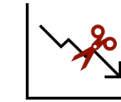


Link to Pandora's Box problem
& Gittins index theory

Principled decision rules



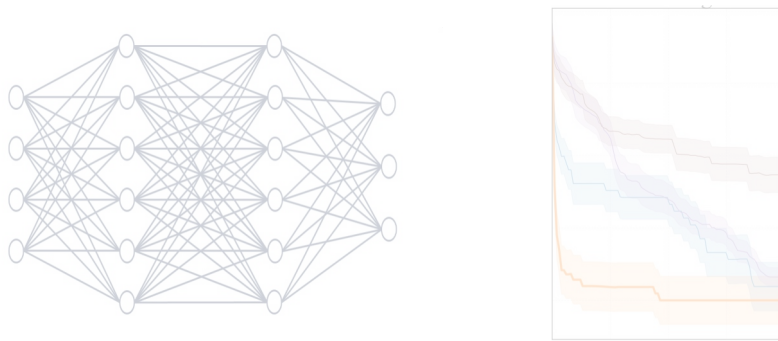
Varying evaluation costs



Adaptive stopping time

Unified framework for
selection and stopping

Competitive empirical performance



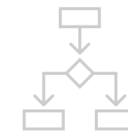
Future potential



Adaptive response sampling



Best-prompt identification

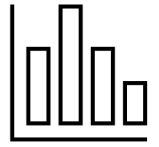


Chain-of-thought selection

Application to efficient LLM

Interests from practitioners (e.g., Meta)

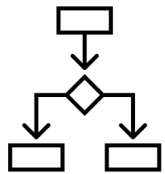
Under-explored Information for Better Decisions



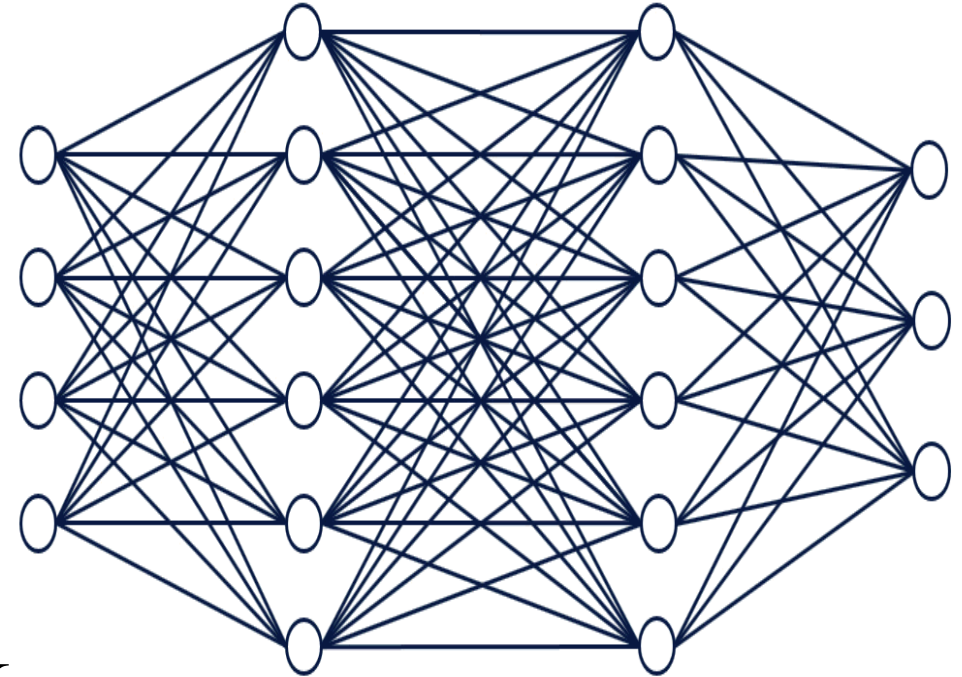
Varying evaluation costs



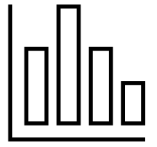
Smart stopping time



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]



