NeurIPS'24 publication

Cost-aware Bayesian Optimization via the Pandora's Box Gittins Index

Qian Xie (Cornell ORIE)

Virtual Seminar Series on Bayesian Decision-making and Uncertainty

Coauthors

Raul Astudillo

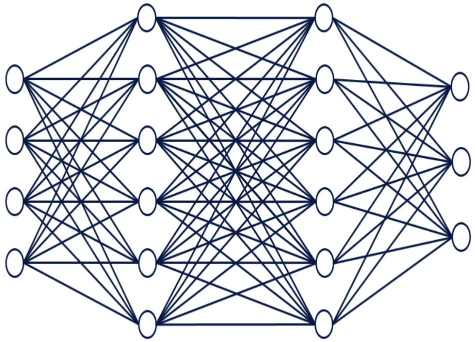
Peter Frazier

Ziv Scully

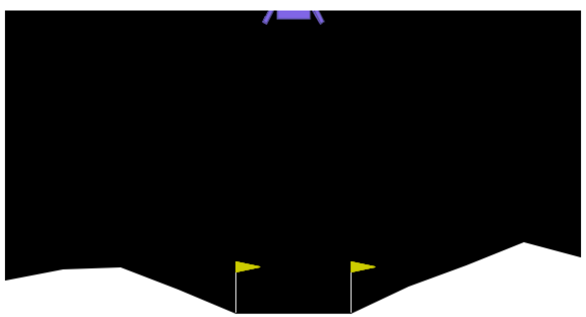
Alexander Terenin

World of Hyperparameter Optimization

Hyperparameter tuning:

Training hyperparameters →  → Accuracy

Control optimization:

Control variables →  → Reward

Adaptive experimentation:

Decision variables → 

→ Revenue

World of Hyperparameter Optimization

Black-box optimization:

Input hyperparameters →  → Performance metric

World of Hyperparameter Optimization

Black-box function:

$x \longrightarrow$

$\longrightarrow f(x)$

$f \sim$Stochastic Process

Optimizing Black-box Functions

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

Goal: $\max_{x \in \mathcal{X}} f(x)$

$f \sim$Stochastic Process

Optimizing Black-box Functions

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$f \sim$Stochastic Process

Grid Search? Random search?

Optimizing Black-box Functions

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

expensive-to-evaluate

Goal: $\max_{x \in \mathcal{X}} f(x)$

$f \sim$ Stochastic Process

Grid Search? Random search?

Optimizing Black-box Functions

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

limited #evaluations

Goal: $\sup_{\text{policy}} \mathbb{E} \max_{t=1,2,\dots,T} f(x_t)$

$f \sim$Stochastic Process

Grid Search? Random search?

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limited #evaluations

Goal: $\sup_{\text{policy}} \mathbb{E} \max_{t=1,2,\ldots,T} f(x_t)$

$f \sim$Stochastic Process

More efficient: Bayesian optimization!

Bayesian Optimization

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

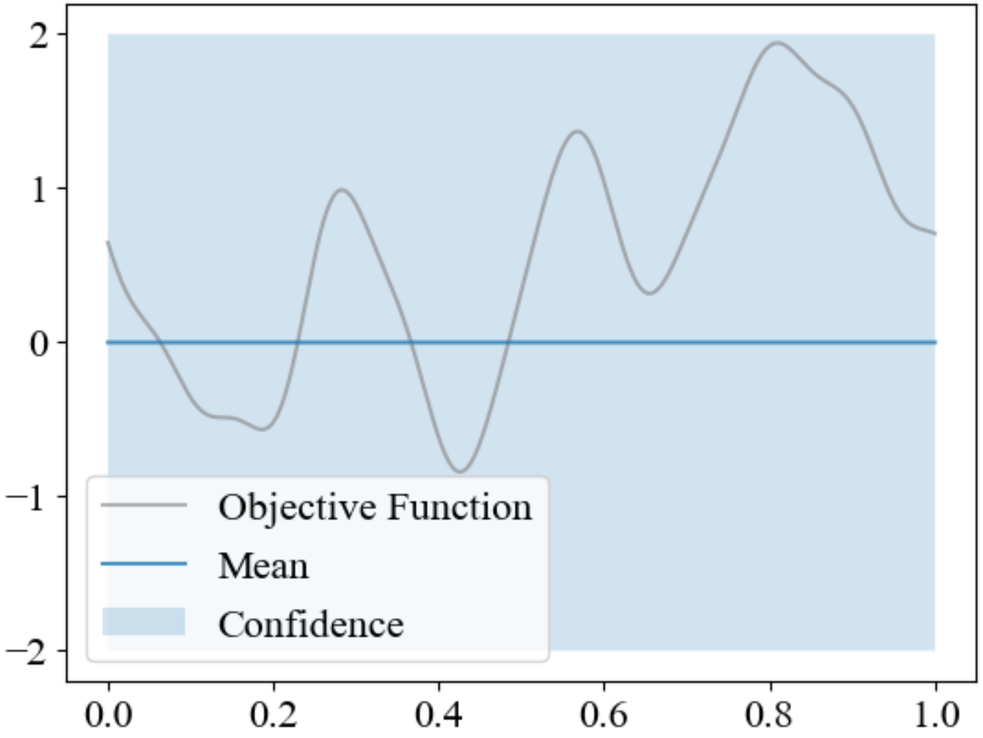
limited #evaluations

Goal: $\sup_{\text{policy}} \mathbb{E} \max_{t=1,2,\ldots,T} f(x_t)$

$f \sim$Gaussian Process

Key idea: maintain posterior belief about f

Bayesian Optimization



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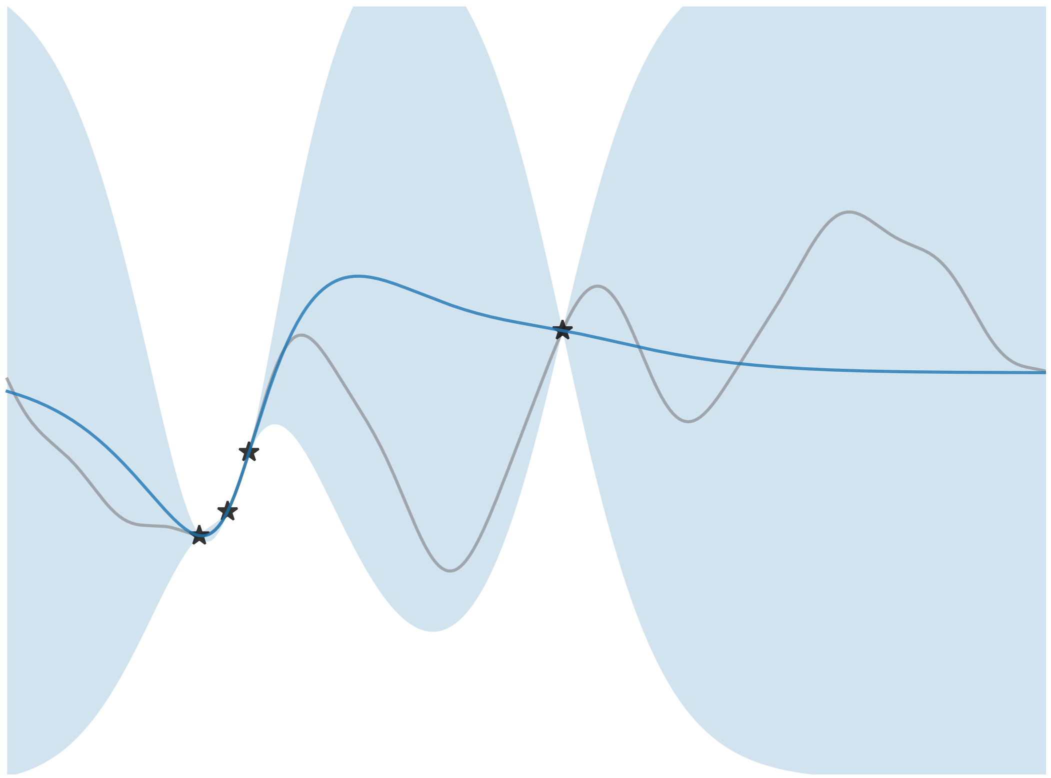
Bayesian Optimization



