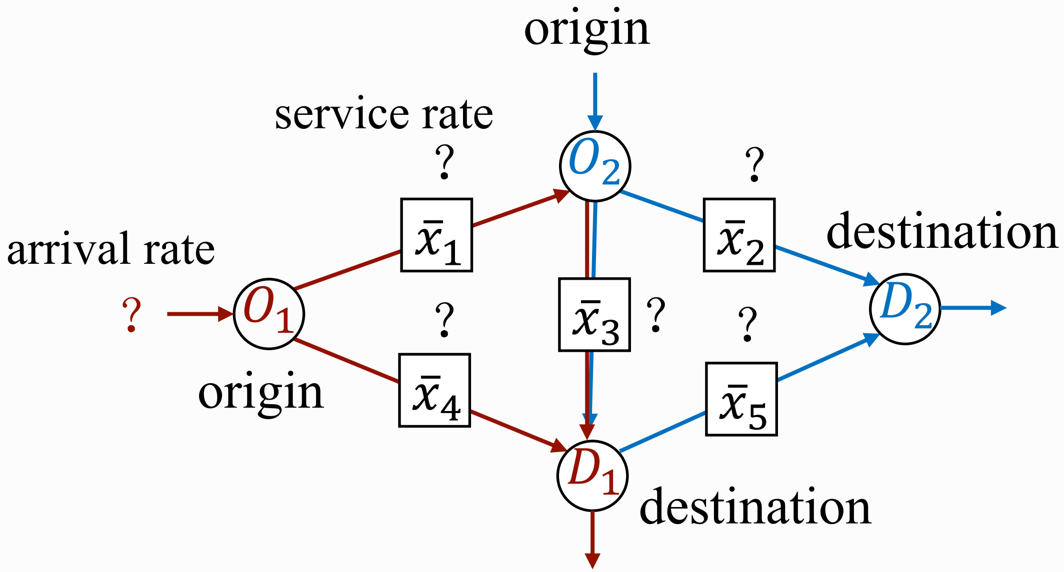
Data-Efficient Decision-making under Uncertainty: AutoML and Beyond

Qian Xie 谢倩 (Cornell)

Job talk for engineering school audiences

Research Overview: Decision-making under Uncertainty

- Earlier: stochastic control (actions chosen to regulate system)
  - Unknown system rates (robust/model-free control) [IEEE TCNS]



"Stabilizing Queuing Networks with Model Data-Independent Control." IEEE TCNS.

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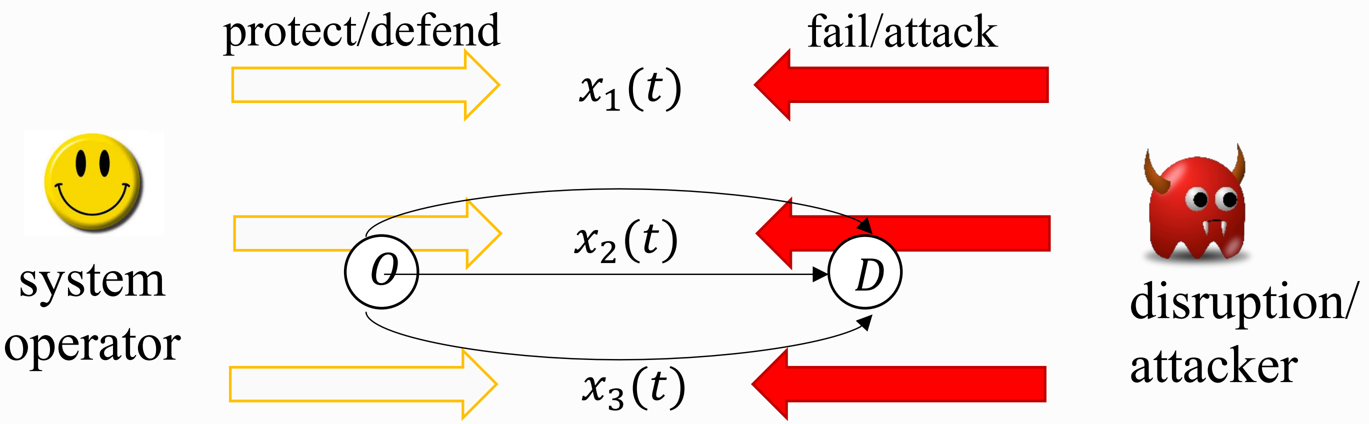

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"Cost-aware Defense for Parallel Server Systems against Reliability and Security Failures." Automatica.

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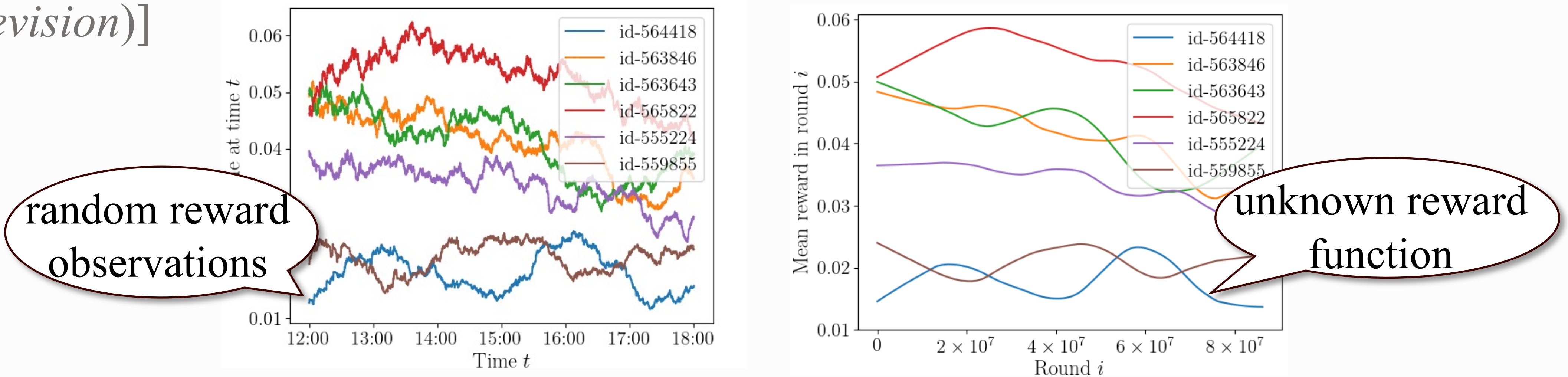

"Smooth Nonstationary Bandits." ICML'23

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  - Unknown objective functions (black-box optimization) with

varying evaluation costs [NeurIPS'24 + INFORMS DM Paper Finalist]

adaptive stopping time [Under review + AutoML'25 (non-archival)]

multi-stage feedback [To be submitted]

multi-source environment information [NeurIPS'25 LAW]

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

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

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This talk's focus

- varying evaluation costs [NeurIPS'24 + INFORMS DM Paper Finalist]
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Motivation: World of Optimization under Uncertainty

ML model training:

≠ parameters
(weights, biases)

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

⟶ Accuracy

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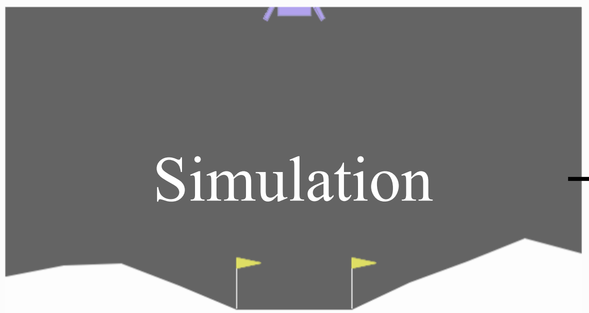
→ Accuracy

Control design:

Control variables
(e.g., position, angle, velocity) →



→ Reward

Motivation: World of Optimization under Uncertainty

non-analytical &
no gradient info

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

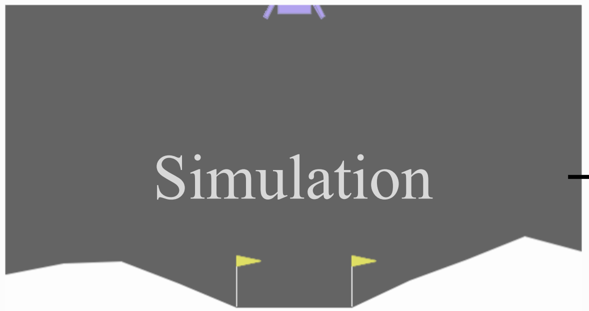
≠ parameters
(weights, biases)

ML model training:

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

⟶ Accuracy

Control design:

Control variables
(e.g., position, angle, velocity) ⟶ 

⟶ Reward

Motivation: World of Optimization under Uncertainty

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

Input x $\longrightarrow$

non-analytical & no gradient info

$\longrightarrow$ Observed outcome $f(x)$

ML model training:

≠ parameters (weights, biases)

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

$\longrightarrow$ Accuracy

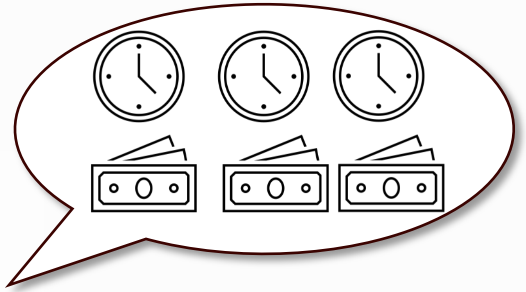
Background: Black-Box Optimization

Black-box optimization:

(gradient-based methods not applicable)

expensive-to-evaluate

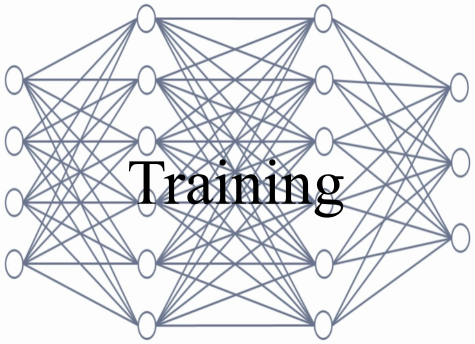
Input x ⟶  ⟶ Observed outcome $f(x)$



Training time

Compute credits

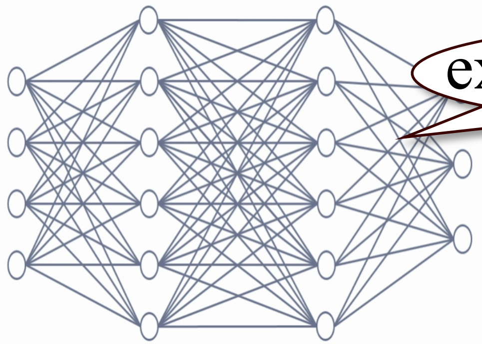
ML model training:

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

⟶ Accuracy

Naïve (Non-Adaptive) Approach: Grid Search

ML model training:

Training hyperparameters →  → Accuracy

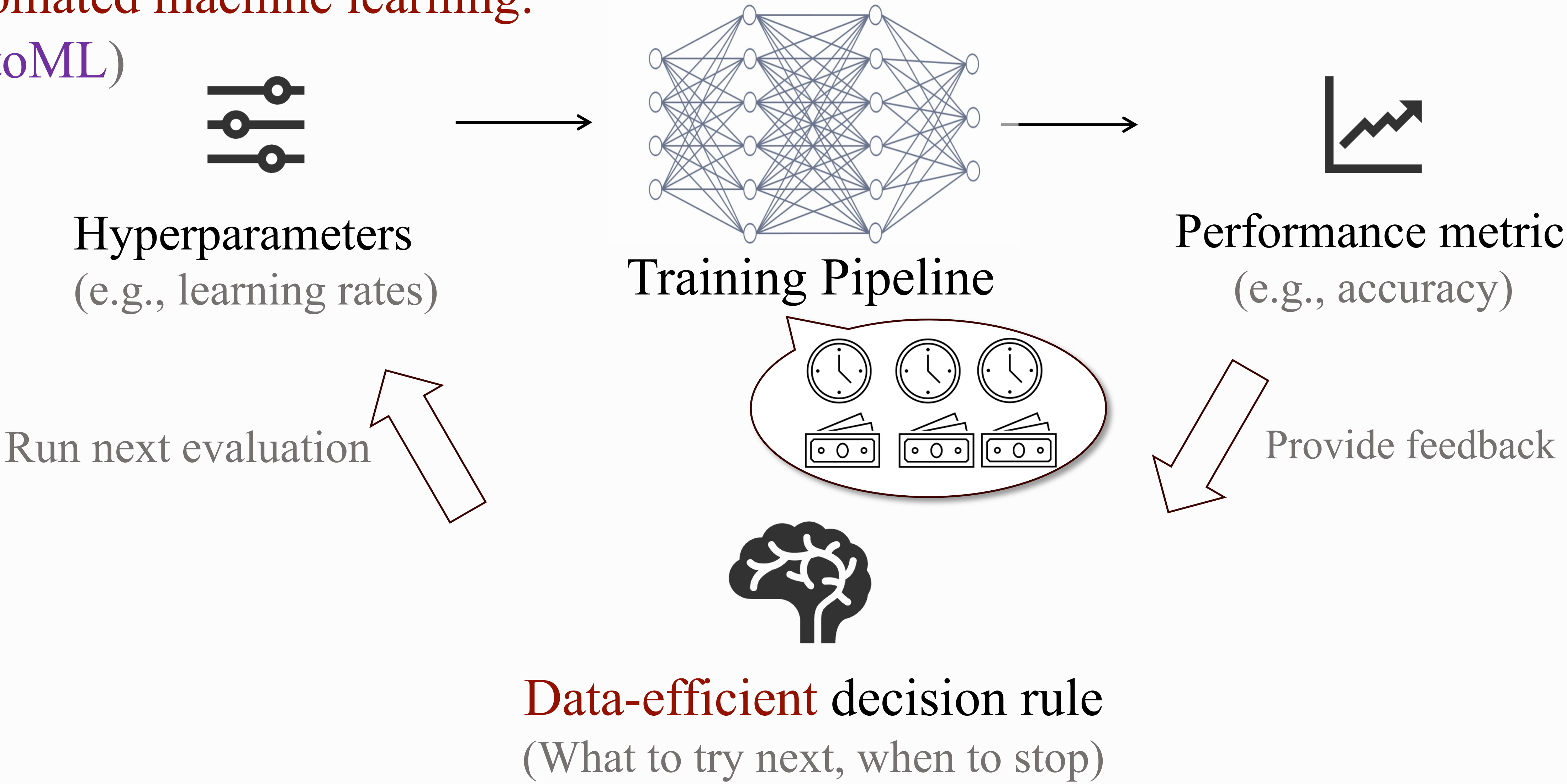
expensive-to-evaluate

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

Automated machine learning: (AutoML)