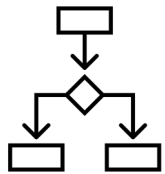
Smart stopping time

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

[Locatelli'97,
Nguyen et al.'17,

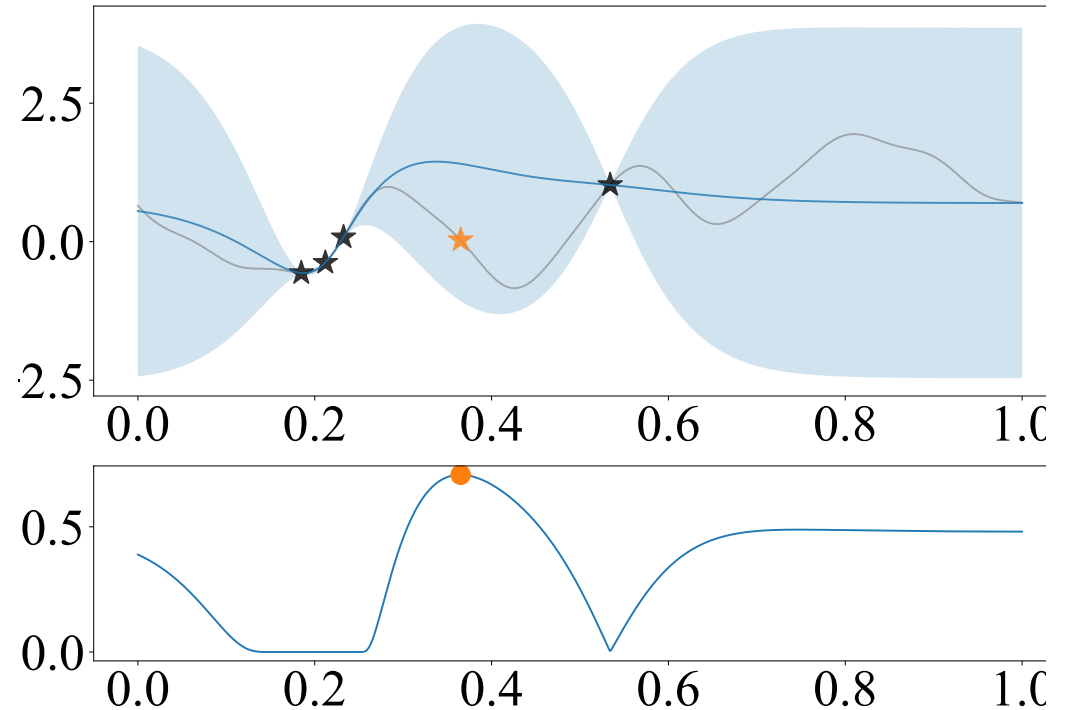
Ishibashi et al.'23]

Which threshold?



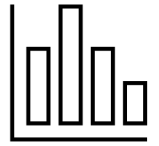
Observable multi-stage feedback

?



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

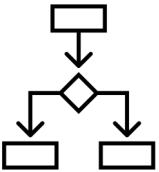
Under-explored Information for Better Decisions



Varying evaluation costs



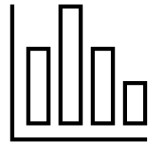
Smart stopping time



Observable multi-stage feedback

New design principle:
Gittins index

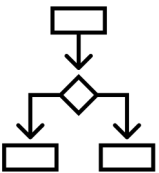
Why Gittins index?



Varying evaluation costs



Smart stopping time

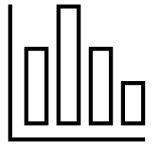


Observable multi-stage feedback

New design principle:
Gittins index

Optimal in related sequential
decision problems

Why Gittins index?



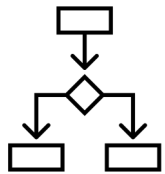
Varying evaluation costs

Features in Pandora's box



Smart stopping time

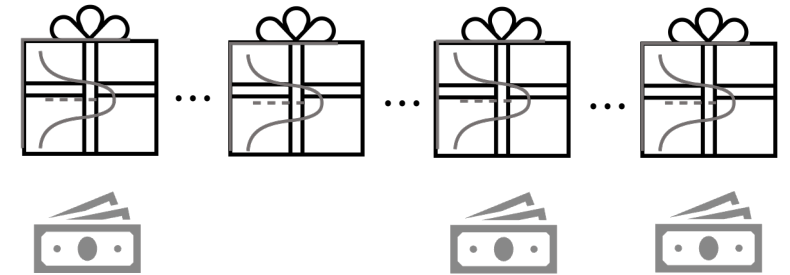
Features in Pandora's box



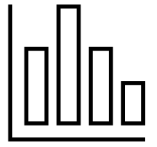
Observable multi-stage feedback

New design principle:
Gittins index

Optimal in related sequential
decision problems



Why Gittins index?