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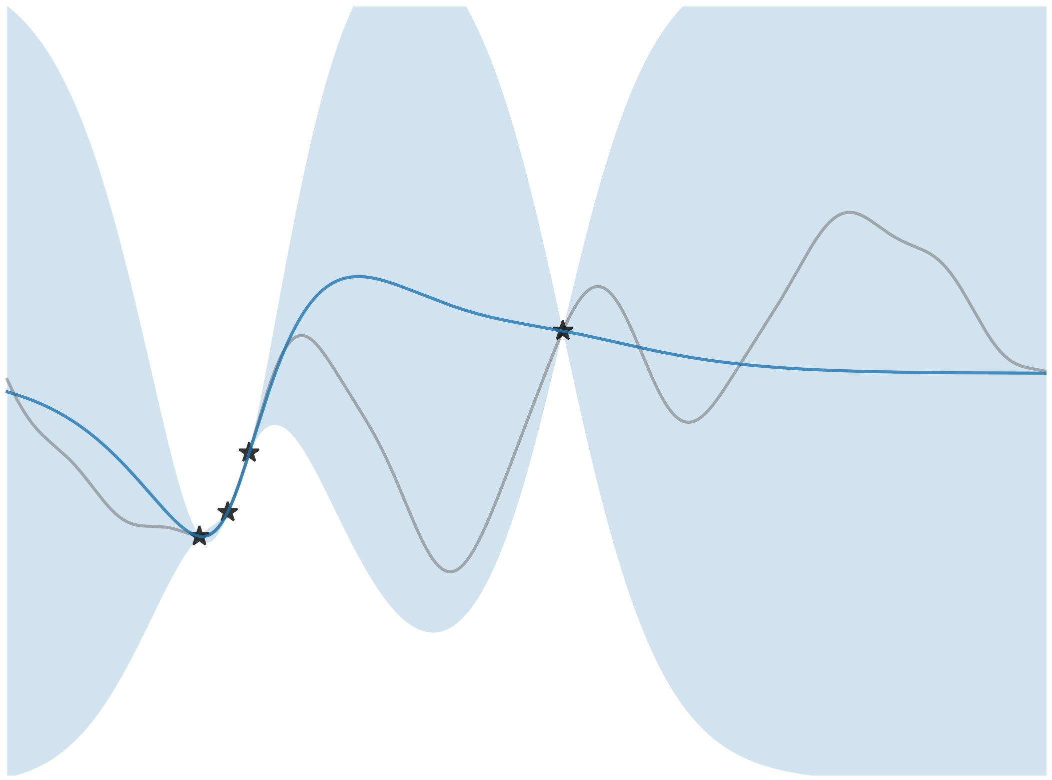
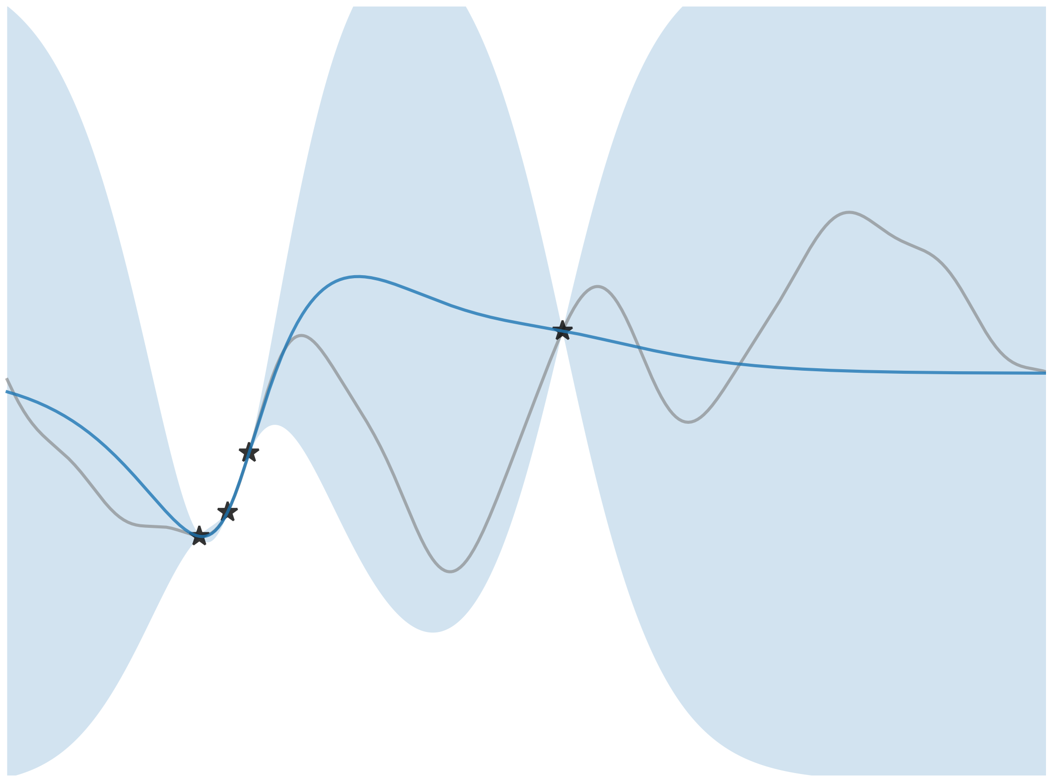
Bayesian Optimization



What to evaluate next?

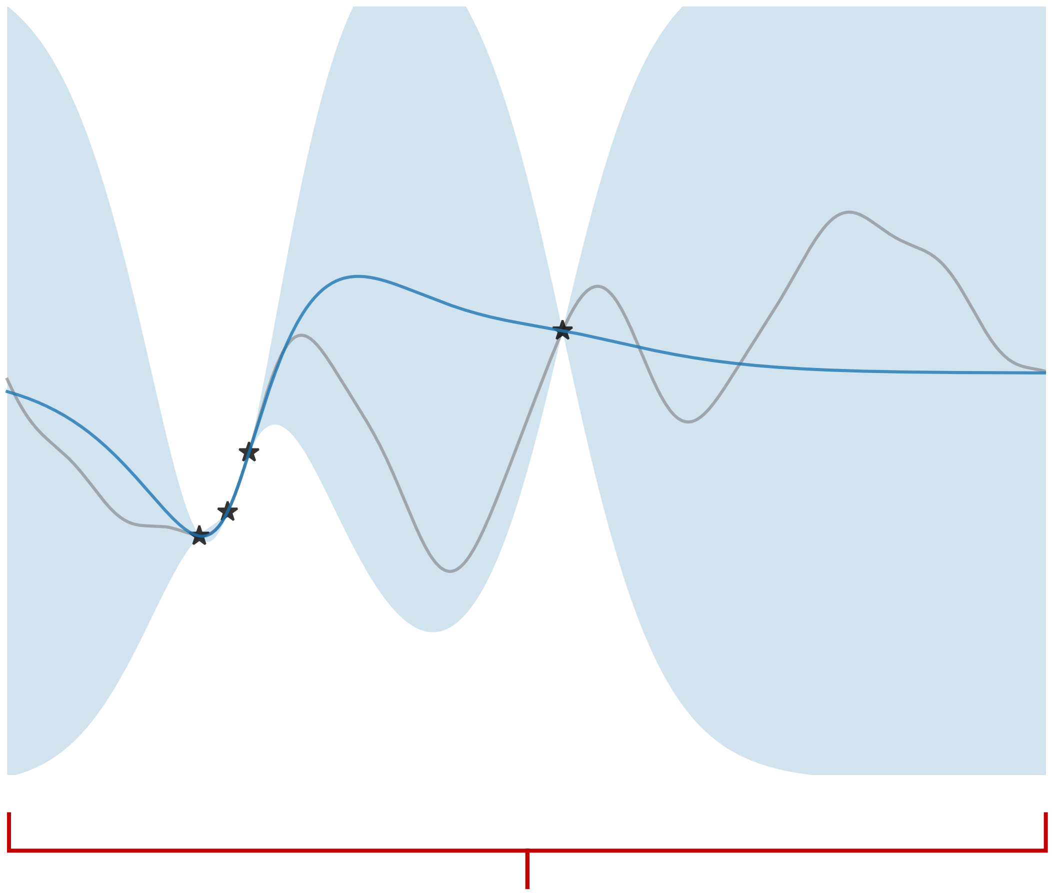
Bayesian Optimization



What to evaluate next?

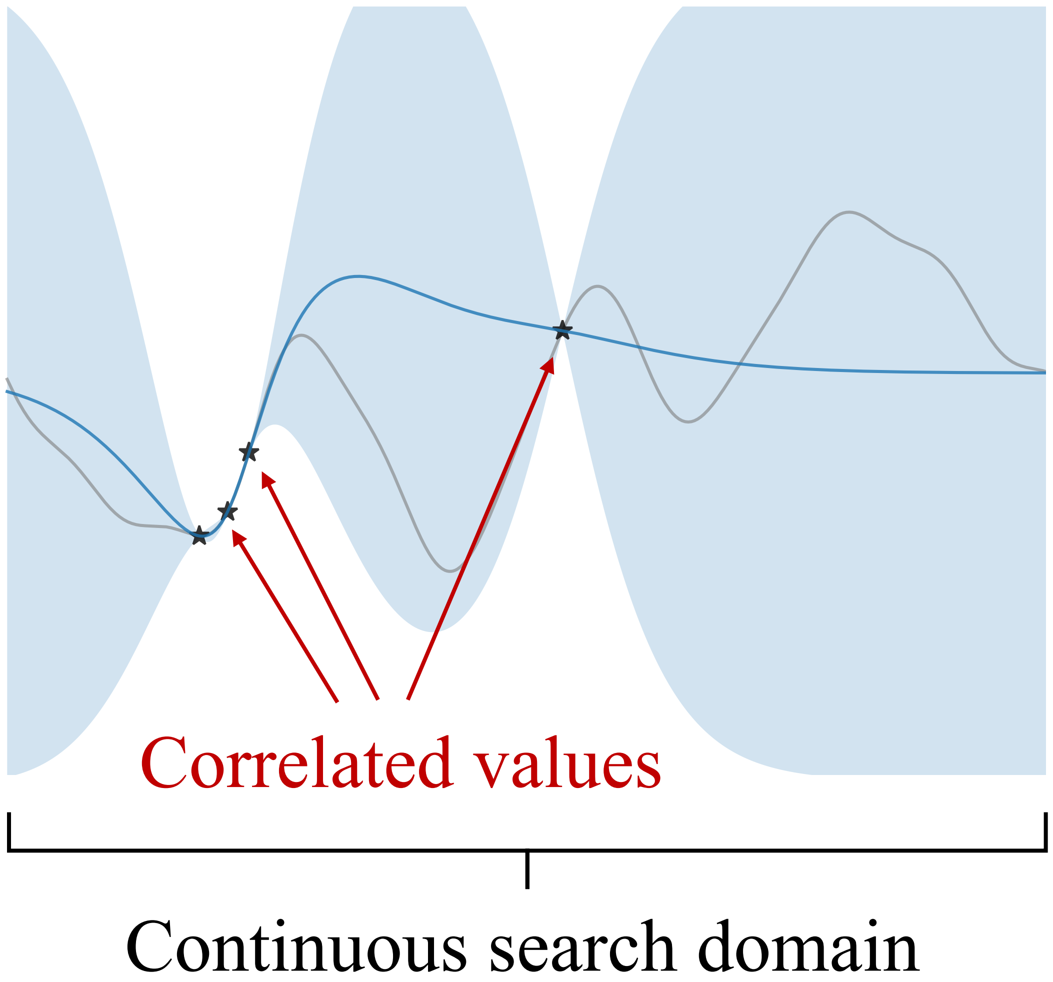
Optimal policy?