Existing Umbrellas of Black-Box Optimization

Naïve (non-adaptive) approaches:	Data-driven (adaptive) approaches:
• Grid search	• Local search (e.g., simulated annealing)
• Random search	• Evolutionary algorithms (e.g., genetic algo)
• Manual tuning	• Bayesian optimization (e.g., EI, UCB, TS)
	• Reinforcement learning (e.g., PPO, ENAS)
	• LLM-based search agent (e.g., GENIUS)

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Limitations in practice:

1. Limited principled guidance (e.g., naïve)

2. Often data-inefficient (e.g., naïve, local search, evolutionary algo)

3. No or ad-hoc incorporation of additional side info (most)

(e.g., varying training time across search space)

Overview of Contributions Across My Work

Naïve (non-adaptive) approaches:	Data-driven (adaptive) approaches:
• Grid search	• Local search
• Random search	• Evolutionary algorithms
• Manual tuning	• Bayesian optimization ★ Part I
	• Reinforcement learning ★
	• LLM-based search agent ★ Part II

Contributions of methods in my work:

1. Principled guidance

2. Competitive empirical performance

3. Principled incorporation of additional side info

★ New methods under this umbrella

Outline

Part I (Recent):

Bayesian Optimization via Gittins Index Design Principle

Part II (Ongoing):

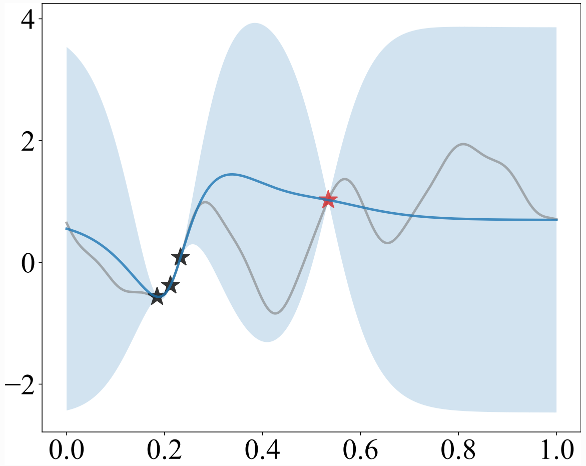
Black-box Optimization Beyond AutoML

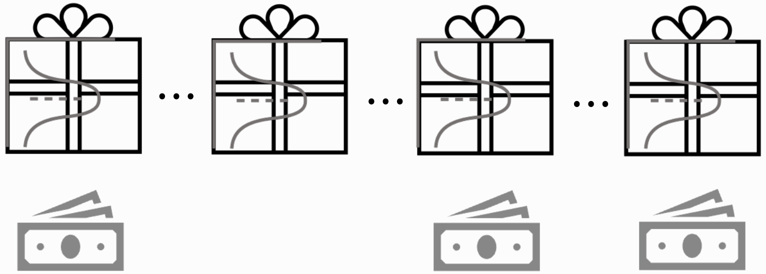
Reinforcement Learning · Engineering Design · Scientific Discovery · LLM

Part I (Recent):

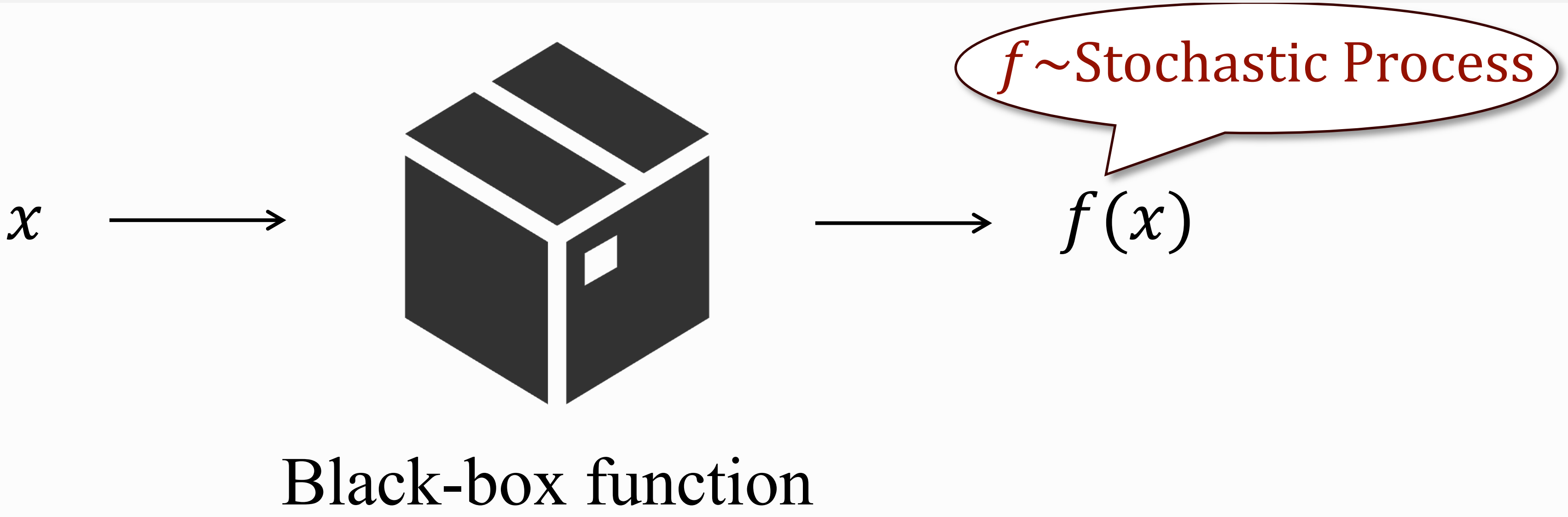
Bayesian Optimization via Gittins Index

Design Principle





Bayesian Optimization



Bayesian Optimization

Time 0

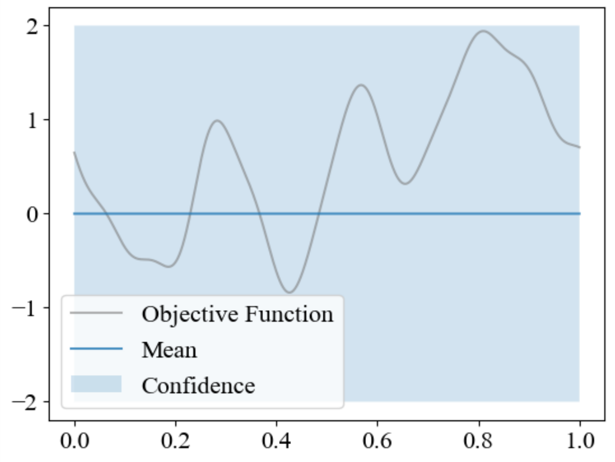
$x \longrightarrow$

$\longrightarrow f(x)$

$f \sim$Stochastic Process

Model belief

Black-box function



Probabilistic model

(e.g., Gaussian process)

Bayesian Optimization

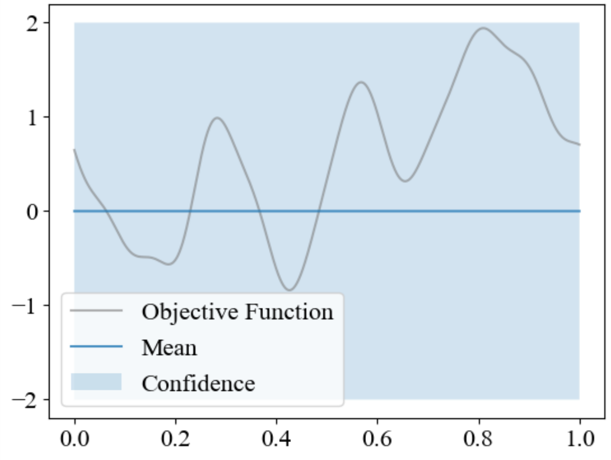
Time t

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

$f \sim$ Stochastic Process

Black-box function

Model belief



Probabilistic model
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Bayesian Optimization

Time t

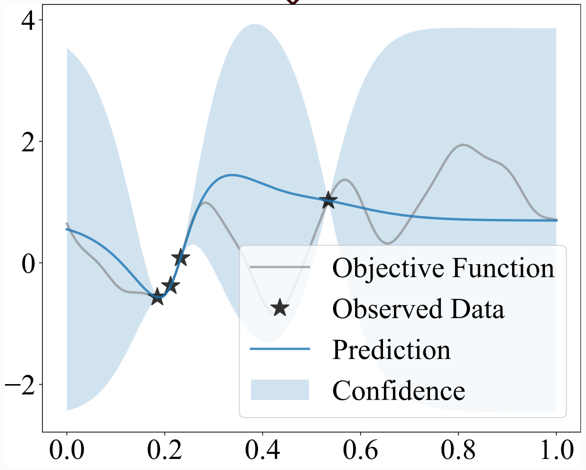
$f \sim$Stochastic Process

$x_1, \dots, x_t \longrightarrow$

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

Black-box function

Update belief
(Bayes' rule)



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Bayesian Optimization

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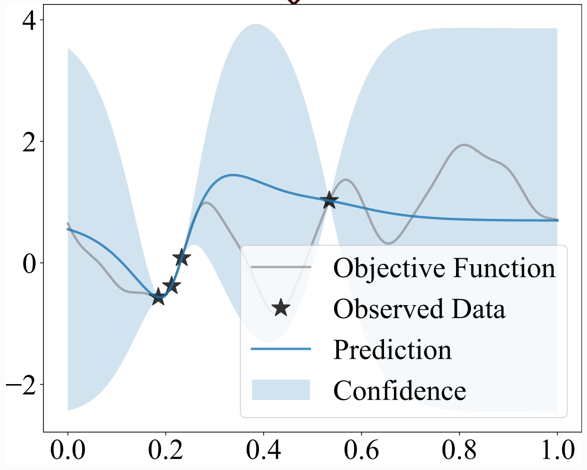

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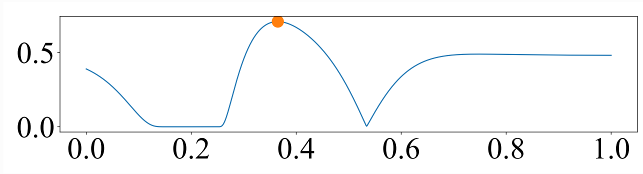


Decision rule
(e.g., EI, UCB, TS)

scoring (worth of each point

Bayesian Optimization

Time t

$x_1, \dots, x_t \longrightarrow$

Black-box function

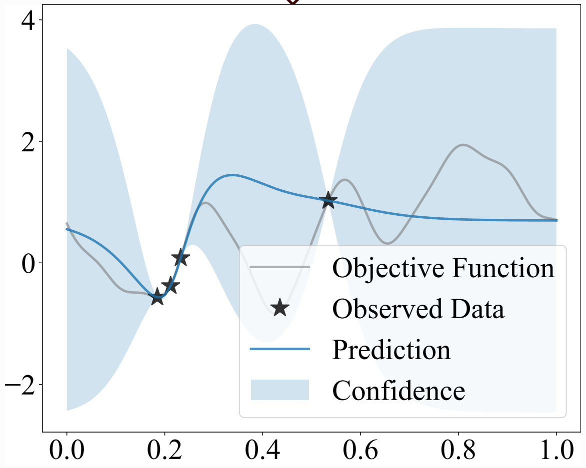
$\longrightarrow f(x_1), \dots, f(x_t)$

Decide next input

(gradient-based optimization)