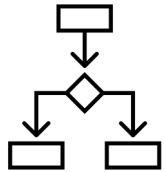
Varying evaluation costs

Features in Pandora's box



Smart stopping time

Features in Pandora's box

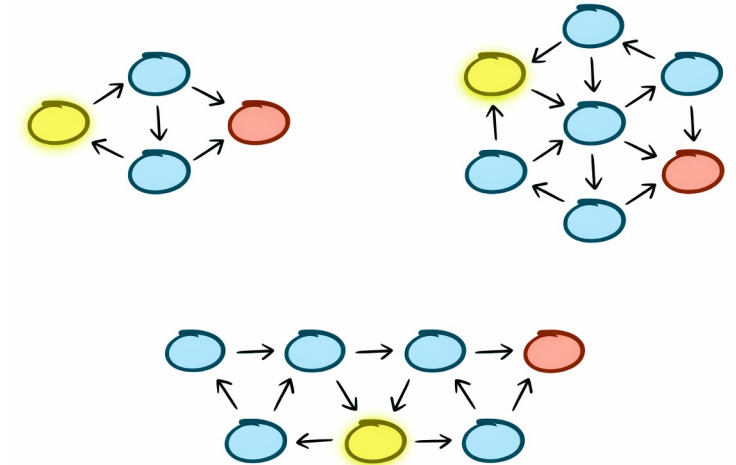


Observable multi-stage feedback

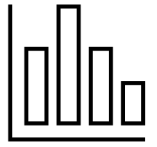
Features in **Markov chain selection**

New design principle:
Gittins index

Optimal in related sequential
decision problems



Why Gittins index?



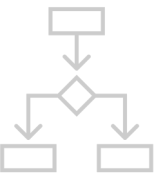
Varying evaluation costs

Features in Pandora's box



Smart stopping time

Features in Pandora's box



Observable multi-stage feedback

Features in Markov chain selection

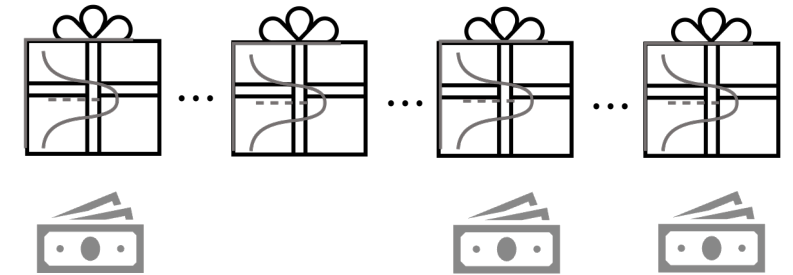


"Cost-aware Bayesian Optimization via the Pandora's Box Gittins Index." NeurIPS'24.