Properties of Bayesian Optimization

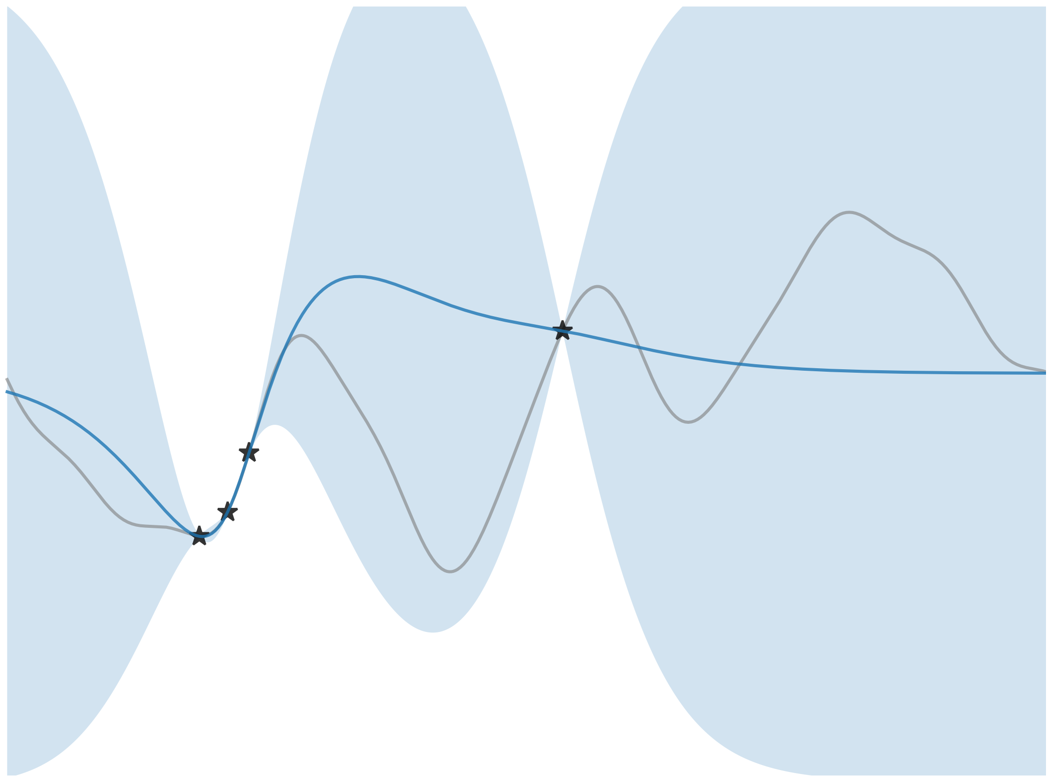


Continuous search domain

Properties of Bayesian Optimization

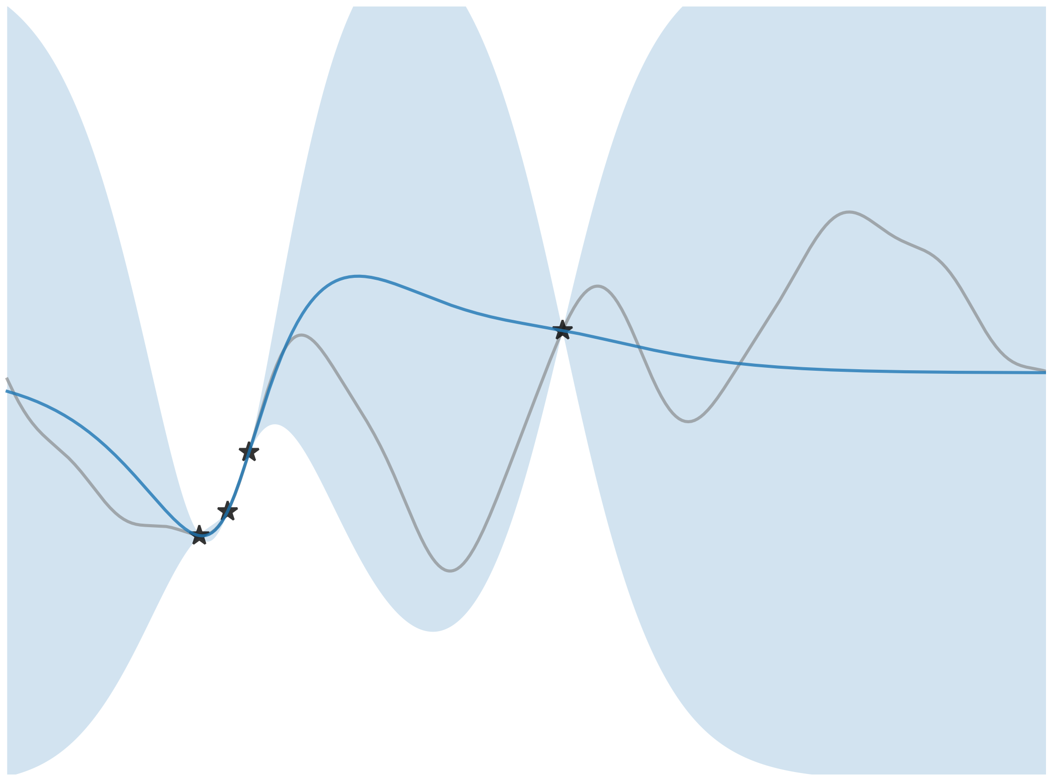


Properties of Bayesian Optimization



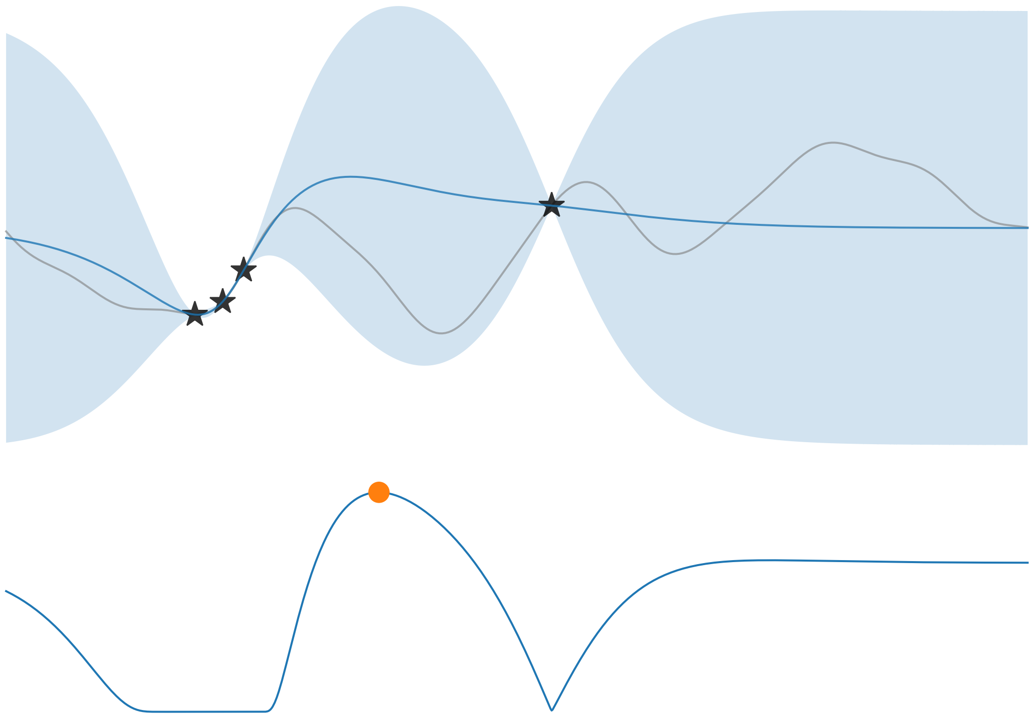
Correlation & continuity $\Longrightarrow$ Intractable MDP

Properties of Bayesian Optimization



Intractable MDP $\Longrightarrow$ Optimal policy unknown

Popular Policy: Expected Improvement

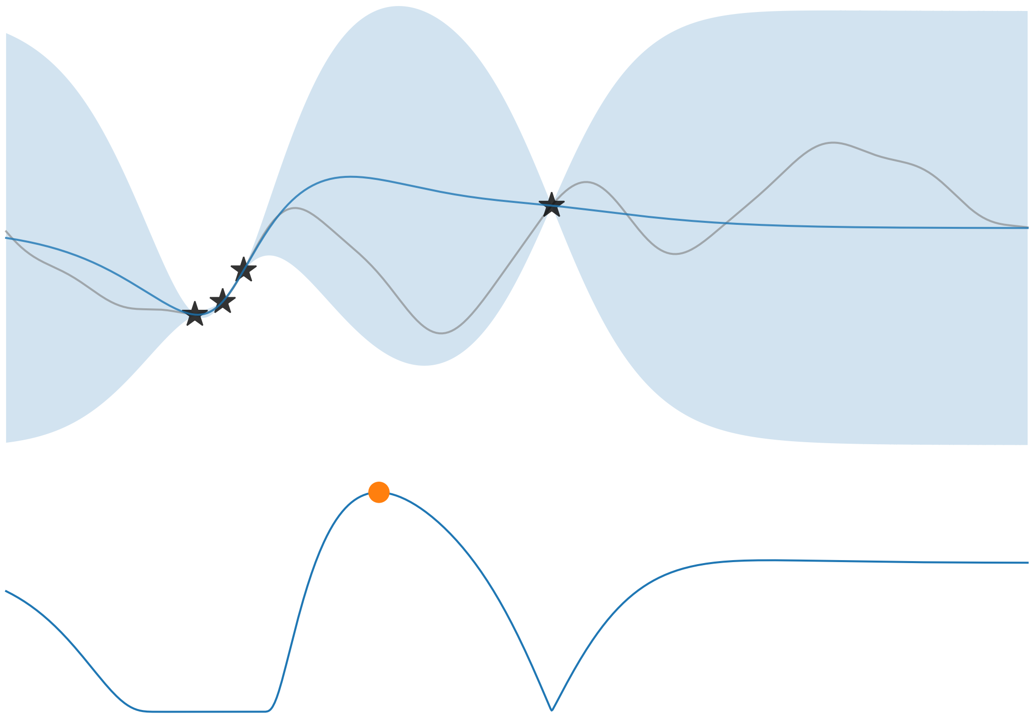


$$\text{EI}(x) = \mathbb{E}[\underbrace{\max(f(x) - \overbrace{y_{\text{best}}}^{\text{current best observed}}, 0)}_{\text{“improvement”}} \mid \overbrace{D}^{\text{data}}]$$

$$\max_x \text{EI}_{\underbrace{f|D}_{\text{posterior distribution}}}(x; y_{\text{best}})$$

One-step approximation to MDP

Popular Policy: Expected Improvement



Other improvement-based policies:

- Probability of Improvement
- Knowledge Gradient
- Multi-step Lookahead EI
- ⋮

multi-step approximation to MDP

Approaches to Bayesian Optimization

- Improvement-based:
  - Expected Improvement
  - Probability of Improvement
  - Knowledge Gradient
  - Multi-step Lookahead EI

Approaches to Bayesian Optimization

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  - Max-value Entropy Search
  - Predictive Entropy Search

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Approaches to Bayesian Optimization

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- Our work: Gittins Index

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Why another approach?