Update belief

(Bayes' rule)



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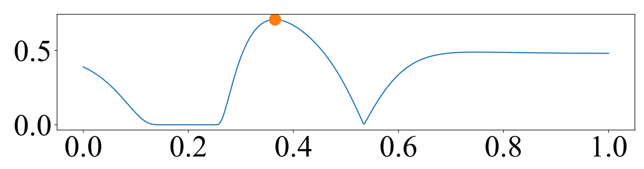


Decision rule

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

Bayesian Optimization

Time $t + 1$

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

Decide next input

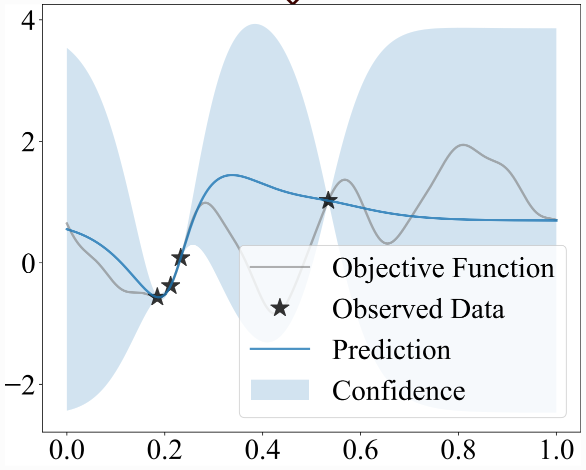
(gradient-based optimization)

Black-box function

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

Update belief

(Bayes' rule)



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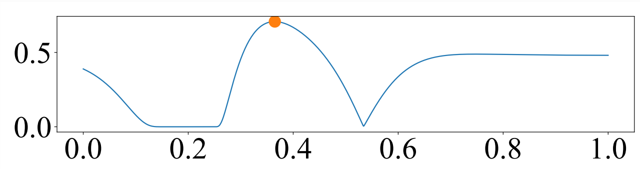

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$f(x_1), \ldots, f(x_{t+1})$

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Probabilistic model
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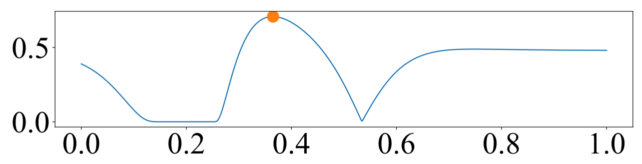
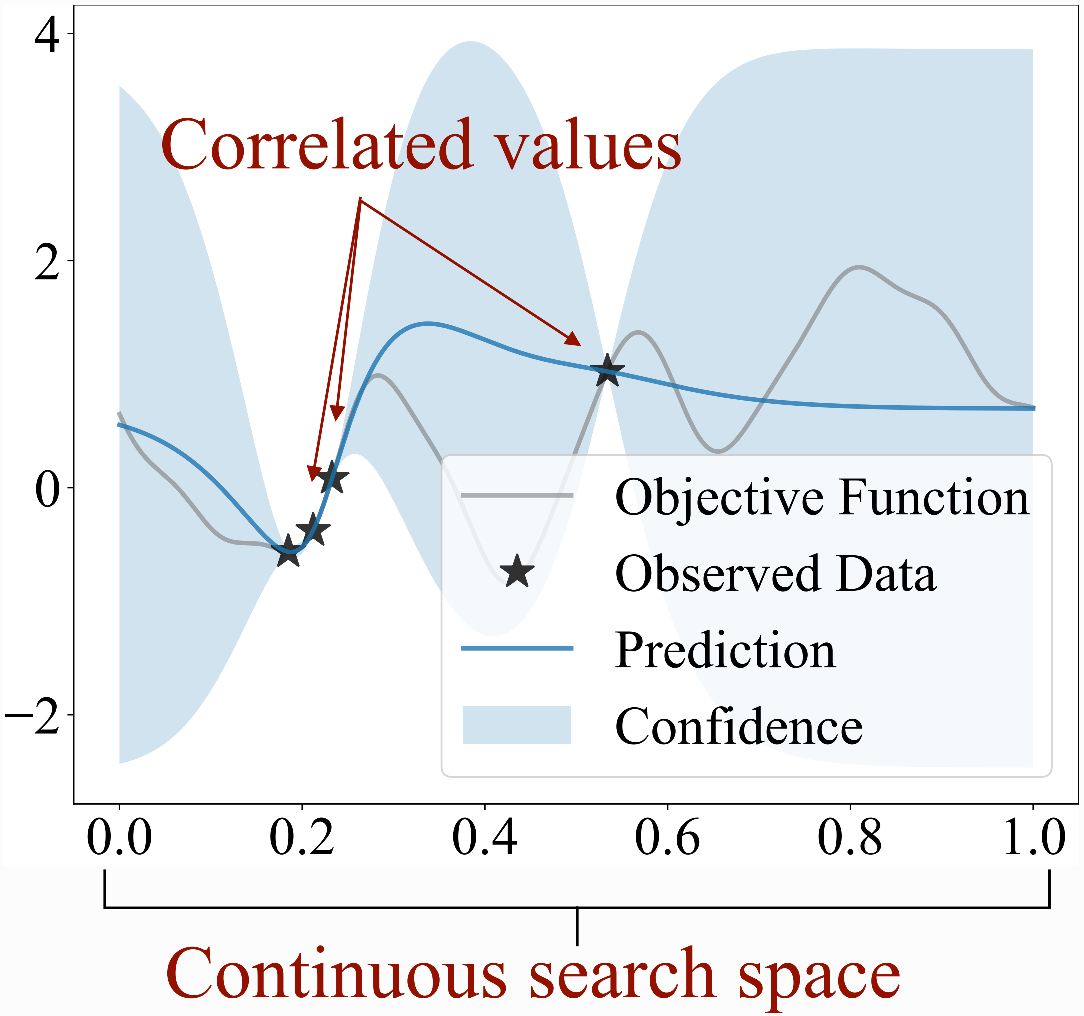


My focus

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

scoring (worth of each point

Challenges in Decision Rule Design



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

Popular Decision Rule: Expected Improvement

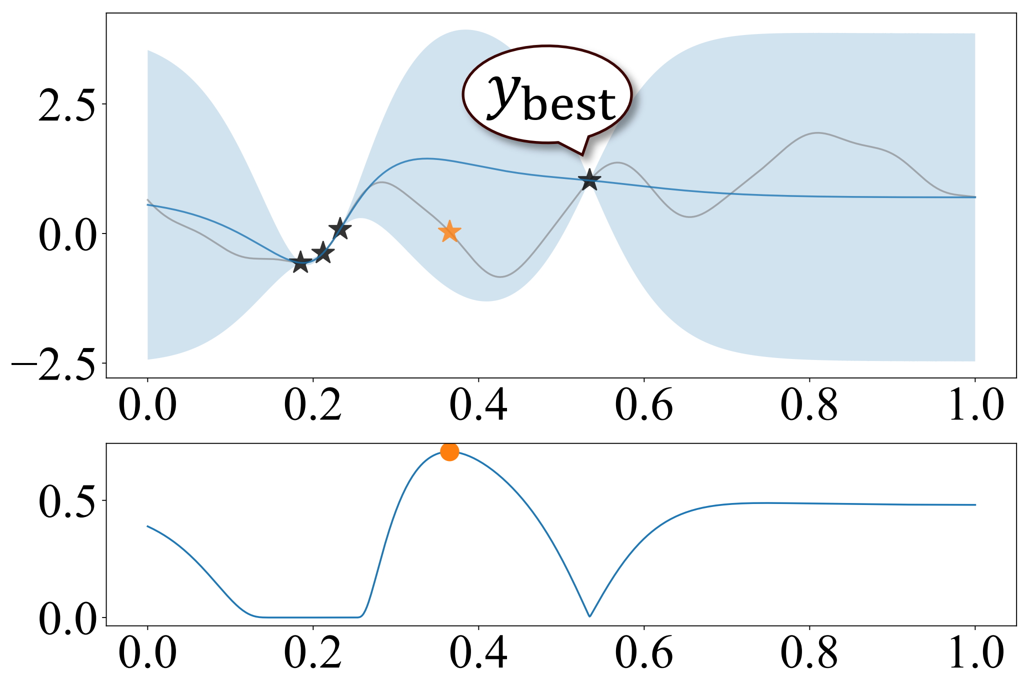
current best observed

data D

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

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

posterior distribution



One-step approximation to MDP

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

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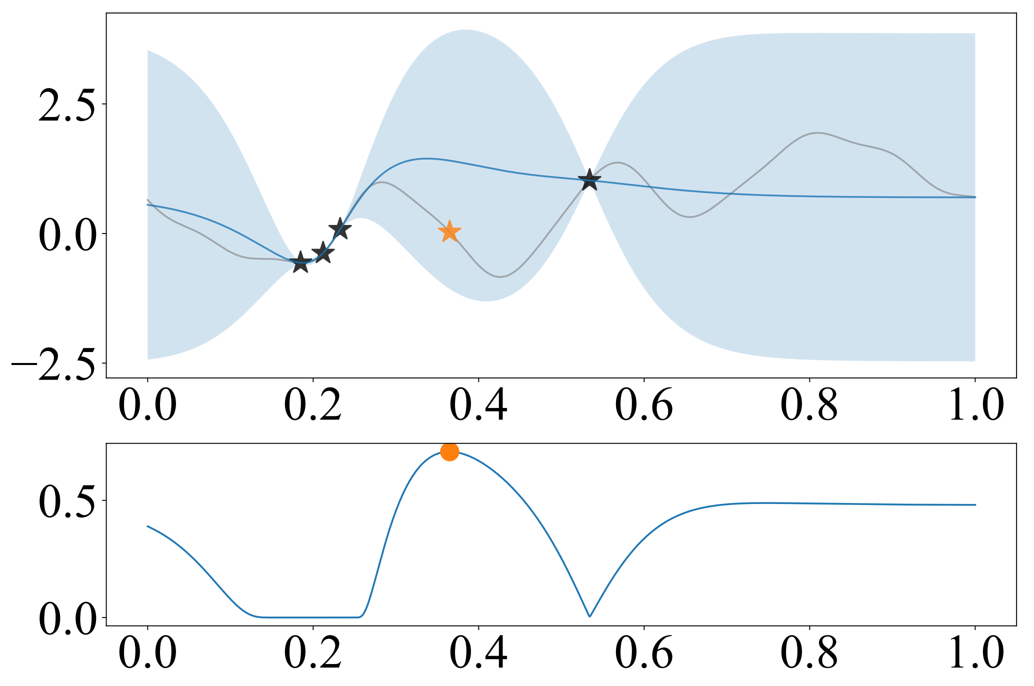
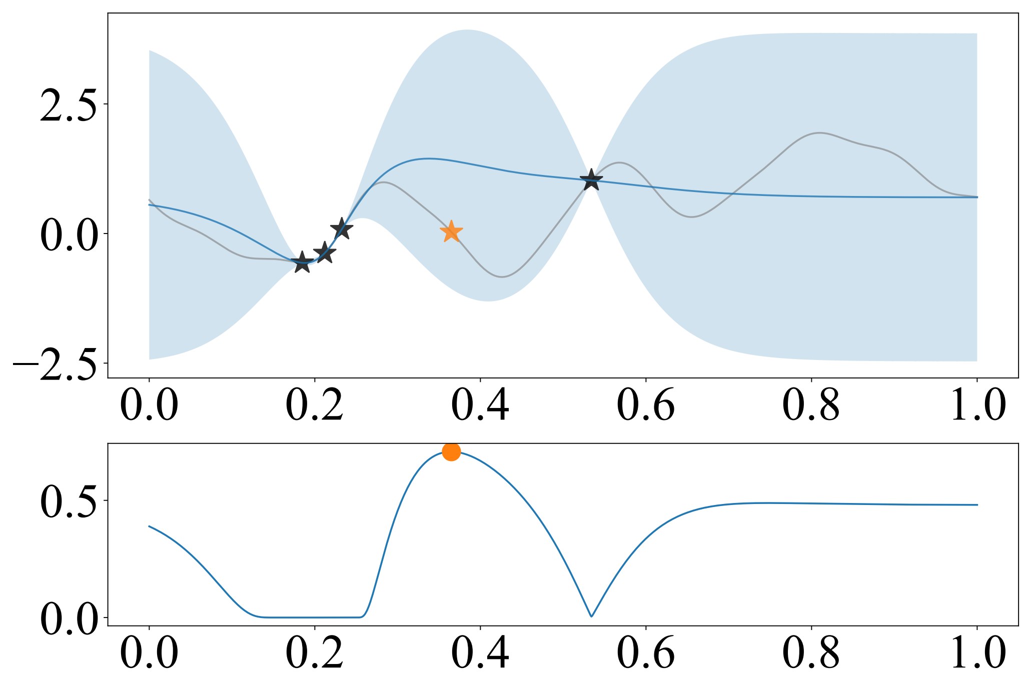


Expected improvement $\mathrm{EI}(x)$

Improvement-based design principle

Existing Design Principles

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



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New Design Principle: Gittins Index