This talk's focus

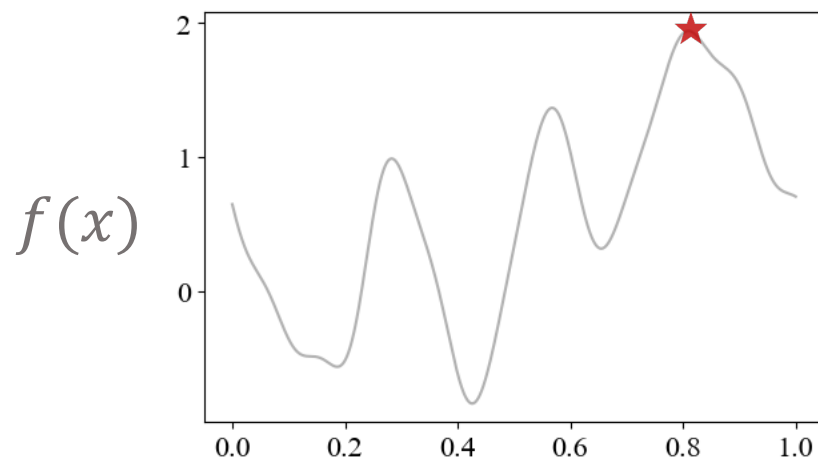
New design principle:
Gittins index

Optimal in related sequential
decision problems



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

Bayesian Optimization



Continuous

Correlated

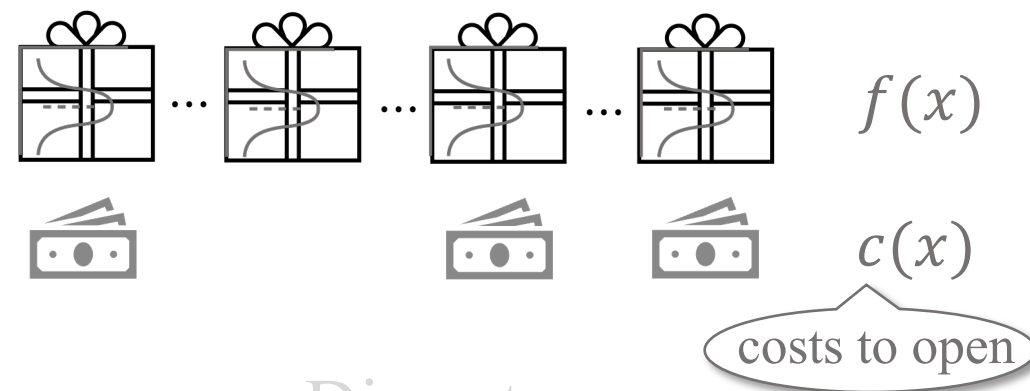
Cost-unaware

Fixed-iteration

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

Pandora's Box

[Weitzman'79]



Discrete

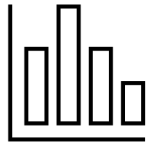
Independent

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

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

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:

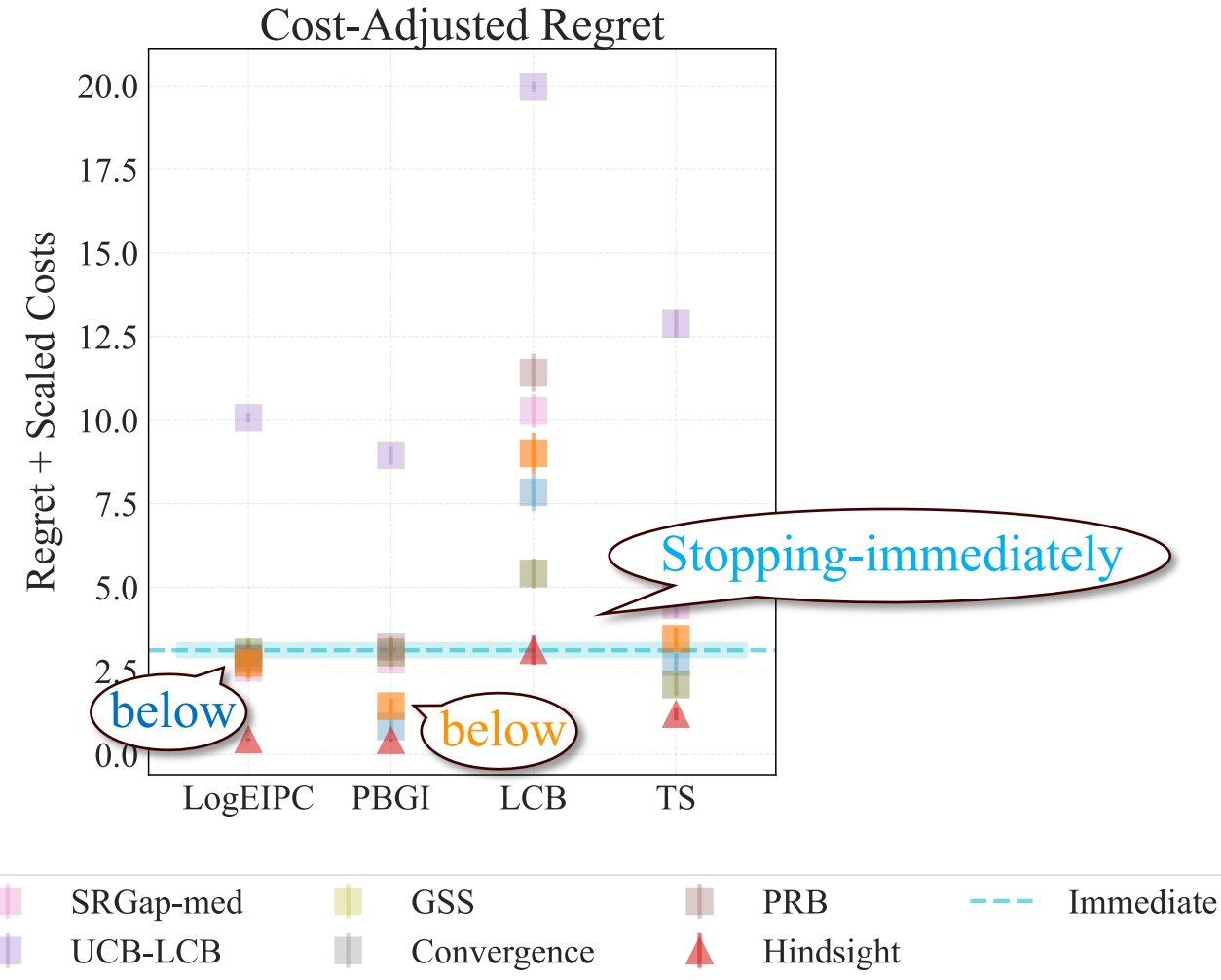
- Matches the **best achievable performance in the worst case** (evaluations are all very costly).