Approaches to Bayesian Optimization

- Improvement-based
- Entropy-based
- Upper Confidence Bound
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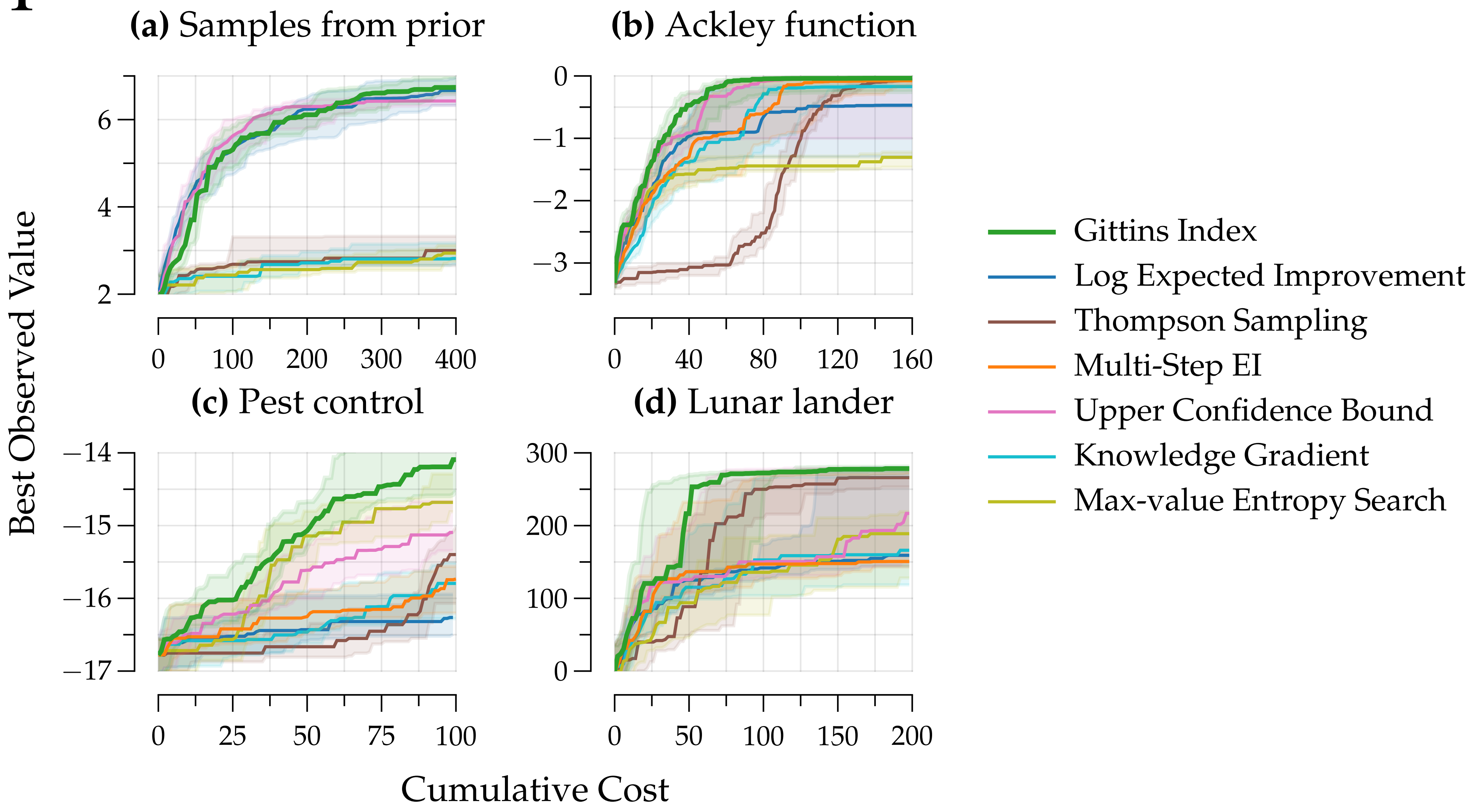
- Our work: Gittins Index

Why another approach?

1. Competitive empirical performance

Experiment Results: Gittins Index vs Baselines



Experiment Setup: Objective Functions

Synthetic

Samples from prior

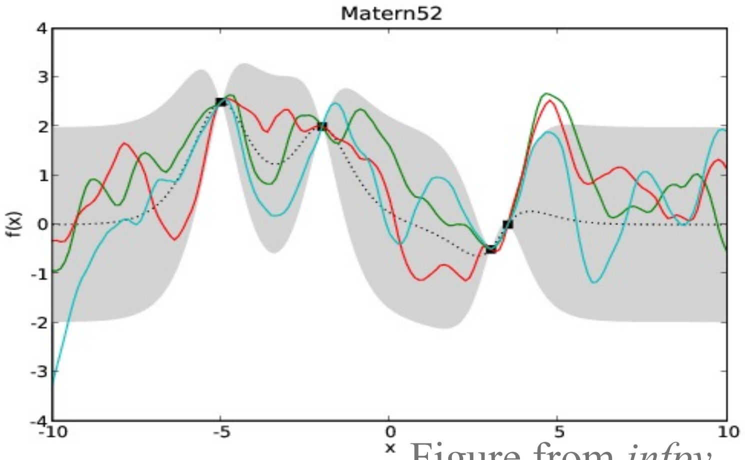


Figure from *infpy*

Ackley function

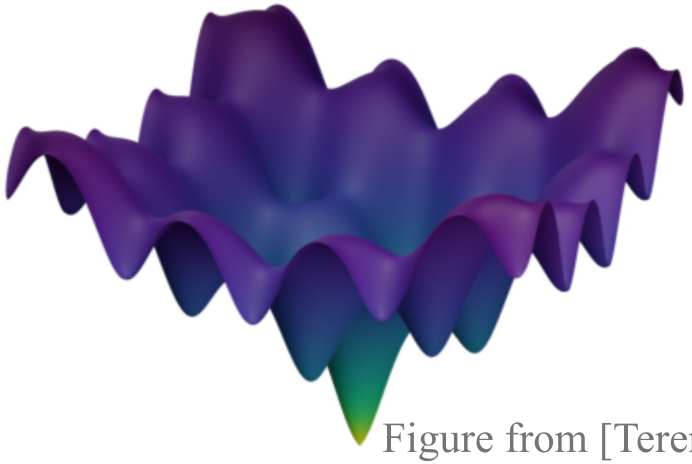


Figure from [Terenin'22]

Empirical

Pest Control

Figure from ChatGPT

Lunar Lander

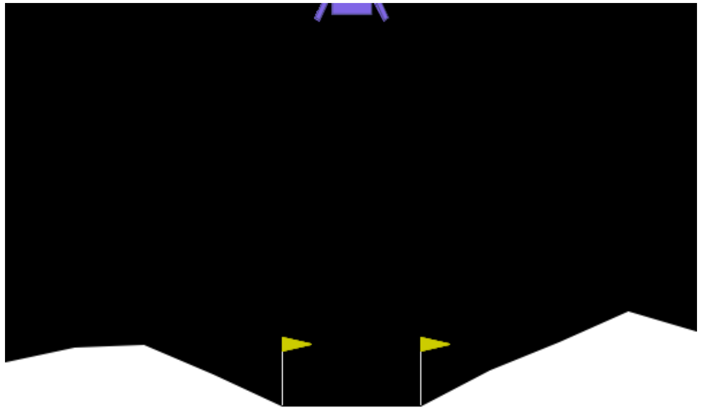


Figure from OpenAI Gym

Approaches to Bayesian Optimization

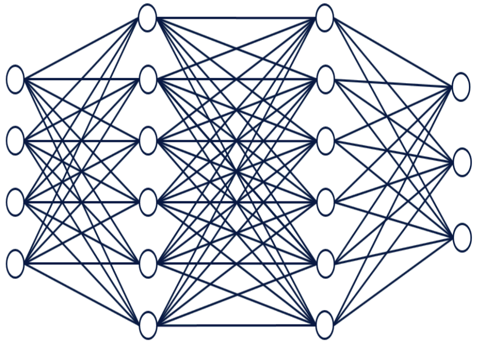
- Improvement-based
- Entropy-based
- Upper Confidence Bound
- Thompson Sampling
- Our work: Gittins Index

Why another approach?