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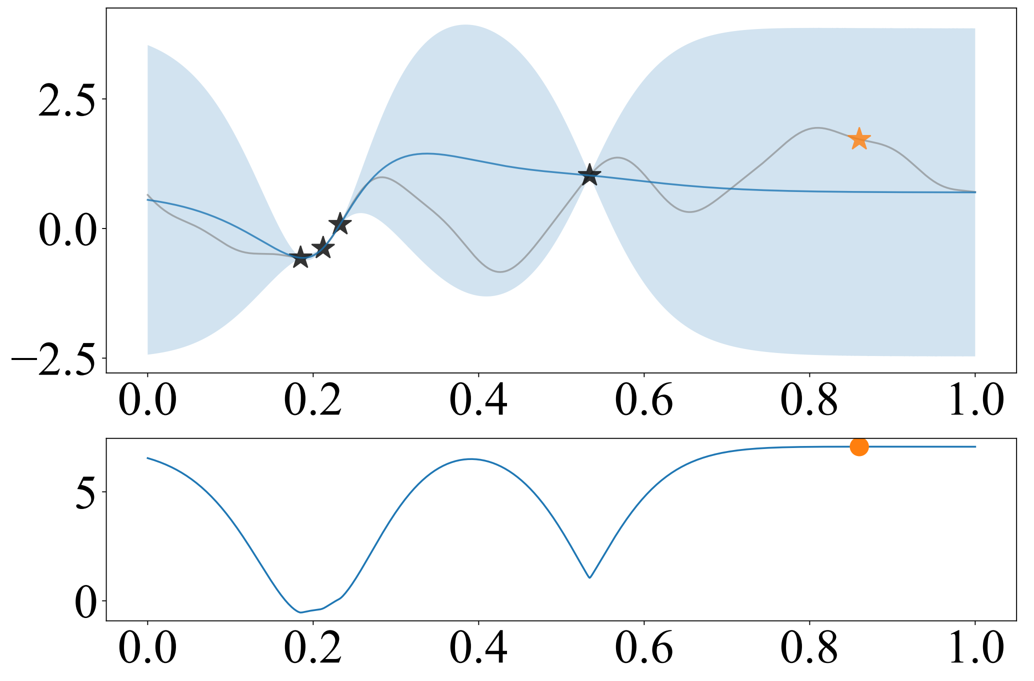

Gittins index $\mathrm{GI}(x)$

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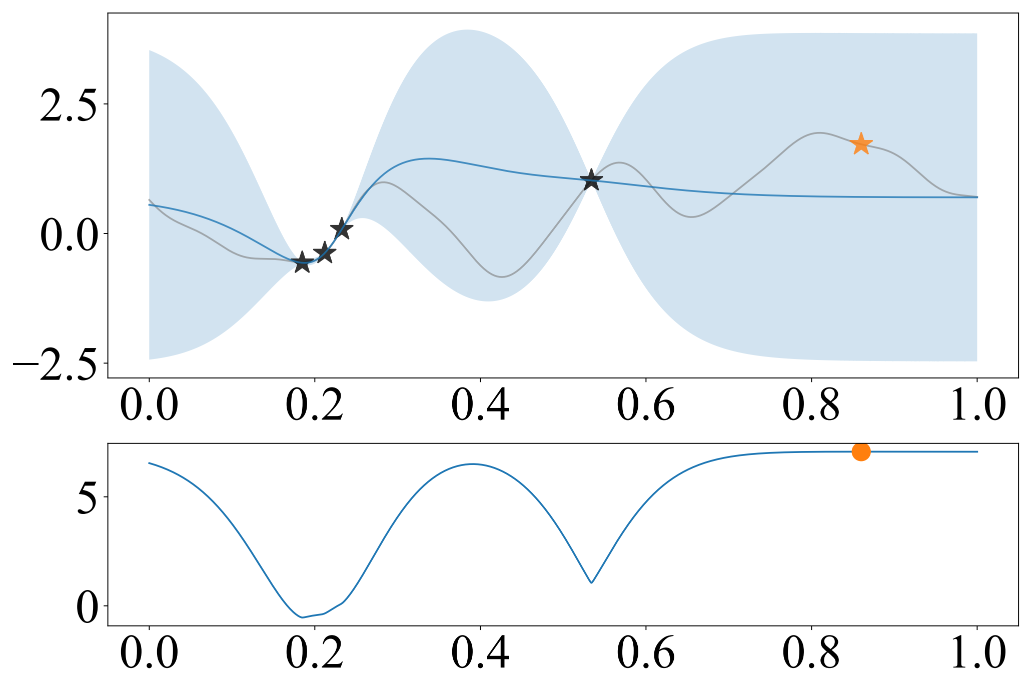

Gittins index $\mathrm{GI}(x)$

? Why another principle?

Our Contribution: Gittins Index Principle

Joint work with Ziv Scully and Alexander Terenin et al.

1. Principled easy-to-compute decision rules

2. Natural incorporation of side info and flexibility

3. Competitive performance on benchmarks

4. Theoretical guarantees

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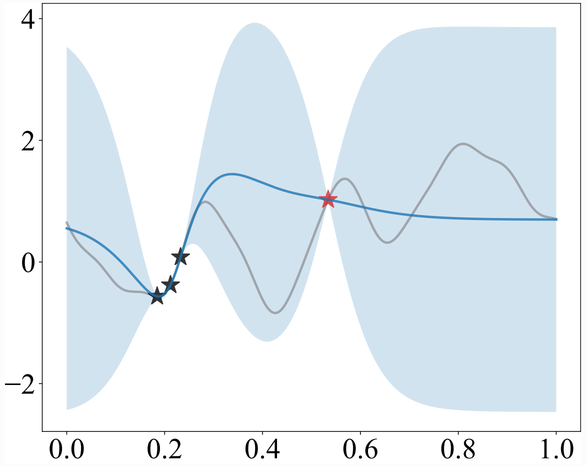
Bayesian Optimization

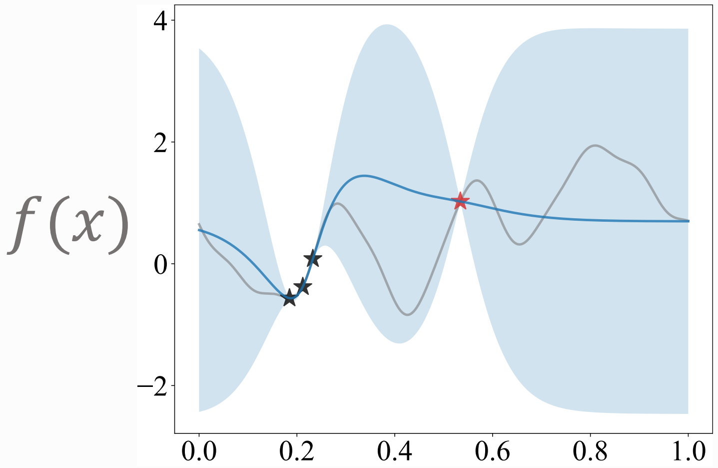
$f(x)$



Continuous search space

Correlated function values

Bayesian Optimization

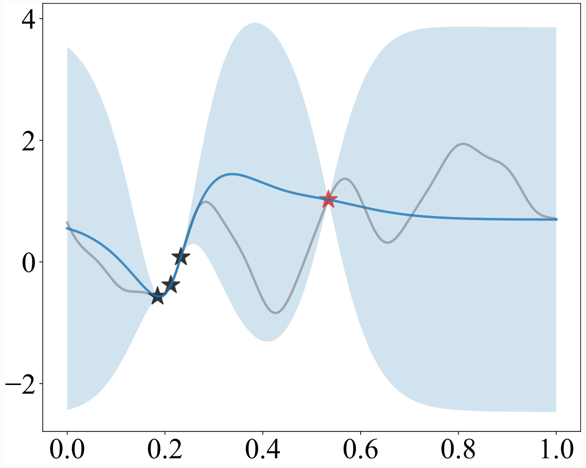


Continuous search space $\Longrightarrow$ Discrete

Correlated function values $\Longrightarrow$ Independent

Bayesian Optimization

$f(x)$

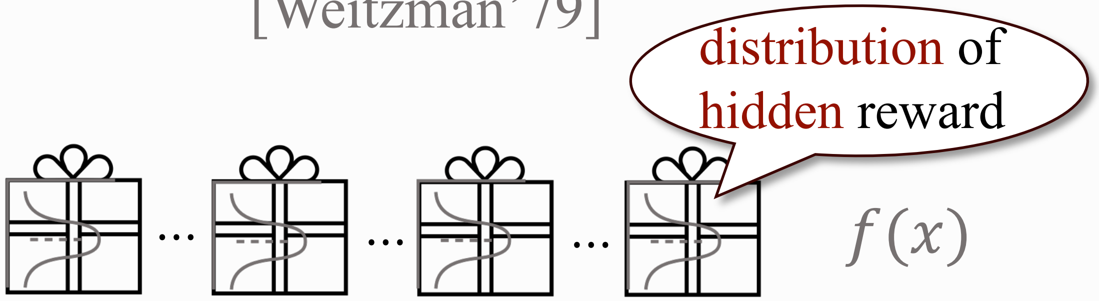


Continuous search space

Correlated function values

Pandora's Box

[Weitzman'79]



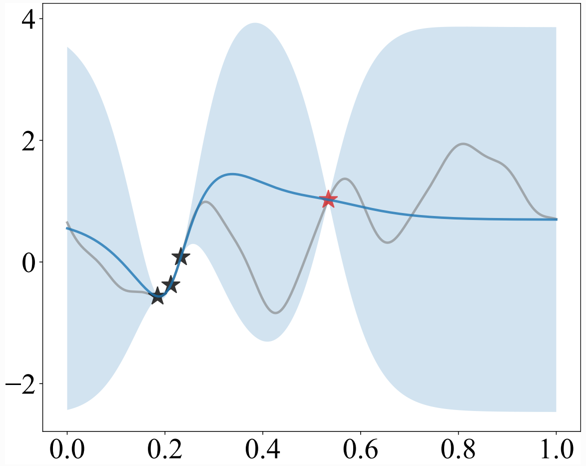
$f(x)$

Discrete

Independent

Bayesian Optimization

$f(x)$



Continuous search space

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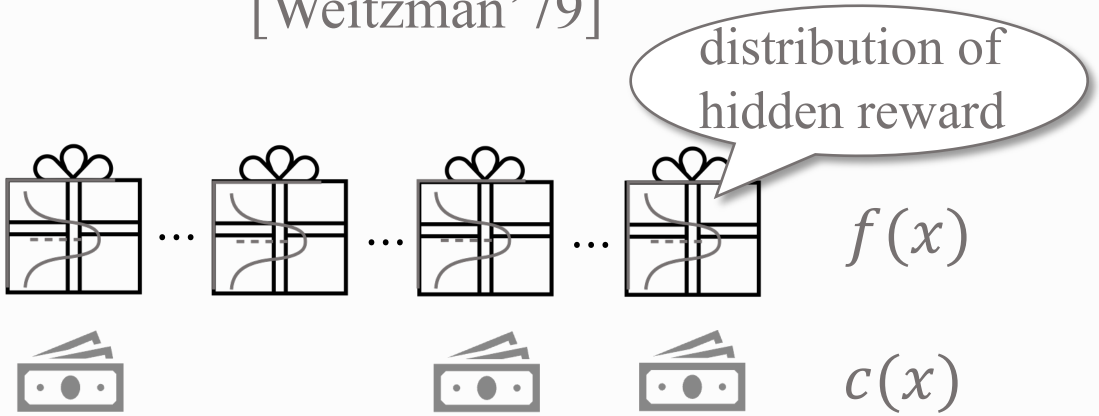


$f(x)$

$c(x)$

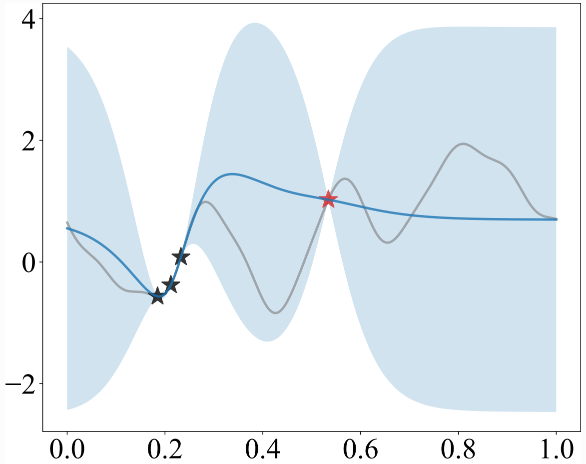
costs to open

Discrete

Independent

Bayesian Optimization

$f(x)$

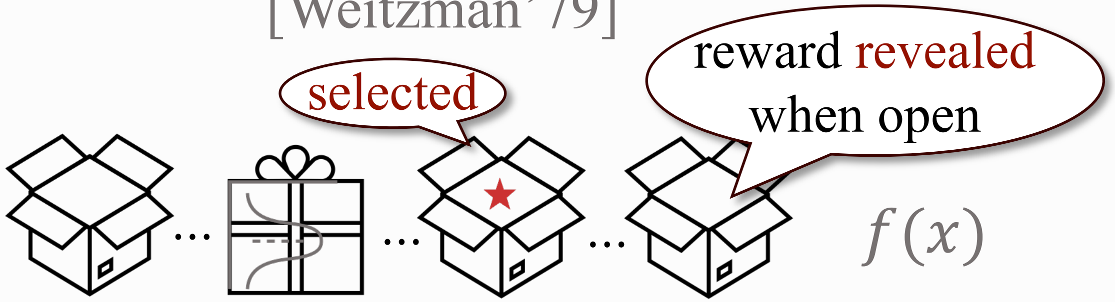


Continuous search space

Correlated function values

Pandora's Box

[Weitzman'79]