- 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



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

Our Contribution: Gittins Index Principle

Novel connection



Link to Pandora's Box problem
& Gittins index theory

Principled decision rules



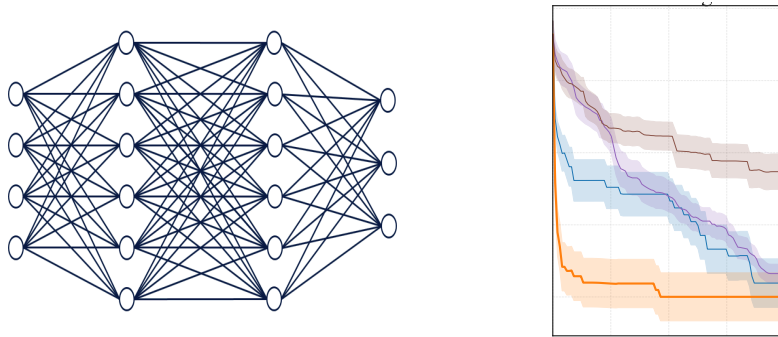
Varying evaluation costs



Adaptive stopping time

Unified framework for
selection and stopping

Competitive empirical performance



Interests from practitioners (e.g., Meta)

Future potential



Adaptive response sampling



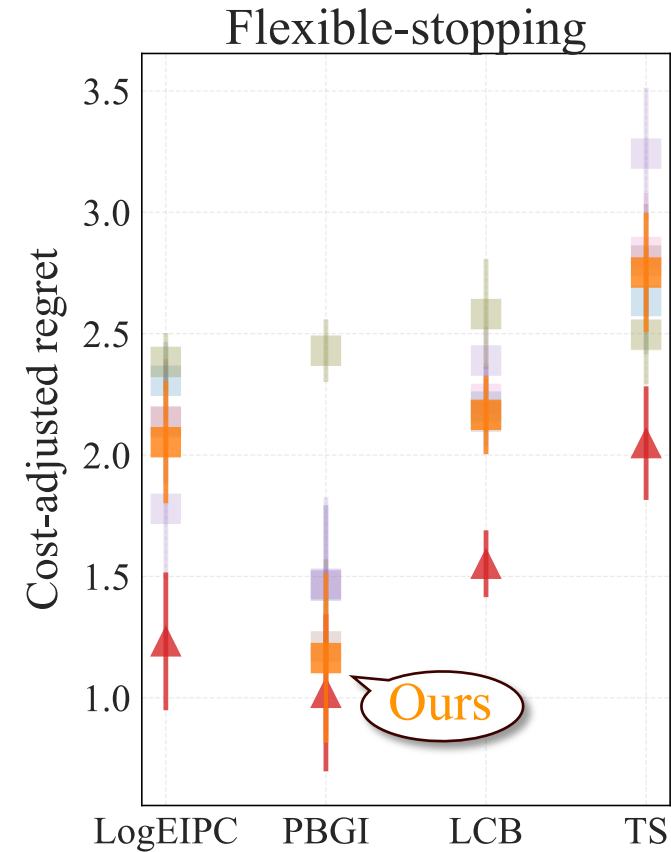
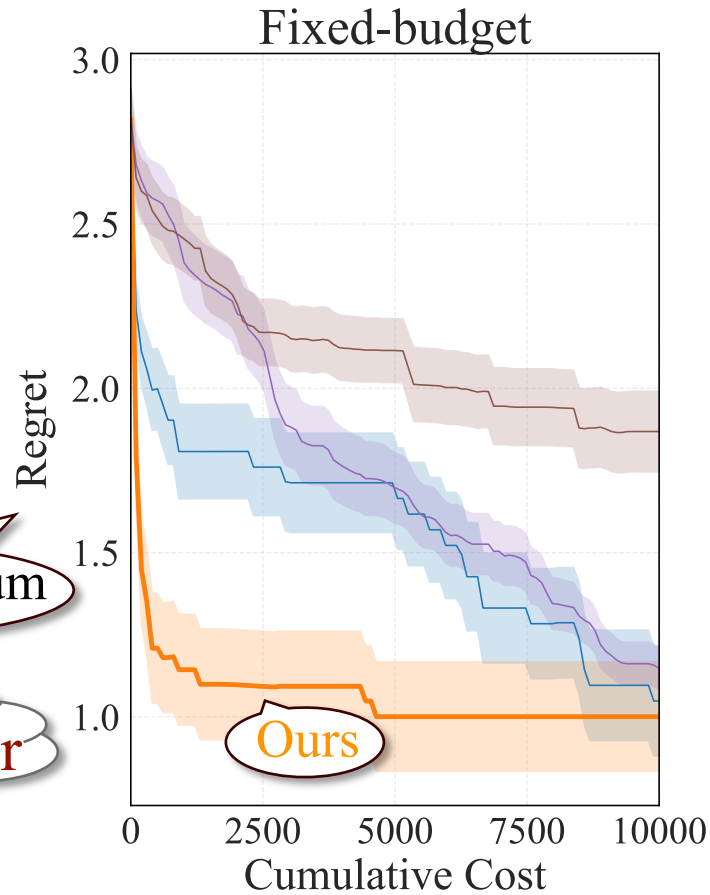
Best-prompt identification