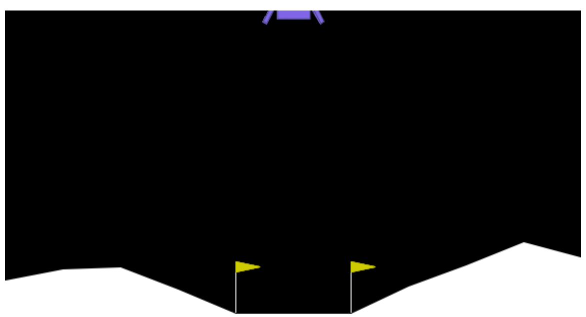
1. Competitive empirical performance
2. Applicable to varying evaluation costs

Examples: Varying Evaluation Time

Hyperparameter tuning:

Training hyperparameters →  → Accuracy

Control optimization:

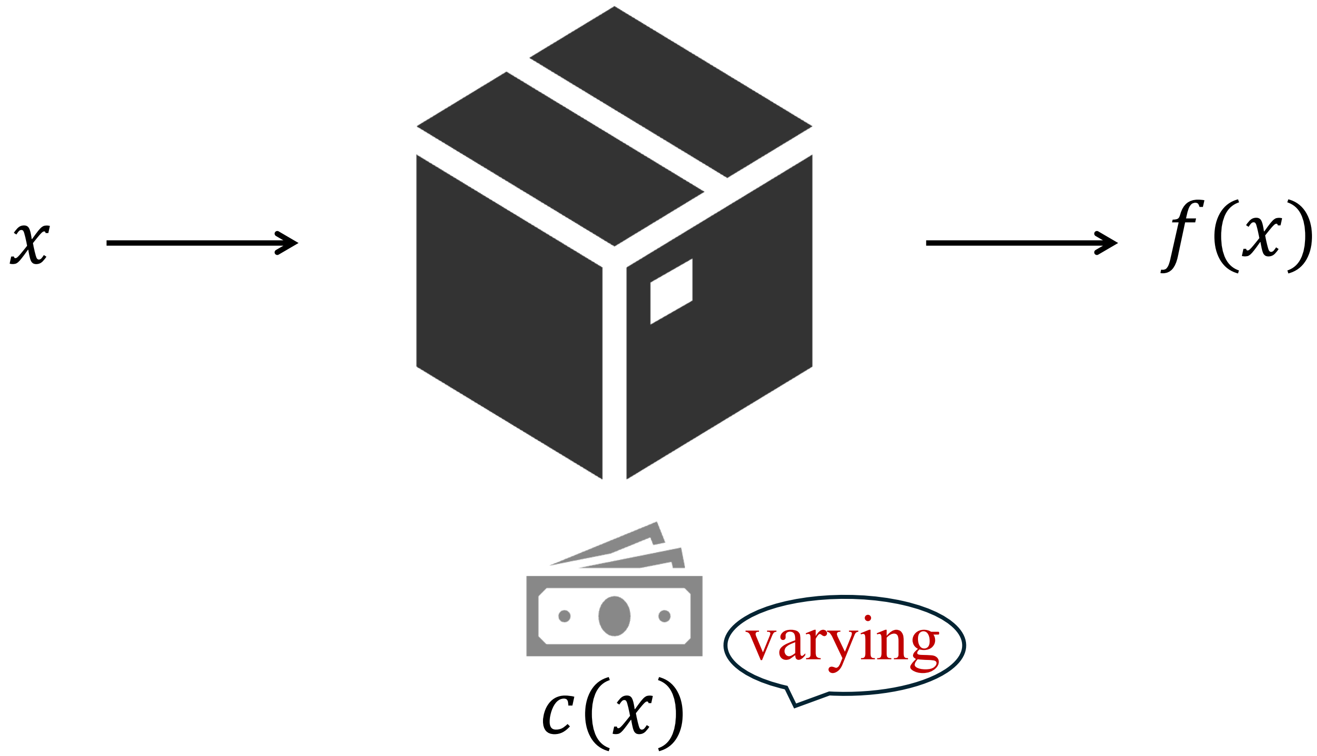
Control variables →  → Reward

Adaptive experimentation:

Decision variables → 

→ Revenue

Varying Evaluation Costs



Cost-aware Bayesian Optimization

[Lee, Perrone, Archambeau, Seeger'21]

$x \longrightarrow$

$\longrightarrow f(x)$

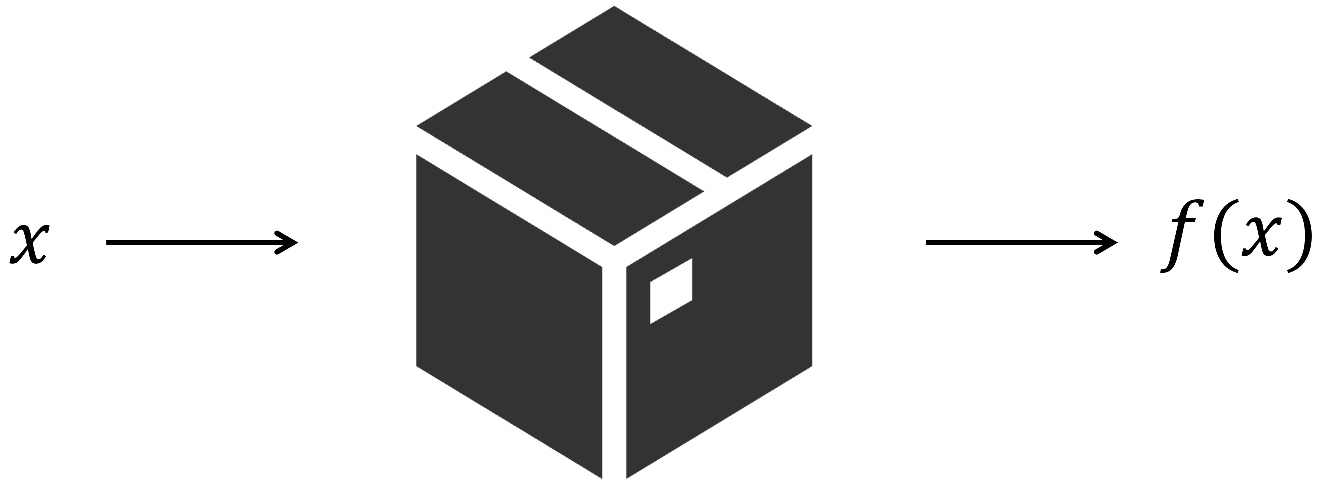
$$\text{Goal: } \sup_{\text{policy}} \mathbb{E} \max_{t=1,2,\dots,T} f(x_t)$$

$$\text{s.t. } \sum_{t=1}^{T} c(x_t) \leq B$$

"Multi-step Budgeted Bayesian Optimization with Unknown Evaluation Costs"
[Astudillo, Jiang, Balandat, Bakshy, Frazier'21]

Cost-aware Bayesian Optimization

[Lee, Perrone, Archambeau, Seeger'21]
[Astudillo, Jiang, Balandat, Bakshy, Frazier'21]



Goal: $\sup_{\text{policy}} \mathbb{E} \max_{t=1,2,\dots,T} f(x_t)$

s.t. $\mathbb{E} \sum_{t=1}^{T} c(x_t) \leq B$

Our work studies expected budget constraint

Cost-aware Bayesian Optimization

	Uniform costs	Varying costs
One-step	Expected improvement $\max_x \mathrm{EI}_{f\mid D}(x; y_{\mathrm{best}})$	

Cost-aware Bayesian Optimization

	Uniform costs	Varying costs
One-step	Expected improvement	Expected improvement per cost
	$\max_x \mathrm{EI}_{f\|D}(x; y_{\text{best}})$	[Snoek, Larochelle, Adams'21]

Cost-aware Bayesian Optimization

	Uniform costs	Varying costs
One-step	Expected improvement	Expected improvement per cost
	$\max_x \mathrm{EI}_{f\|D}(x; y_{\mathrm{best}})$	$\max_x \mathrm{EI}_{f\|D}(x; y_{\mathrm{best}}) / c(x)$

Cost-aware Bayesian Optimization

	Uniform costs	Varying costs
One-step	Expected improvement	Expected improvement per cost
	$\max_x \mathrm{EI}_{f\|D}(x; y_{\text{best}})$	$\max_x \mathrm{EI}_{f\|D}(x; y_{\text{best}})/c(x)$

Why divide?

Cost-aware Bayesian Optimization

	Uniform costs	Varying costs
One-step	Expected improvement	Expected improvement per cost
	$\max_x \mathrm{EI}_{f\mid D}(x; y_{\text{best}})$	$\max_x \mathrm{EI}_{f\mid D}(x; y_{\text{best}})/c(x)$

arbitrarily bad

[Astudillo, Jiang, Balandat, Bakshy, Frazier'21]

Cost-aware Bayesian Optimization

	Uniform costs	Varying costs
One-step	Expected improvement	Expected improvement per cost
Multi-step	Multi-step Lookahead EI	Budgeted Multi-step Lookahead EI

slow

[Astudillo, Jiang, Balandat, Bakshy, Frazier'21]

Cost-aware Bayesian Optimization

	Uniform costs	Varying costs
One-step	Expected improvement	Expected improvement per cost
Multi-step	Multi-step Lookahead EI	Budgeted Multi-step Lookahead EI
	Upper Confidence Bound	?
	Thompson Sampling	?