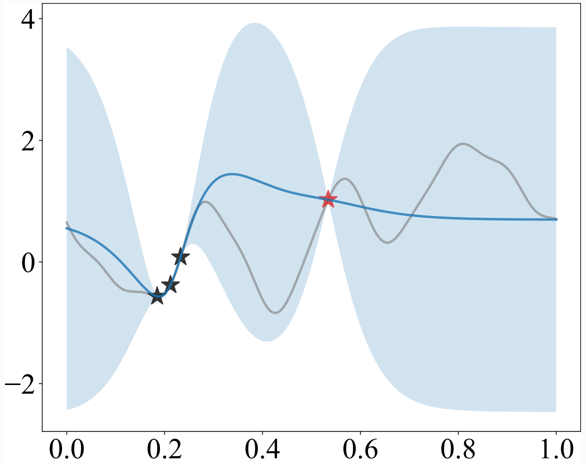


Discrete

Independent

Bayesian Optimization

$f(x)$



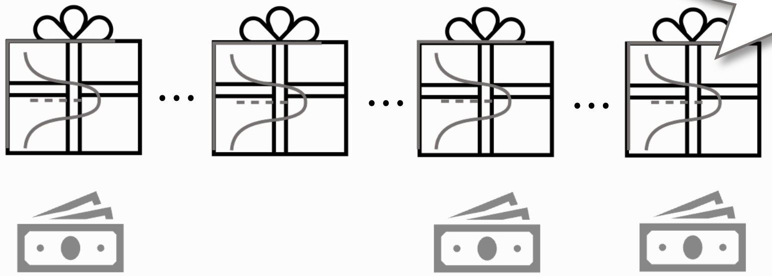
Continuous search space

Correlated function values

Pandora's Box

[Weitzman'79]

distribution of hidden reward



$f(x)$

$c(x)$

costs to open

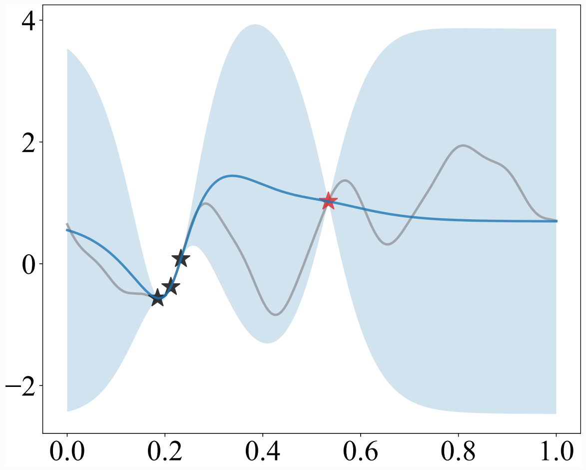
Discrete

Independent

Optimal policy: Gittins index

Bayesian Optimization

$f(x)$



Continuous search space

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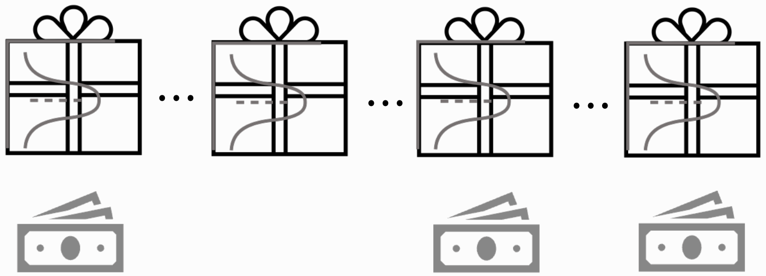

$f(x)$

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costs to open

Discrete

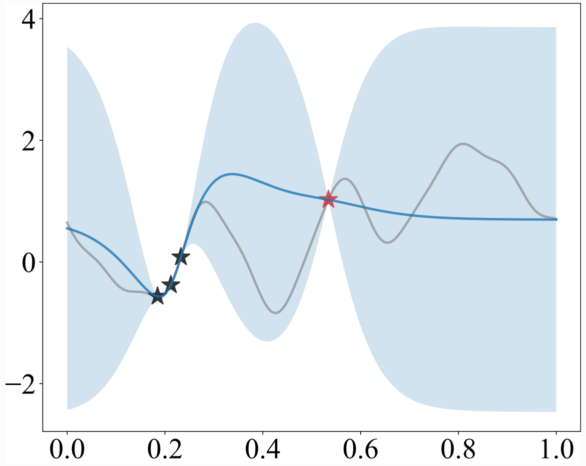
Independent

How to translate?

$\Longleftarrow$ Optimal policy: Gittins index

Bayesian Optimization

$f(x)$

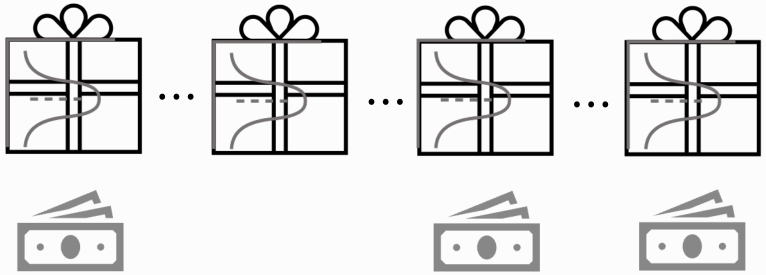


Continuous search space

Correlated function values

Pandora's Box

[Weitzman'79]



$f(x)$

$c(x)$

costs to open

Discrete

Independent

New!

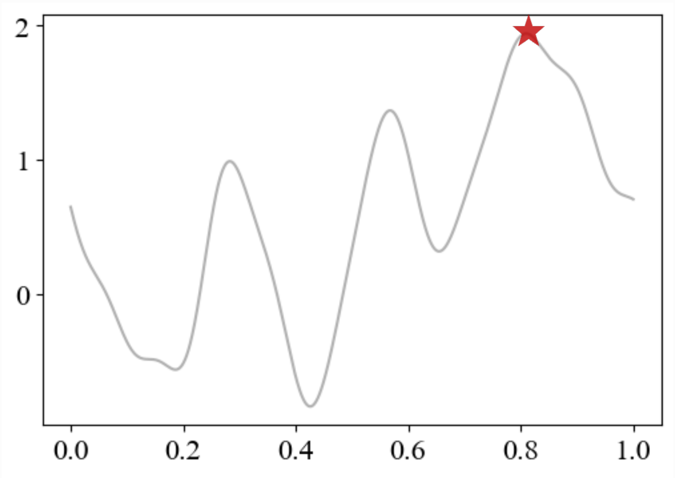
incorporate posterior

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

take continuum limit

Bayesian Optimization

$f(x)$

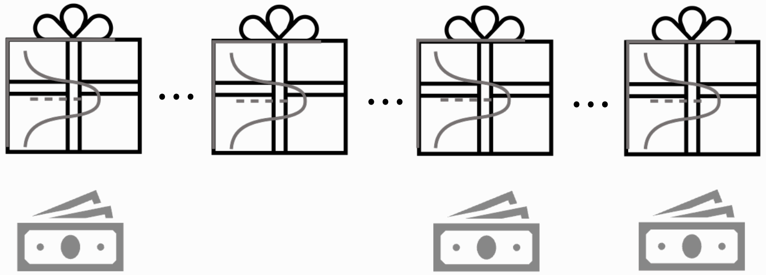


Continuous

Correlated

Pandora's Box

[Weitzman'79]



$f(x)$

$c(x)$

costs to open

Discrete

Independent

incorporate posterior

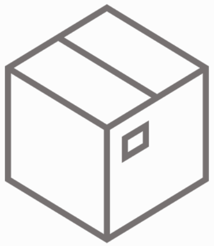
Our policy: $\mathrm{GI}_{f|D}(x; c(x))$ $\Longleftarrow$ Optimal policy: $\mathrm{GI}_{f}(x; c(x))$

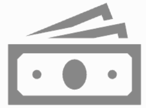
take continuum limit

How to compute?

Intuition

Exploration | Exploitation

$f(x)$  vs. 

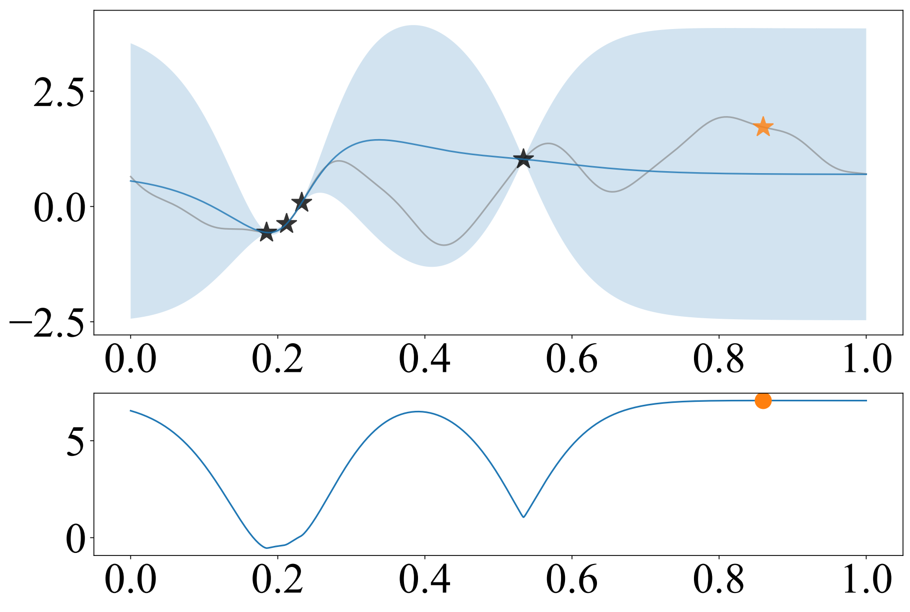
$c(x)$ 

Open closed box | Take opened box

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

Should one open box? Depend on g!

Gittins Index



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

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

Intuition

Exploration | Exploitation

$f(x)$ vs. g

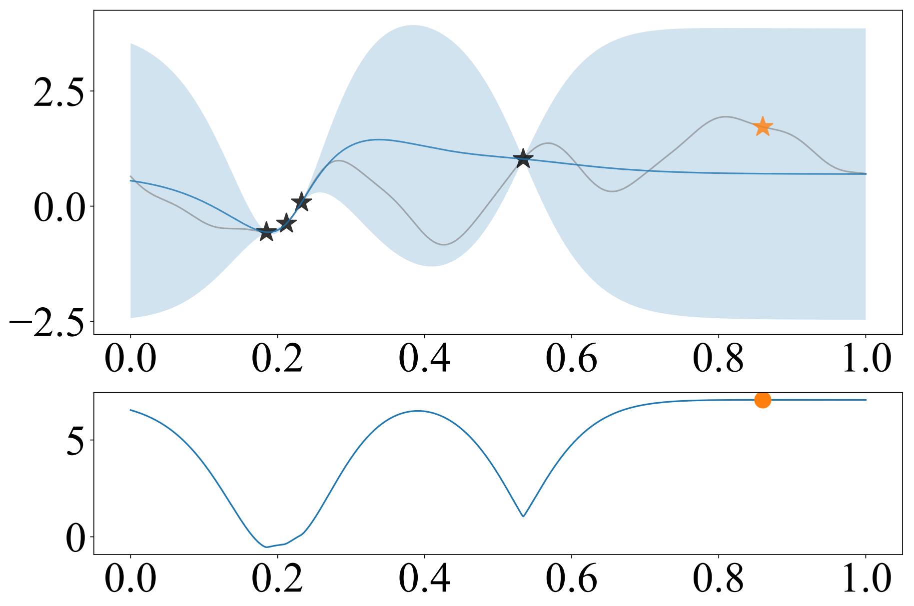
$c(x)$

Open closed box | Take opened box

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

Should one open box? Depend on g!