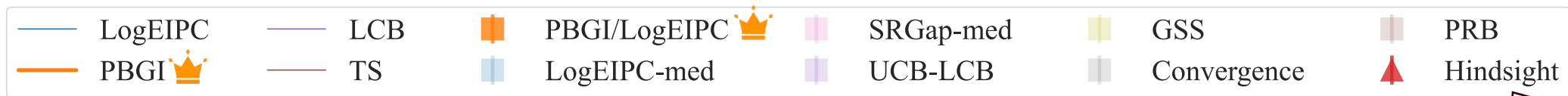
Chain-of-thought selection

Application to efficient LLM

Gittins Index vs Baselines on AutoML Benchmark



Lower the better



Selection rules

Stopping rules

Not a real baseline

Our Contribution: Gittins Index Principle

Novel connection



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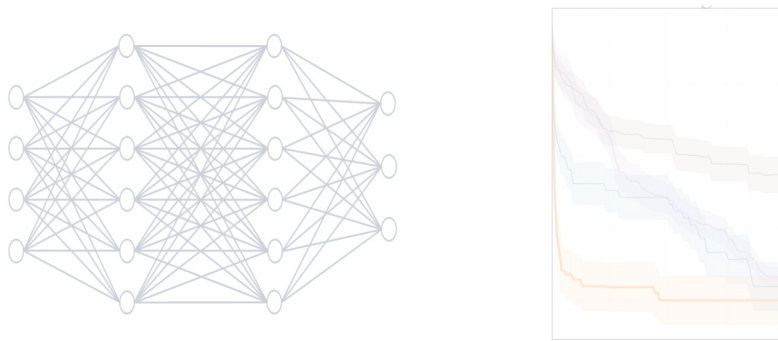
Varying evaluation costs



Adaptive stopping time

Unified framework for cost-aware
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Competitive empirical performance

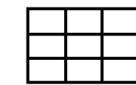


Interests from practitioners (e.g., Meta)