Cost-aware Bayesian Optimization

	Uniform costs	Varying costs
One-step	Expected improvement	Expected improvement per cost
Multi-step	Multi-step Lookahead EI	Budgeted Multi-step Lookahead EI
	Upper Confidence Bound	?
	Thompson Sampling	?
	⋮	⋮

Our view: lack of a guidance to incorporate costs

Cost-aware Bayesian Optimization

	Uniform costs	Varying costs
One-step	Expected improvement	Expected improvement per cost
Multi-step	Multi-step Lookahead EI	Budgeted Multi-step Lookahead EI
	Upper Confidence Bound	?
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	⋮	⋮

New design principle: Gittins Index

Cost-aware Bayesian Optimization

	Uniform costs	Varying costs
One-step	Expected improvement	Expected improvement per cost
Multi-step	Multi-step Lookahead EI	Budgeted Multi-step Lookahead EI
	Upper Confidence Bound	?
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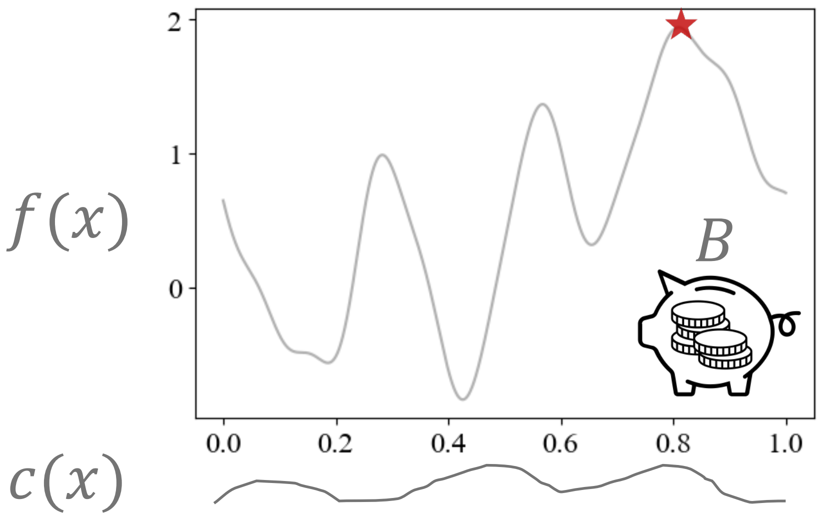
	⋮	⋮

New design principle: Gittins Index

inherently cost-aware

Cost-aware Bayesian Optimization



Continuous

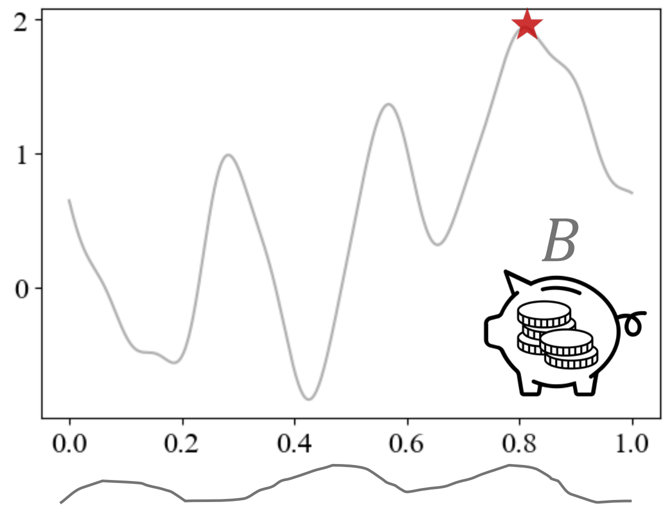
Correlated

Cost-aware Bayesian Optimization

Pandora's Box

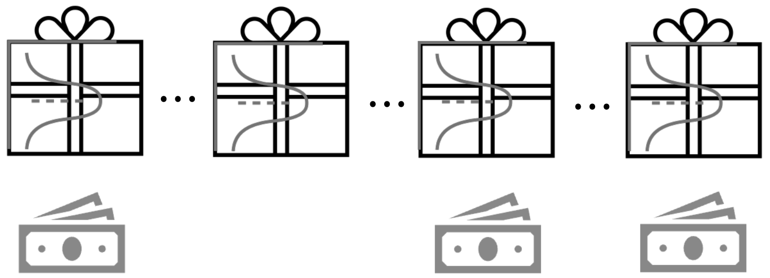
[Weitzman'79]

$f(x)$



$c(x)$

$\Longrightarrow$



$f(x)$

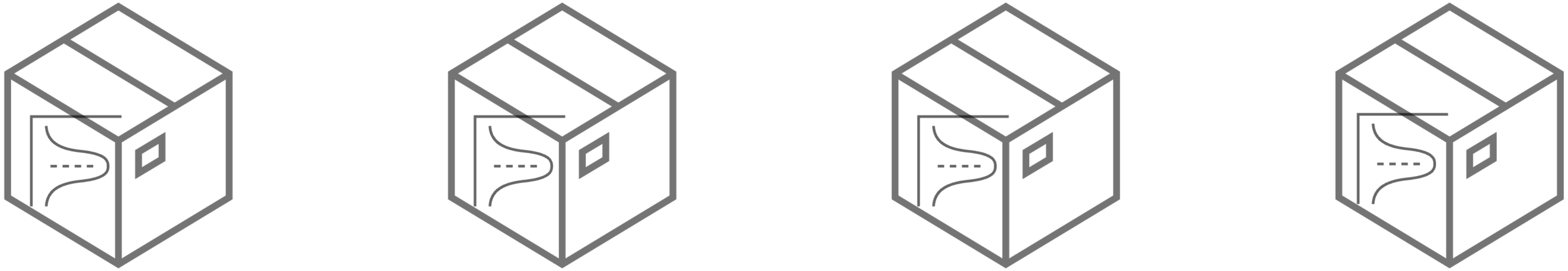
$c(x)$

Continuous $\Longrightarrow$ Discrete

Correlated $\Longrightarrow$ Independent

Pandora’s Box

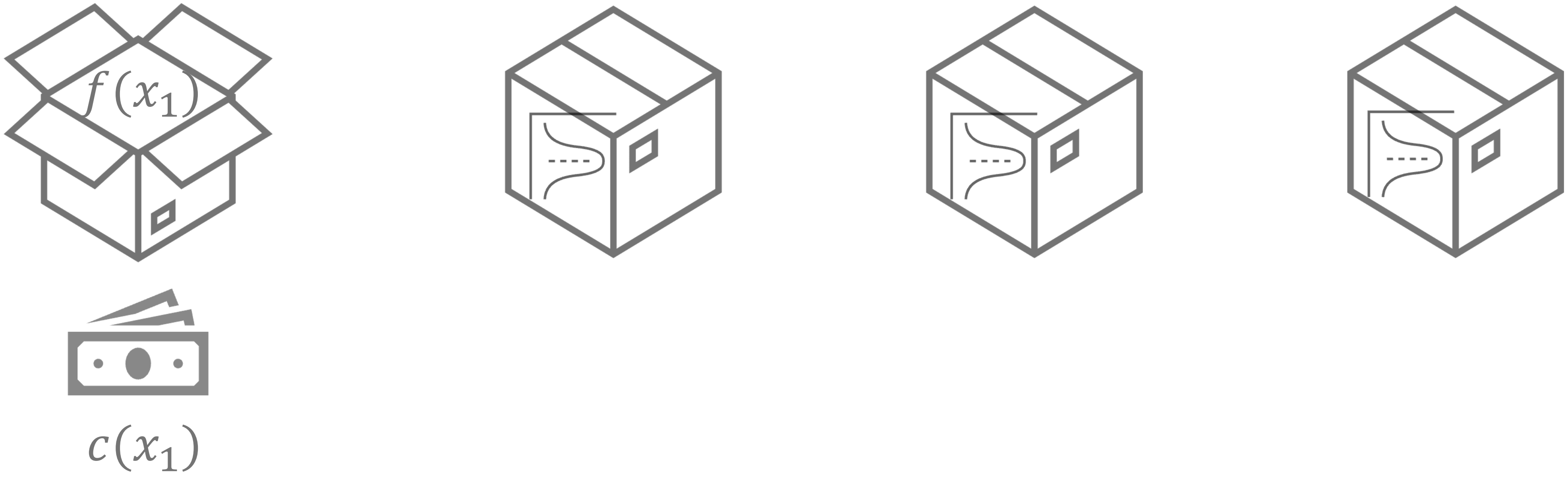
$t = 0$



$$\sup_{\text{policy}} \mathbb{E}\left(\max_{t=1,2,\ldots,T} f(x_t) - \sum_{t=1}^{T} c(x_t) \right)$$

Pandora’s Box

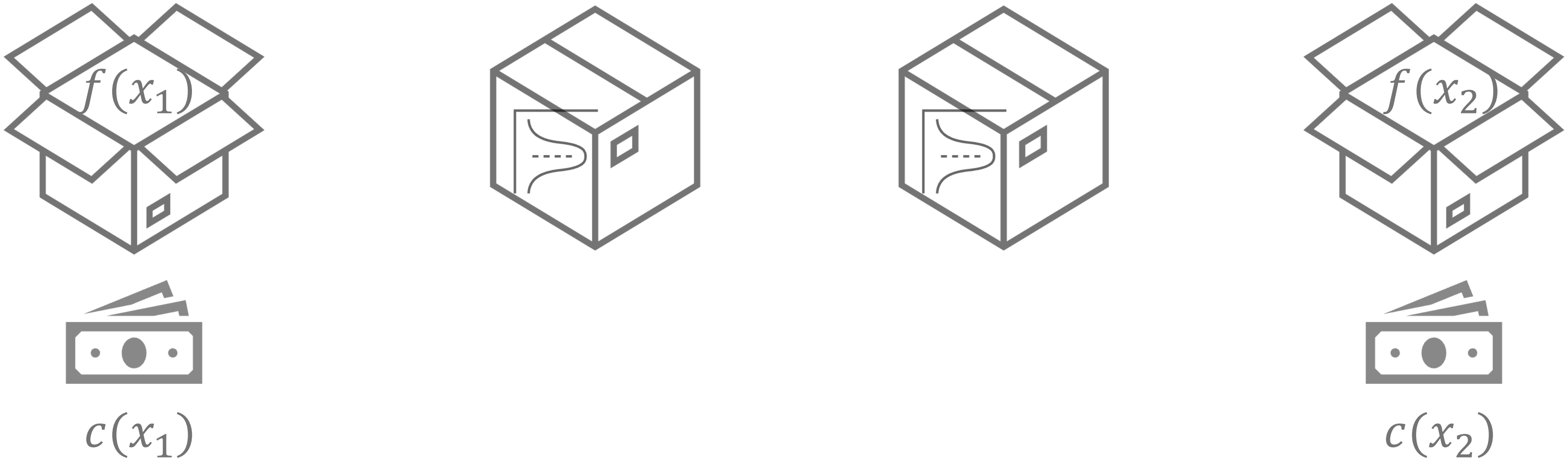
$t = 1$



$$\sup_{\text{policy}} \ \mathbb{E}\left(\max_{t=1,2,\ldots,T} f(x_t) - \sum_{t=1}^{T} c(x_t) \right)$$