Gittins Index



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

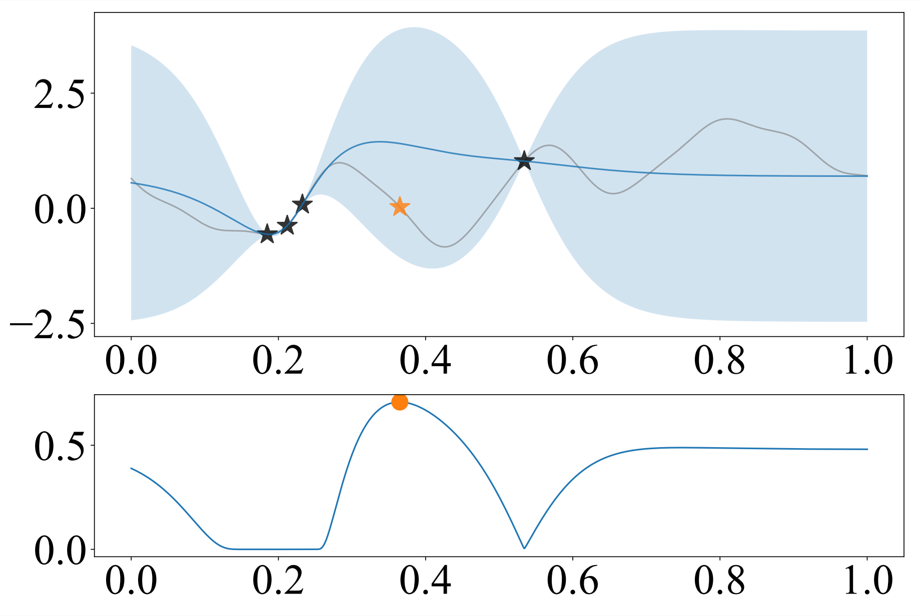
$$\mathbb{E}[\max(f(x), g) \mid D] - c(x) = g$$

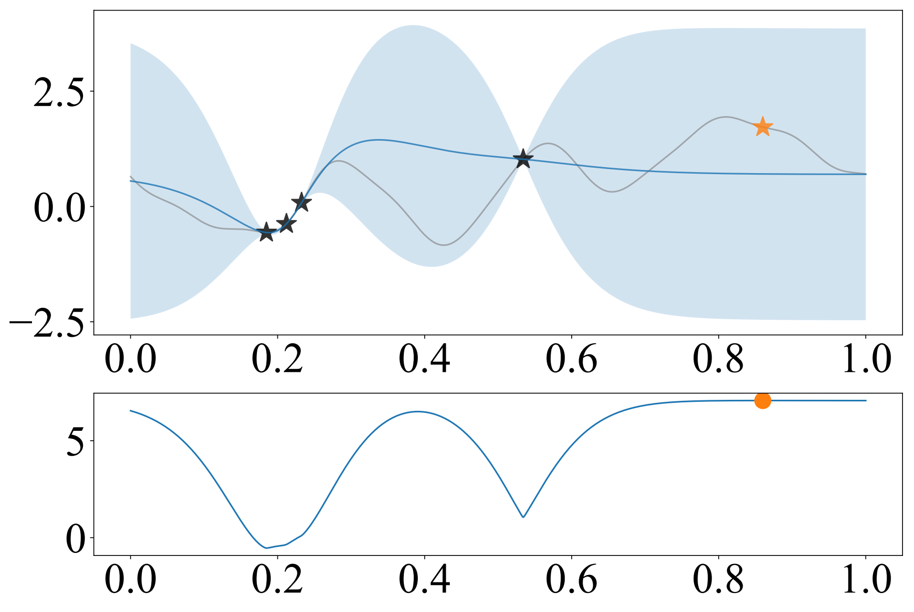
$$\Leftrightarrow \mathbb{E}[\max(f(x) - g, g - g) \mid D] - c(x) = 0$$

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

Expected Improvement

Gittins Index



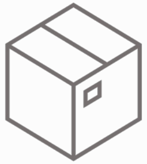


$$\mathrm{EI}_{f|D}(x) := \mathbb{E}[\max(f(x) - y_{\mathrm{best}}, 0) \mid D]$$

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

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

$f(x)$

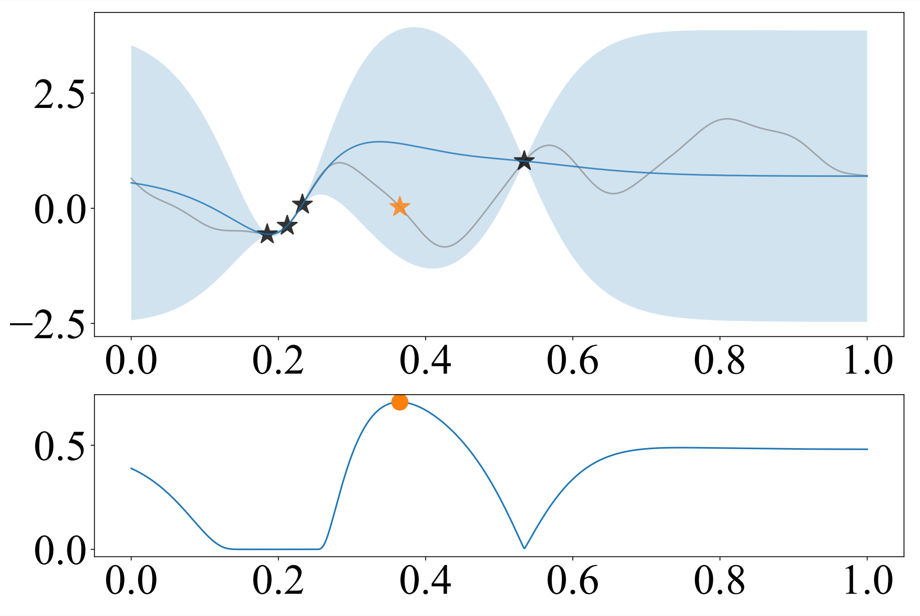


vs.

$c(x)$

Exploration Exploitation

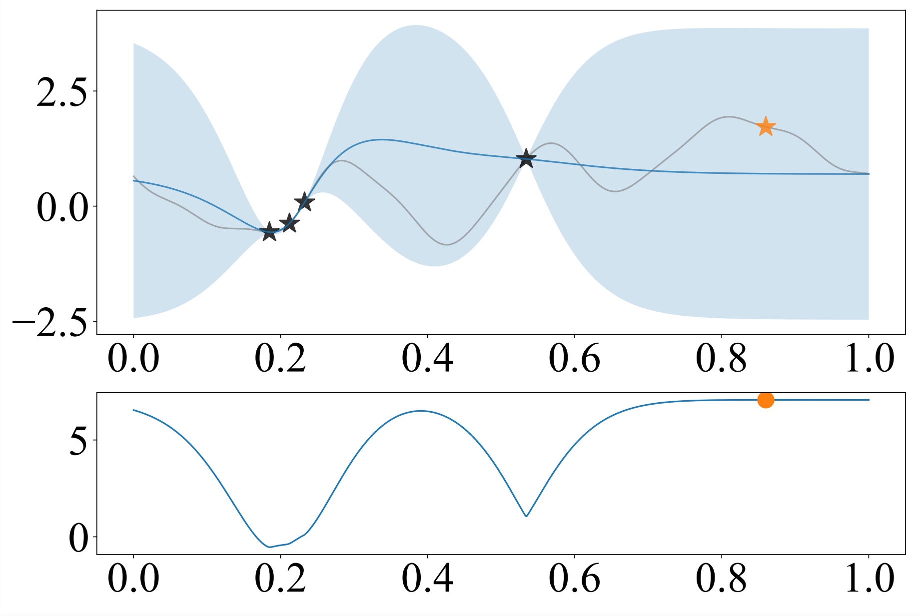
Expected Improvement



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

Temporal simplification to MDP
(One-step)

Gittins Index

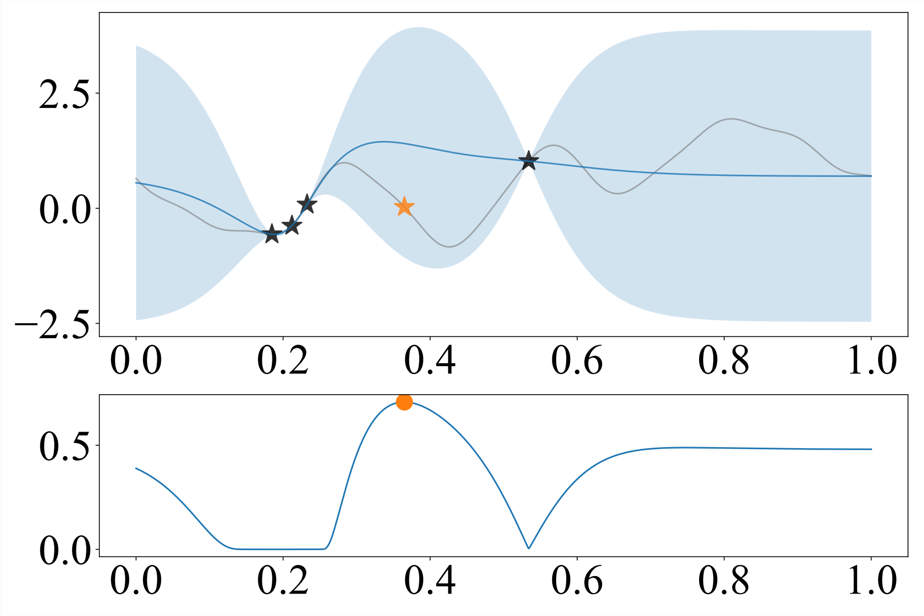


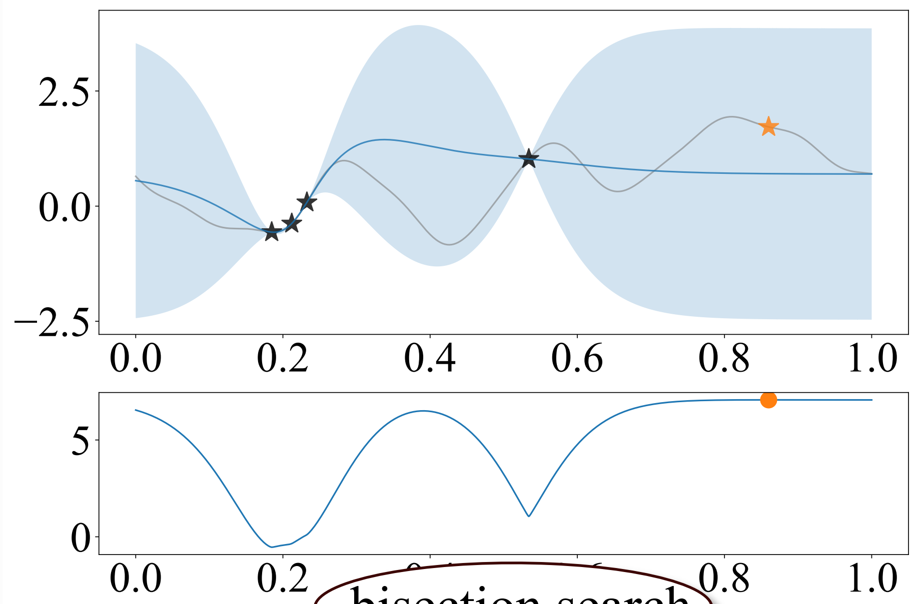
$\mathrm{GI}_{f|D}(x; c) :=$ solution g s.t. $\mathrm{EI}_{f|D}(x; g) = c(x)$
where $\mathrm{EI}_{f|D}(x; g) := \mathbb{E}[\max(f(x) - g, 0) \mid D]$

Spatial simplification to MDP

Expected Improvement

Gittins Index





bisection search

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

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

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

analytical expression

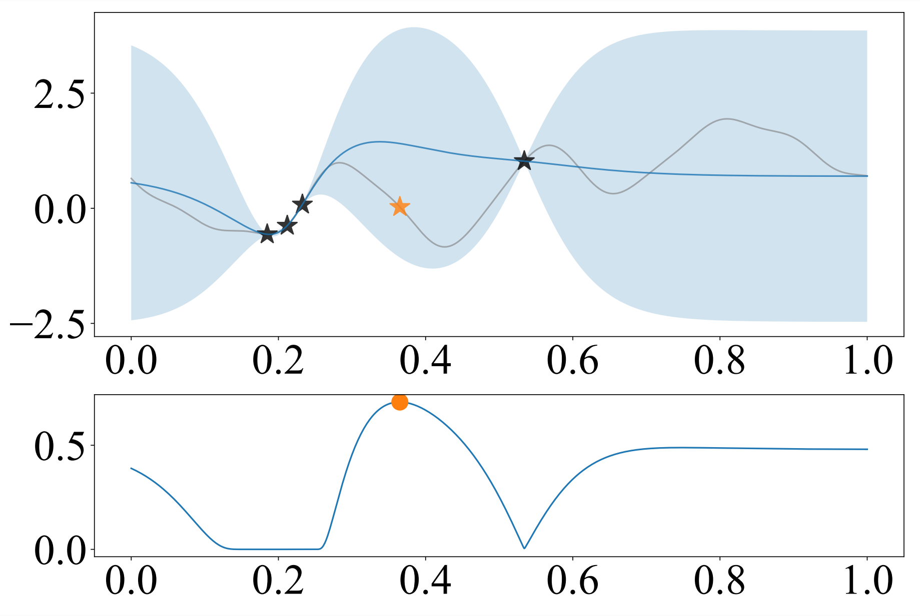
Temporal simplification to MDP

Spatial simplification to MDP

Both are principled and easy-to-compute!