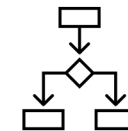
Future potential



Adaptive response sampling



Best-prompt identification

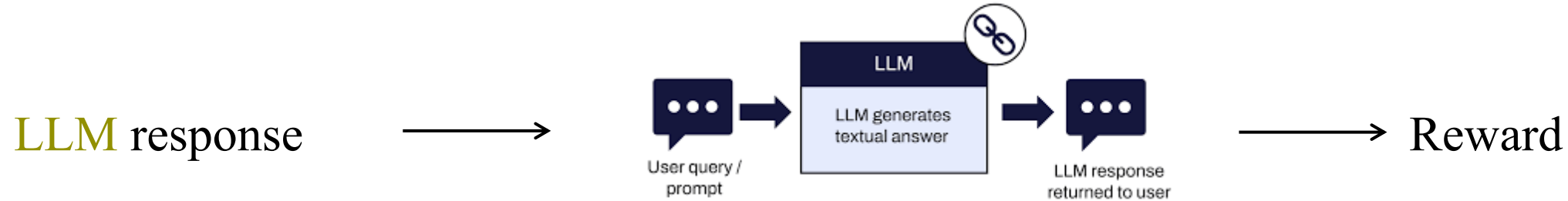


Chain-of-thought selection

Application to **efficient LLM**

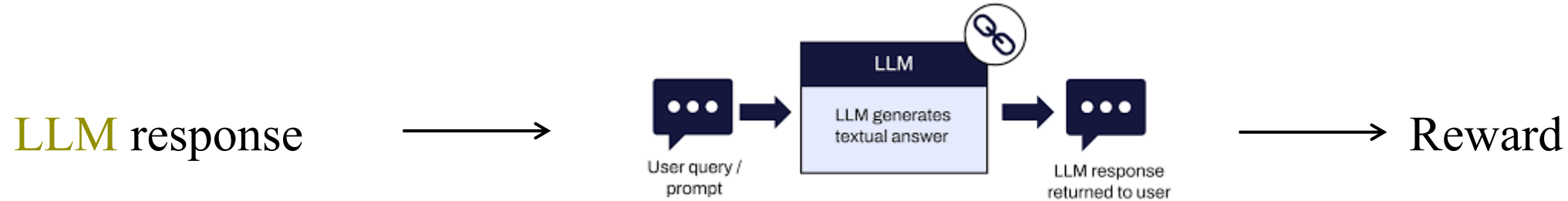
Adaptive Response Sampling in LLM Inference

LLM inference time alignment (optimization):



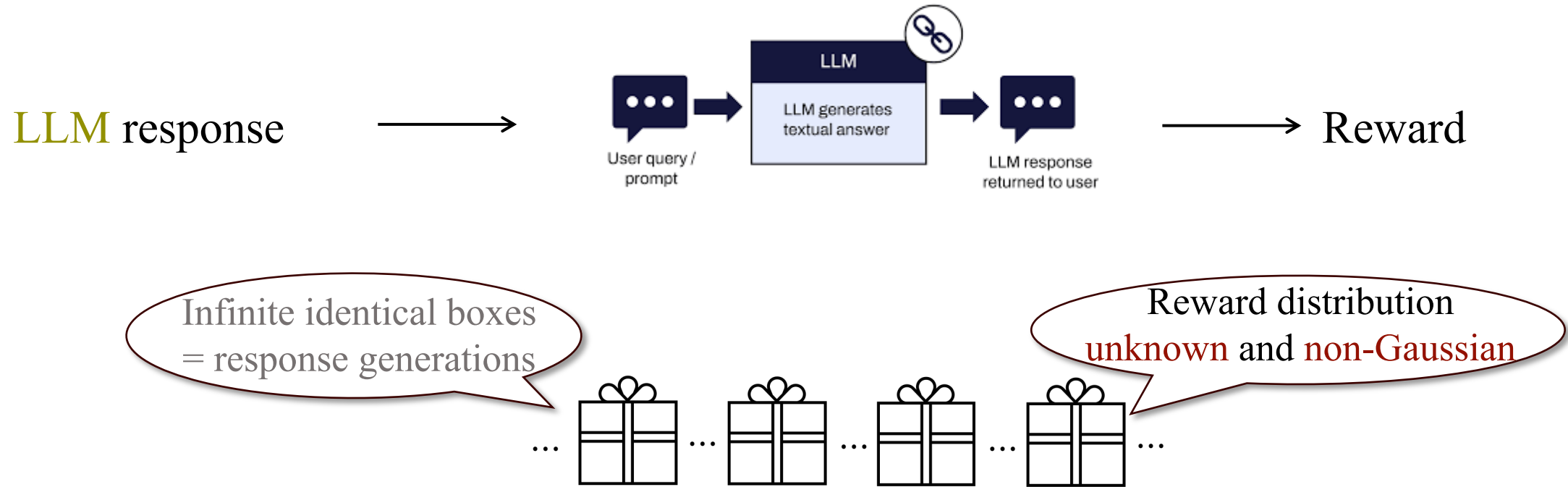
Adaptive Response Sampling in LLM Inference

LLM inference time alignment (optimization):