Pandora's Box

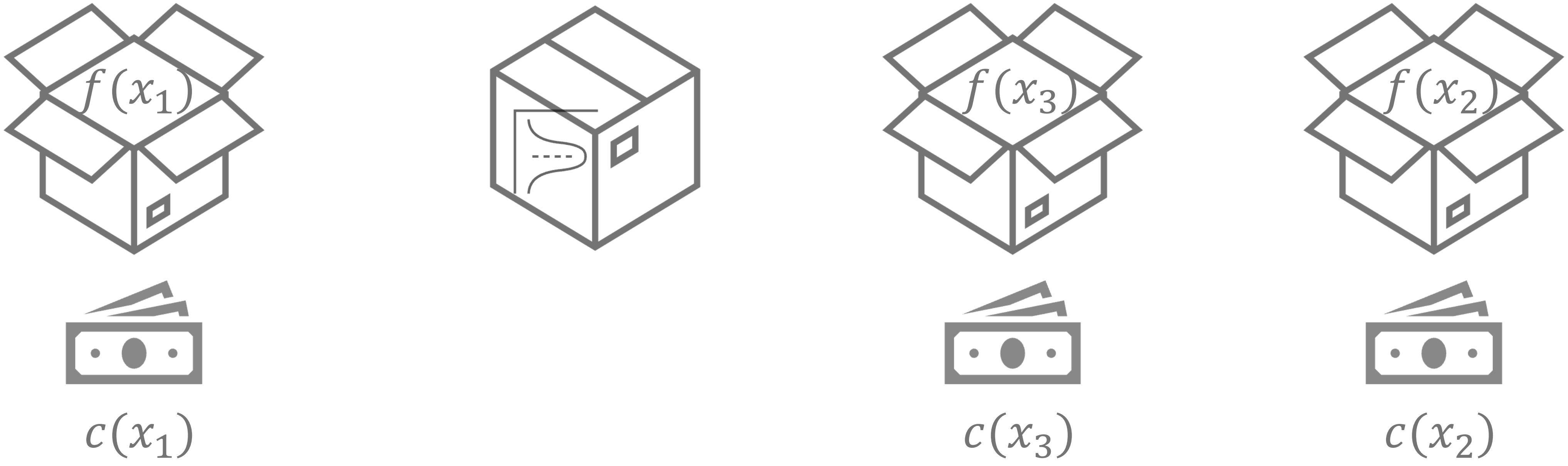
$t = 2$



$$\sup_{\text{policy}} \mathbb{E}\left(\max_{t=1,2,\ldots,T} f(x_t) - \sum_{t=1}^{T} c(x_t) \right)$$

Pandora's Box

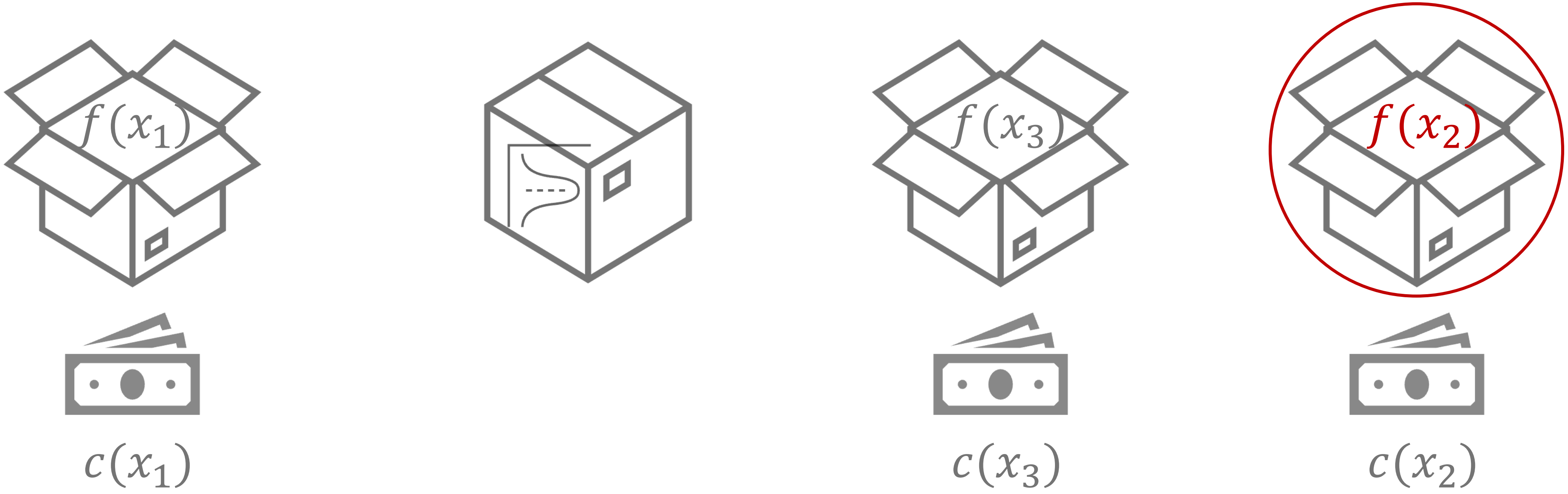
$t = 3$



$$\sup_{\text{policy}} \mathbb{E}\left(\max_{t=1,2,\dots,T} f(x_t) - \sum_{t=1}^{T} c(x_t) \right)$$

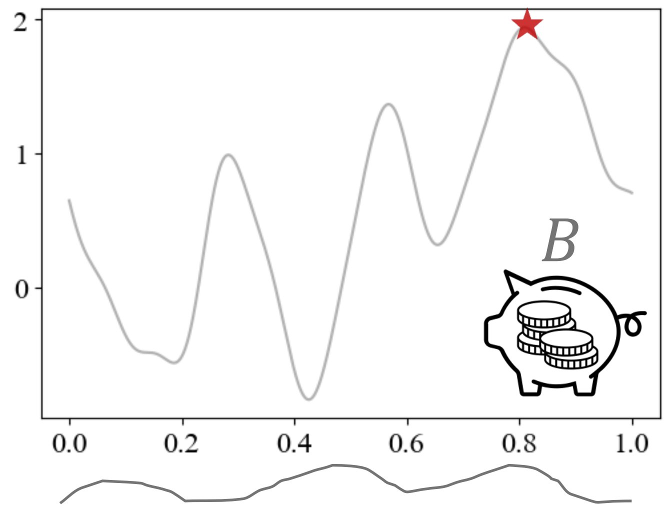
Pandora's Box

$t = T$, stop



$$\sup_{\text{policy}} \mathbb{E}\left(\max_{t=1,2,\ldots,T} f(x_t) - \sum_{t=1}^{T} c(x_t) \right)$$

Cost-aware Bayesian Optimization



Continuous

Correlated

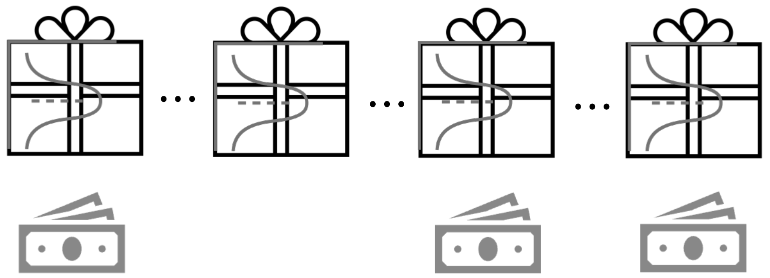
Expected-budget-constrained

$$\sup_{\text{policy}} \mathbb{E} \max_{t=1,2,\dots,T} f(x_t)$$

$$\text{s.t. } \mathbb{E} \sum_{t=1}^{T} c(x_t) \le B$$

Pandora's Box

[Weitzman'79]



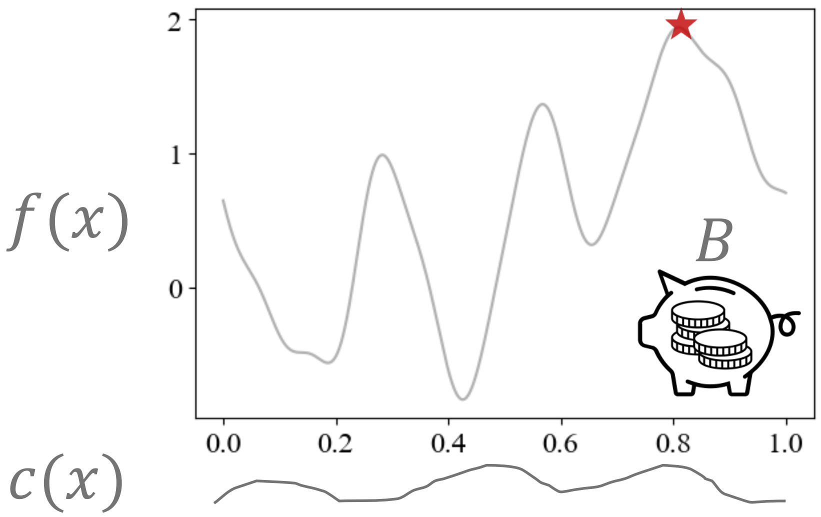
Discrete

Independent

Cost-per-sample

$$\sup_{\text{policy}} \mathbb{E} \left(\max_{t=1,2,\dots,T} f(x_t) - \sum_{t=1}^{T} c(x_t) \right)$$

Cost-aware Bayesian Optimization



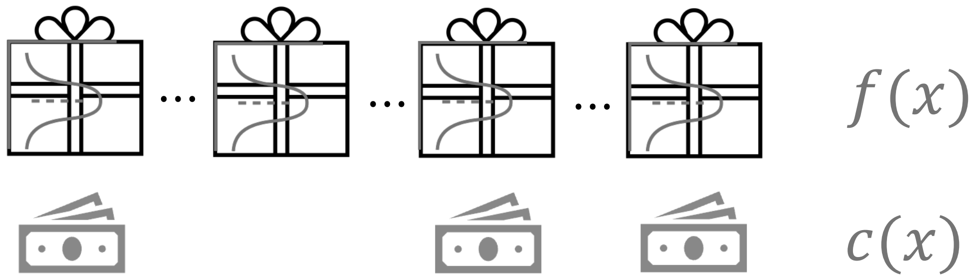
Continuous

Correlated

Expected-budget-constrained

Pandora's Box

[Weitzman'79]