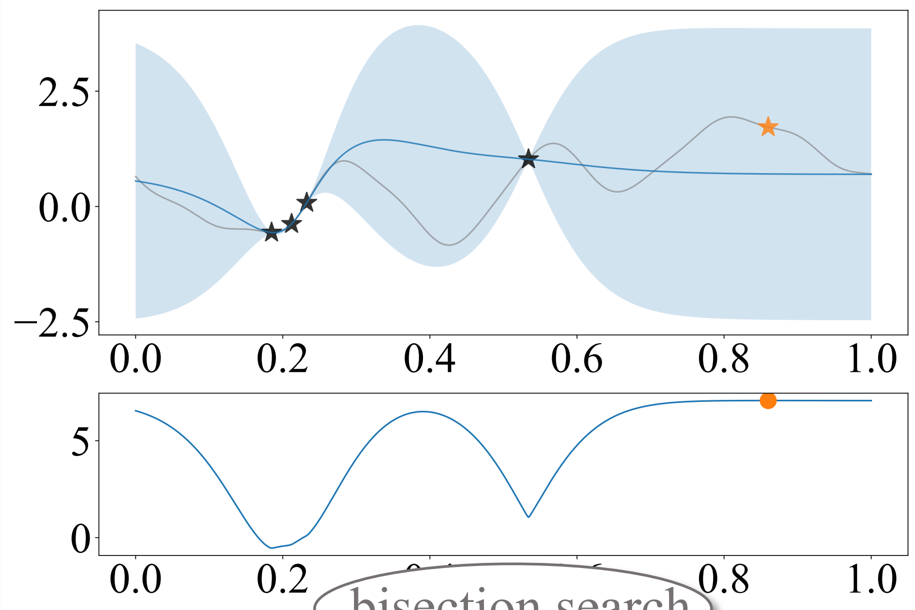
"Cost-aware Bayesian Optimization via the Pandora's Box Gittins Index." NeurIPS'24.

Expected Improvement



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

Gittins Index



bisection search

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

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

Google DeepMind

FunBO: Discovering new acquisition functions for Bayesian Optimization with FunSearch

hard to discover GI

Our Contribution: Gittins Index Principle

Joint work with Ziv Scully and Alexander Terenin et al.

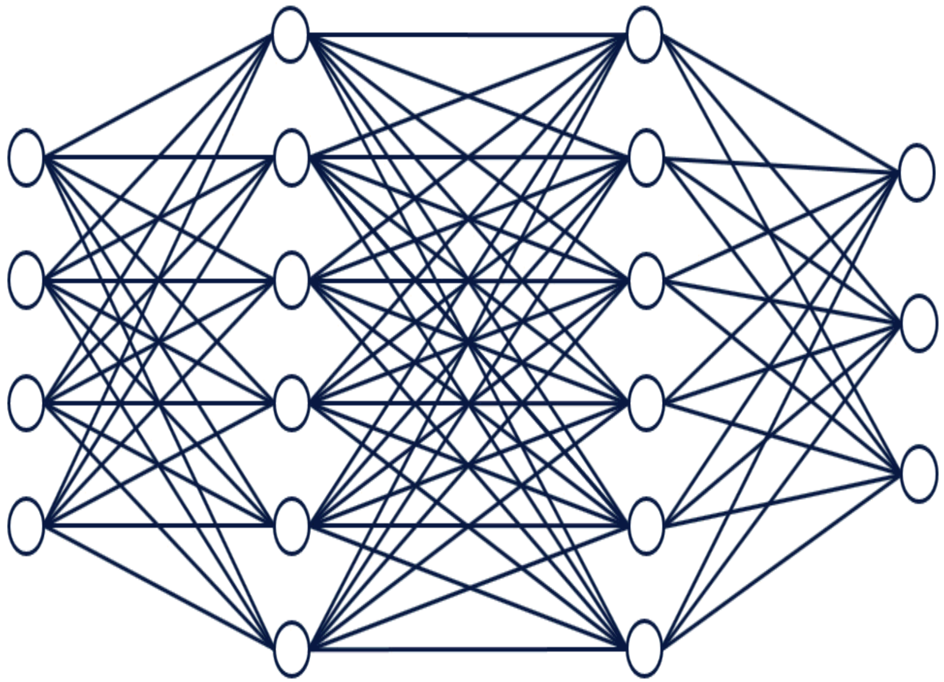
GI (Ours)	EI
1. Principled easy-to-compute decision rules	✓
2. Natural incorporation of side info and flexibility	✗
3. Competitive performance on benchmarks	✓✗
4. Theoretical guarantees	✓✗

Under-explored Side Info and Practical Flexibility

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

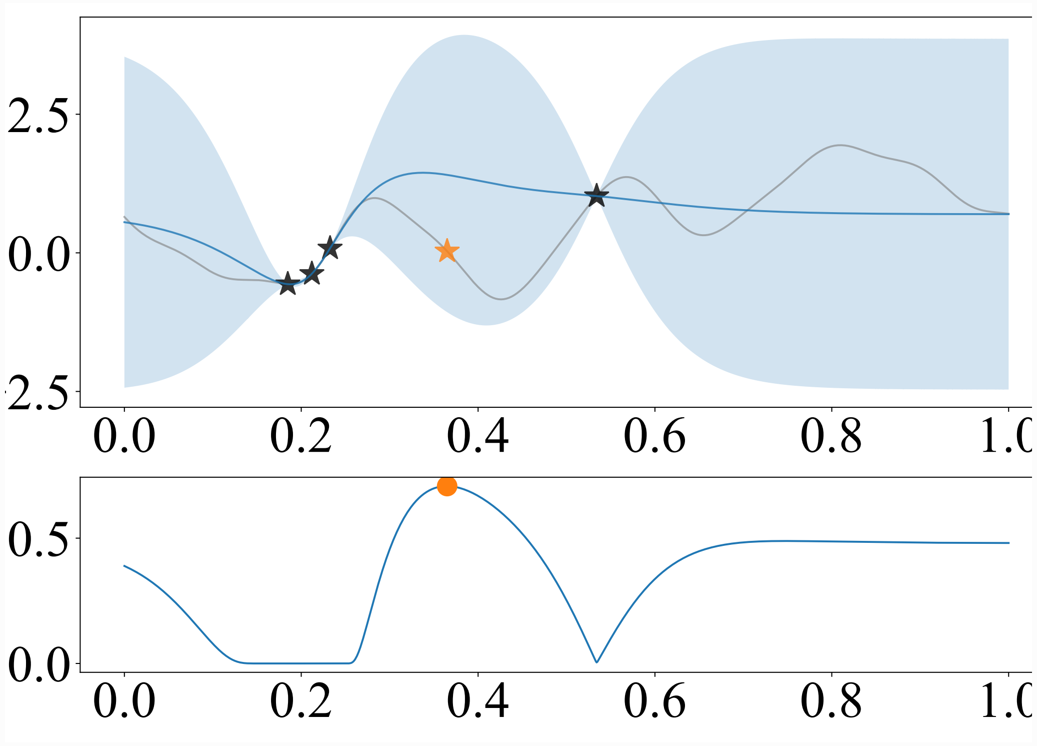
$\tau\text{: } \text{EI}(x_\tau) \leq \theta$

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

Which threshold?

Observable multi-stage feedback

?



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

Under-explored Side Info and Practical Flexibility

- Varying evaluation costs
- Smart stopping time
- Observable multi-stage feedback

New design principle:
Gittins index

Why Gittins index?

Varying evaluation costs

Smart stopping time

Observable multi-stage feedback

New design principle:
Gittins index

Optimal in related sequential decision problems

Why Gittins index?

Varying evaluation costs

Features in Pandora's box

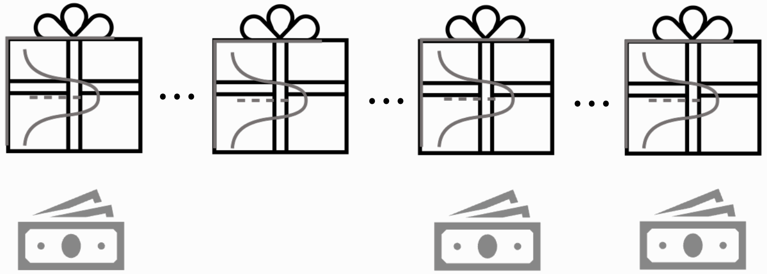
Smart stopping time

Features in Pandora's box

Observable multi-stage feedback

New design principle:
Gittins index

Optimal in related sequential decision problems



Why Gittins index?

Varying evaluation costs

Features in Pandora's box

Smart stopping time

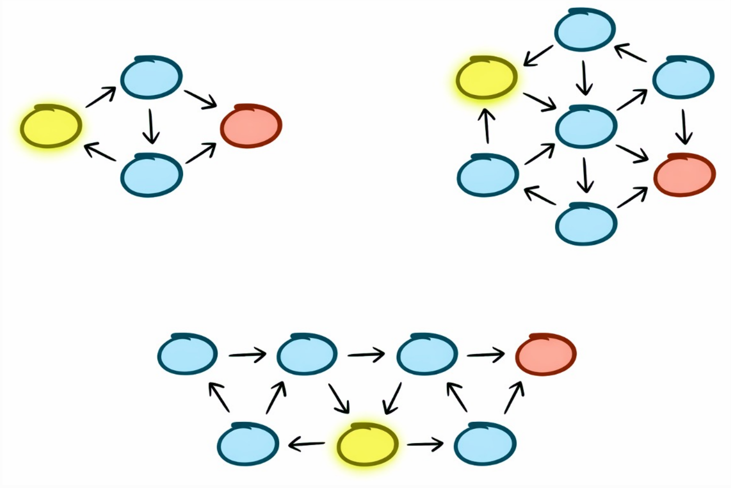
Features in Pandora's box

Observable multi-stage feedback

Features in Markov chain selection

New design principle:
Gittins index

Optimal in related sequential decision problems



Why Gittins index?

Varying evaluation costs

Features in Pandora’s box

This talk’s focus

Smart stopping time

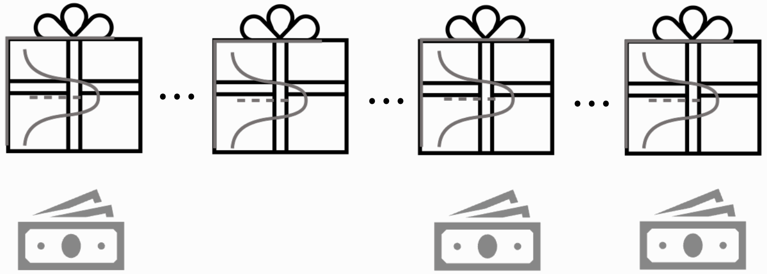
Features in Pandora’s box

Observable multi-stage feedback

Features in Markov chain selection

New design principle:
Gittins index

Optimal in related sequential decision problems

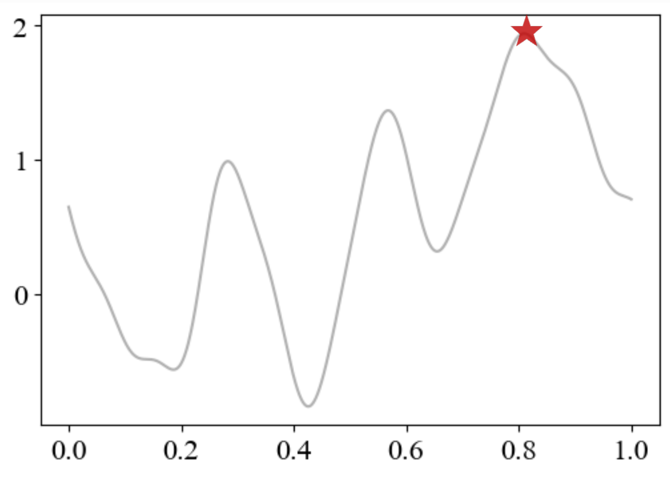


"Cost-aware Bayesian Optimization via the Pandora's Box Gittins Index.” NeurIPS’24.

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

Bayesian Optimization

$f(x)$



Continuous

Correlated

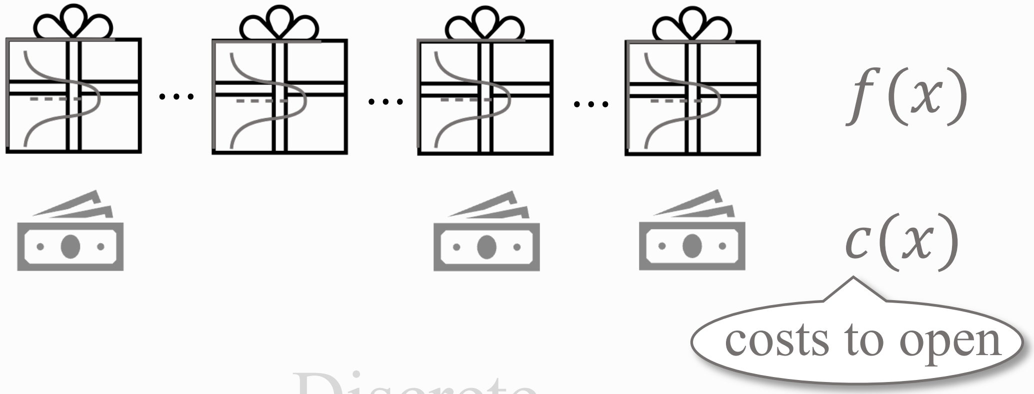
Fixed-iteration

Cost-unaware

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

Pandora's Box

[Weitzman'79]



Discrete

Independent

Flexible-stopping

Cost-aware

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

Expected Improvement vs Gittins Index

Varying evaluation costs

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

Arbitrarily bad

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

naturally incorporates costs

Smart stopping time

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

Which threshold?