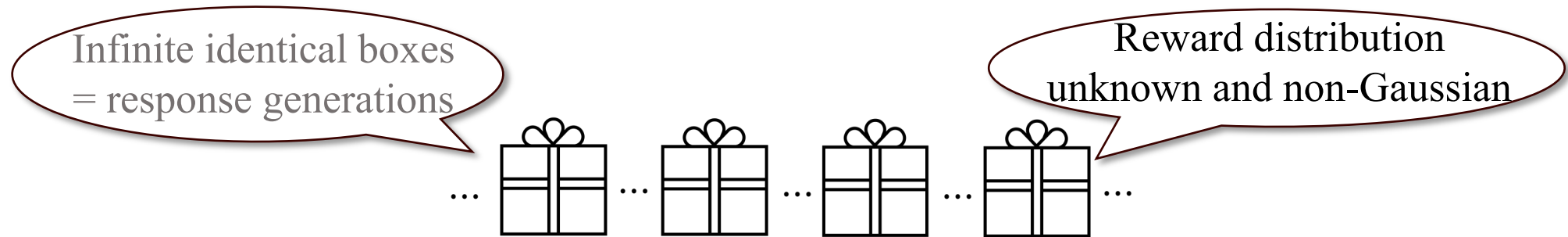
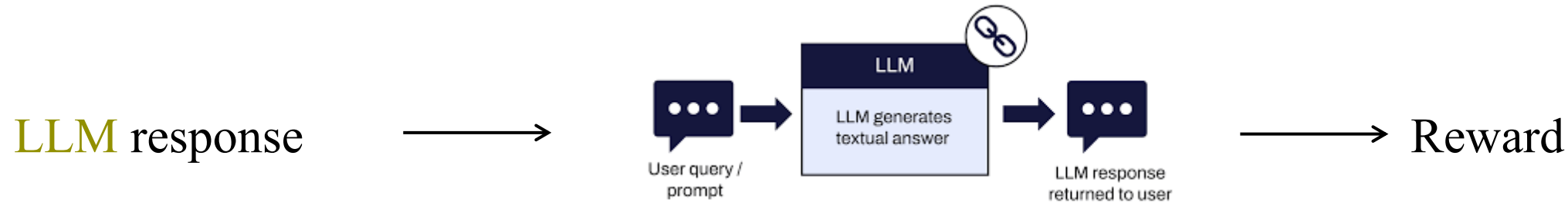
Adaptive stopping vs. fixed budget (best-of- N)
(Kalayci et al. 2025)

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**

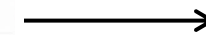
Best-prompt Identification in LLM Evaluation

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 permance
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:

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	Zero-shot	Few-shot	CoT	RAG	Revise
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Gemini 1.5 Pro	★★★★★	★★★	?	★★★★	★★★★★
deepseek	?	?	★★★★	?	★★★★
Llama 3.1-70B	?	?	★★★★	?	★★★
Mistral Large	?	?	★★★	?	★



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



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

Average performance
of (LLM, prompt) pairs

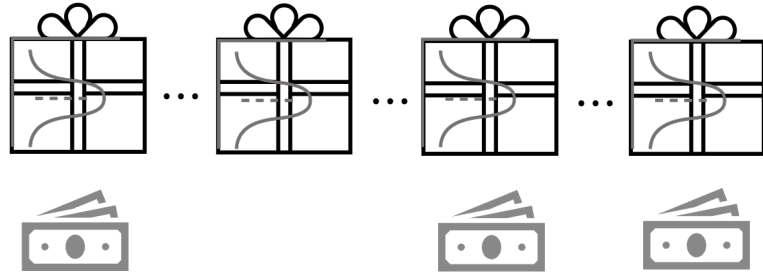
Boxes = entries



Applicable to tensors

Ours: BayesOpt + Gittins
(supports multi-selection)

Novel connection

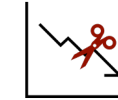


Link to **Pandora's Box** problem
& **Gittins index** theory

Principled decision rules



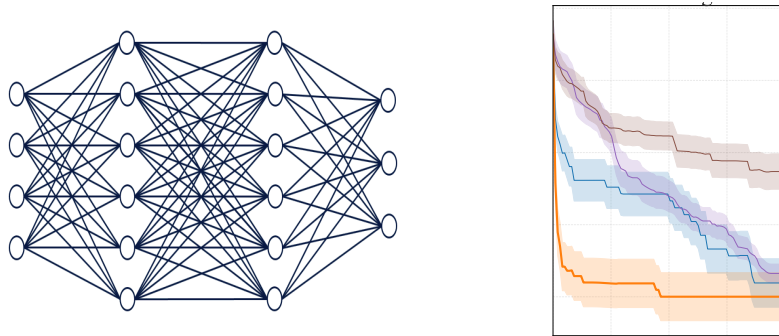
Varying evaluation costs



Adaptive stopping time

Unified framework for
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Competitive empirical performance



Interests from practitioners (e.g., Meta)

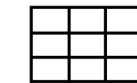


"Cost-aware Bayesian Optimization via the
Pandora's Box Gittins Index." NeurIPS'24.

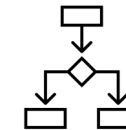
Future potential



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.



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