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

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

derived shared stopping rule

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

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

Our Contribution: Gittins Index Principle

Joint work with Ziv Scully and Alexander Terenin et al.

GI (Ours)	EI

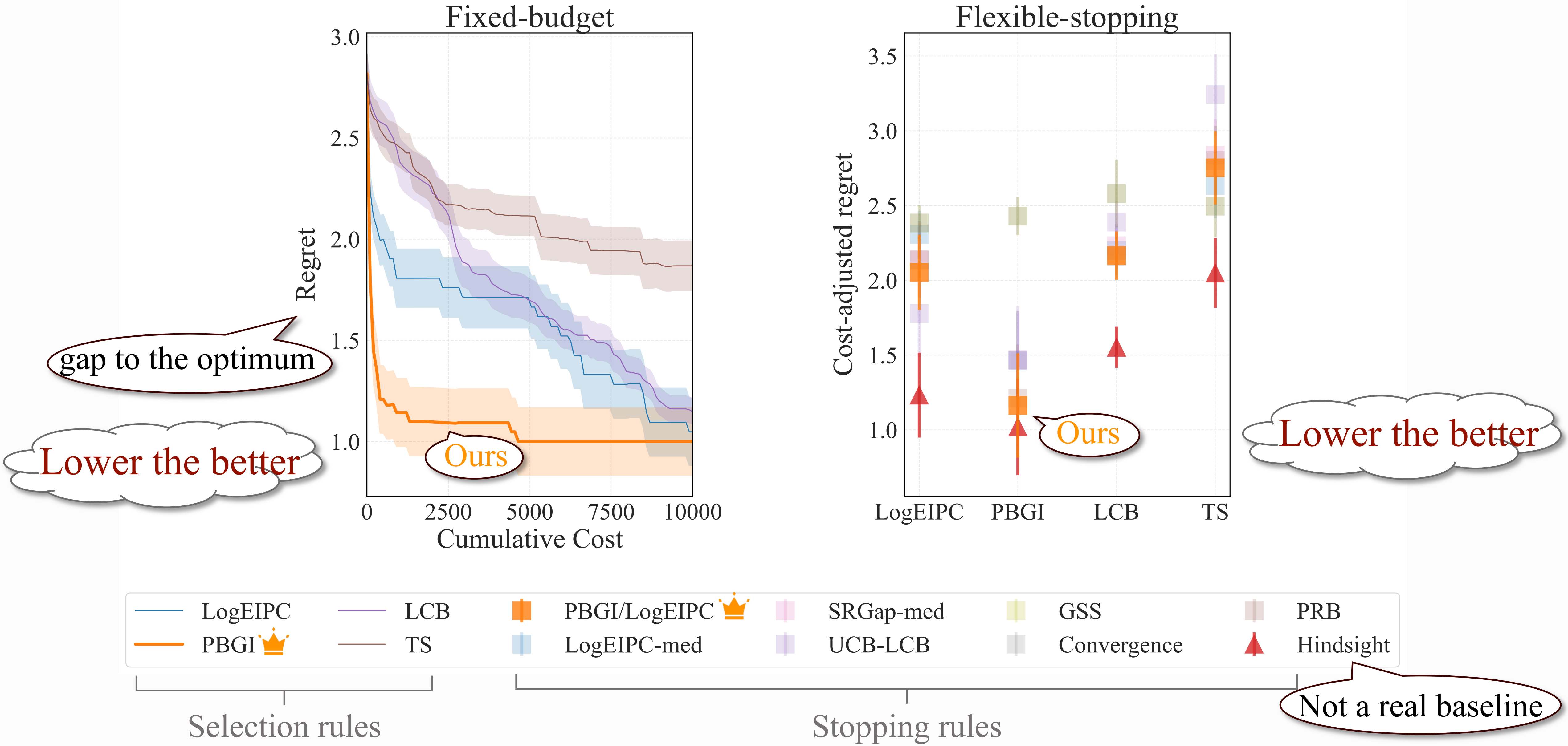
1. Principled easy-to-compute decision rules ✓

2. Natural incorporation of side info and flexibility ✗

3. Competitive performance on benchmarks

4. Theoretical guarantees

Gittins Index vs Baselines on AutoML Benchmark



Our Contribution: Gittins Index Principle

Joint work with Ziv Scully and Alexander Terenin et al.

GI (Ours)

EI

1. Principled easy-to compute decision rules ✓

2. Natural incorporation of side info and flexibility ✗

3. Competitive performance on benchmarks

4. Theoretical guarantees

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

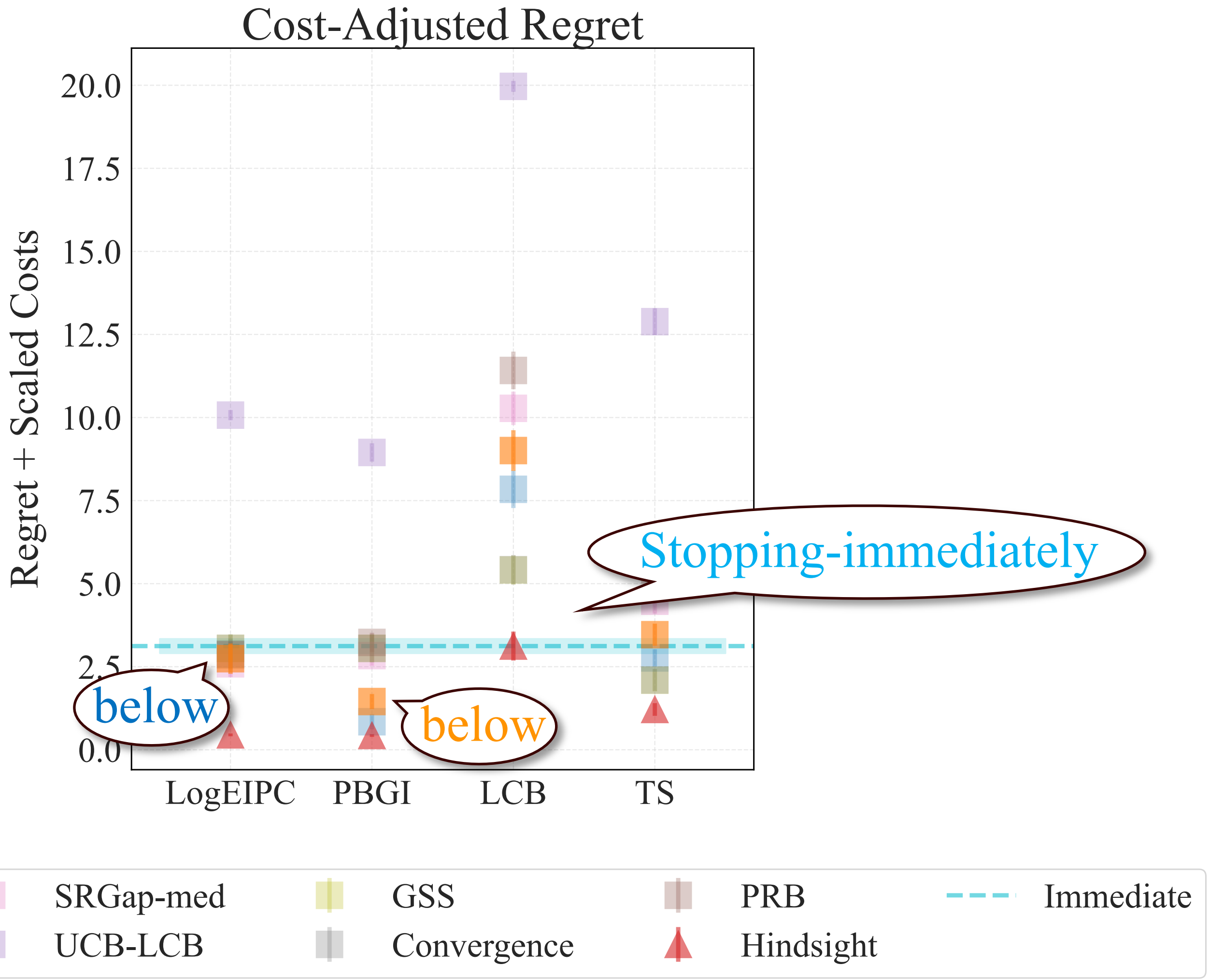
Implication:

- 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

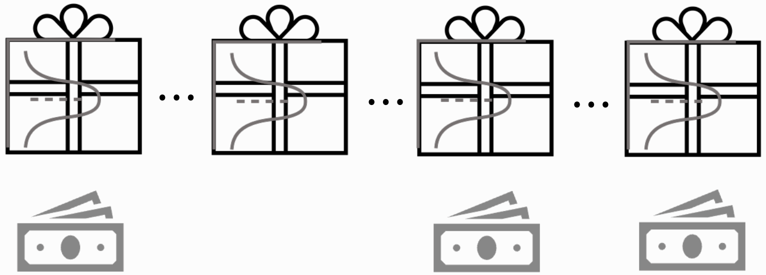
Proof idea: For all $t < \tau$, $\mathrm{EI}(x_{t+1}) \geq c(x_{t+1})$.

stopping time



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

Principled decision rules



Link to Pandora's Box problem
& Gittins index theory

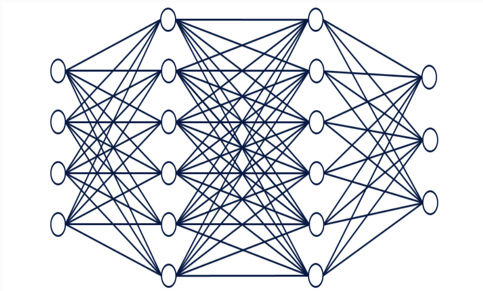
Natural incorporation of side info

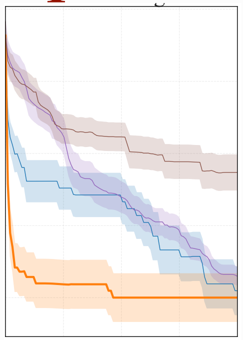
Varying evaluation costs

Adaptive stopping time

Multi-stage feedback

Competitive empirical performance





Interests from practitioners (e.g., Meta)

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

Theoretical guarantees

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

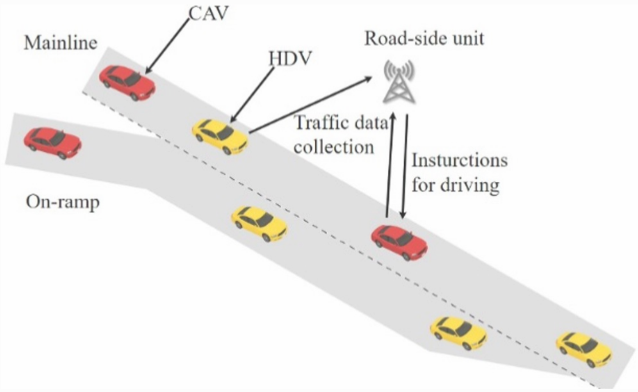
Ongoing: regret bound

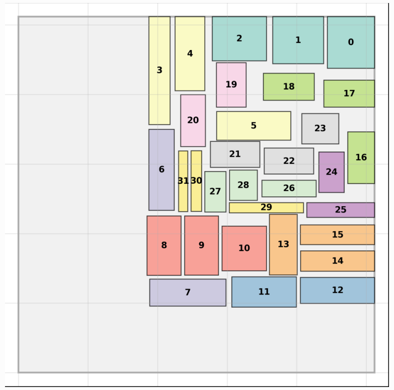
"Cost-aware Stopping for Bayesian Optimization." Under review.

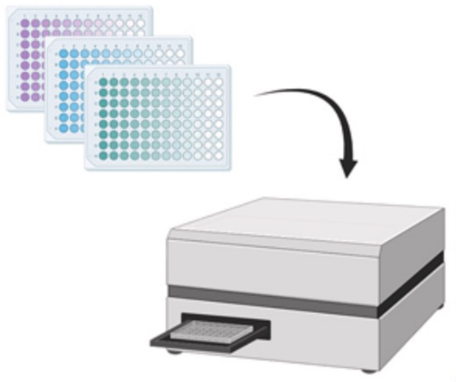
Part II (Ongoing):

Black-box Optimization Beyond AutoML

Reinforcement Learning · *Engineering Design* ·
Scientific Discovery · *Emerging AI Systems (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	?	?	★★★	?	★