Discrete

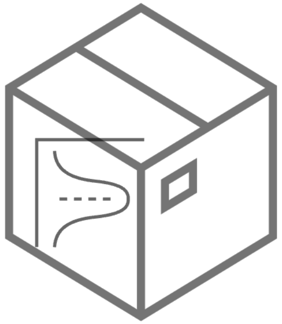
Independent

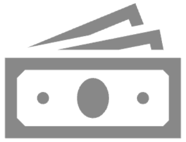
Cost-per-sample

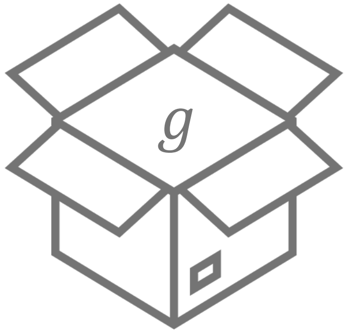
Optimal policy: Gittins index

Optimal Policy: Gittins Index

Step 1: Assign each box a Gittins index (higher is better)

$f(x)$ 

$c(x)$ 



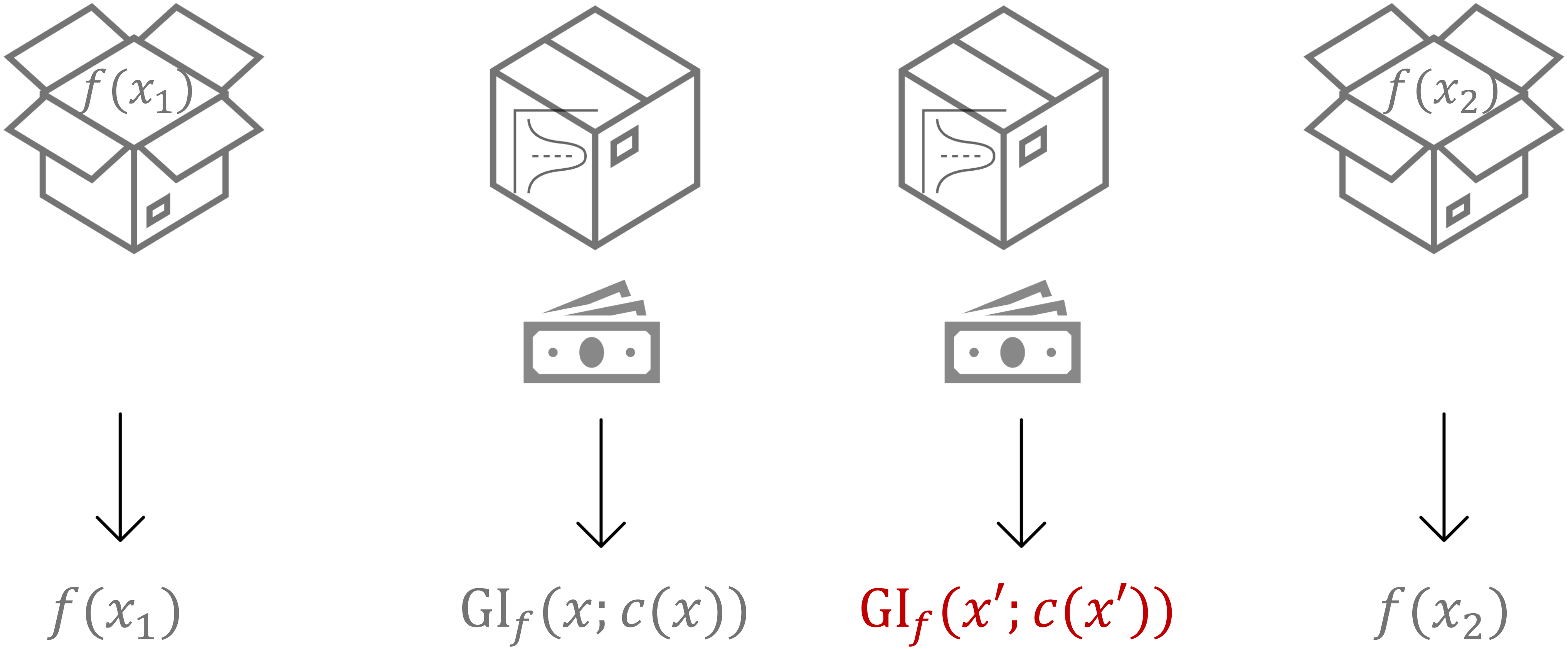
$$\downarrow \qquad\qquad \downarrow$$

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

g

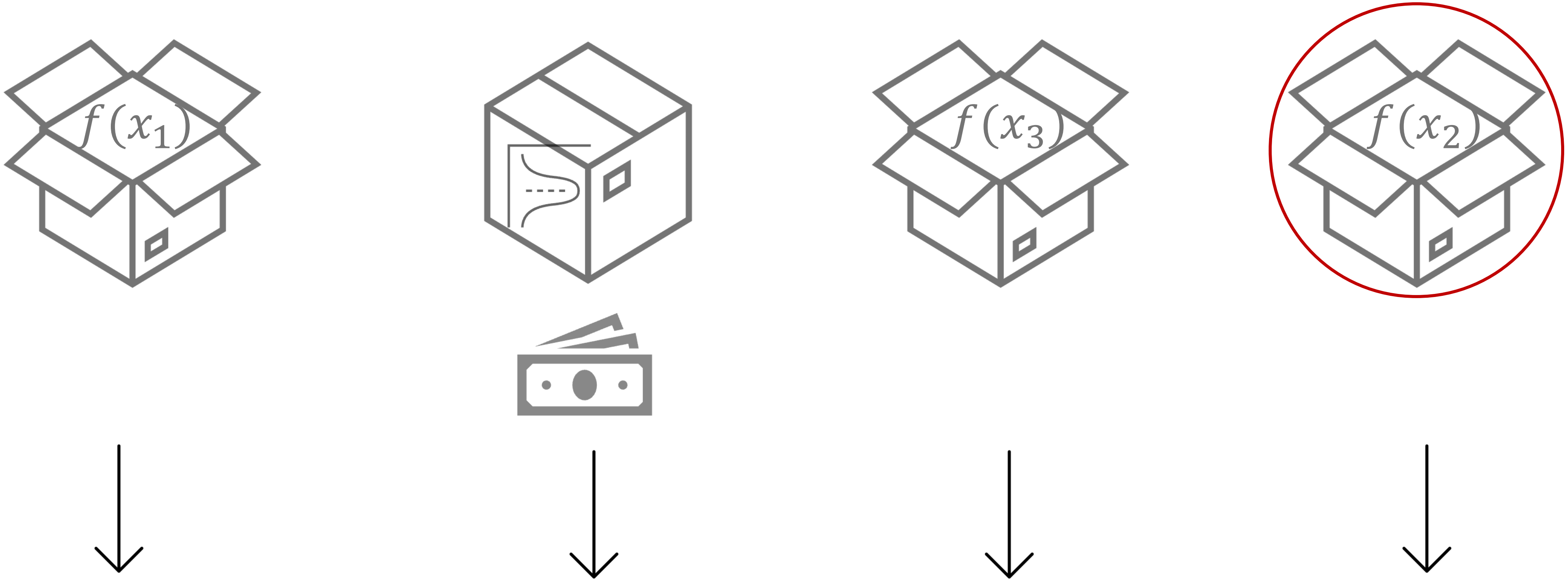
Optimal Policy: Gittins Index

Step 2: Open the box with highest index if it is closed



Optimal Policy: Gittins Index

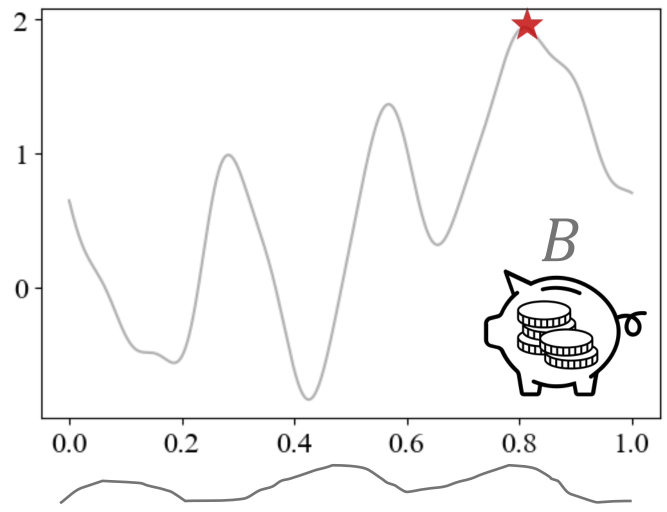
Step 2’: Select the box with highest index if it is opened and stop



$f(x_1)$ $\mathrm{GI}_f(x; c(x))$ $f(x_3)$ $f(x_2)$

Cost-aware Bayesian Optimization

$f(x)$



$c(x)$

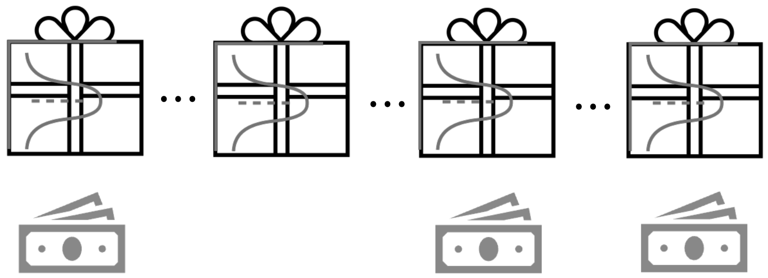
Continuous

Correlated

Expected-budget-constrained

Pandora's Box

[Weitzman'79]



$f(x)$

$c(x)$

Discrete

Independent

Cost-per-sample

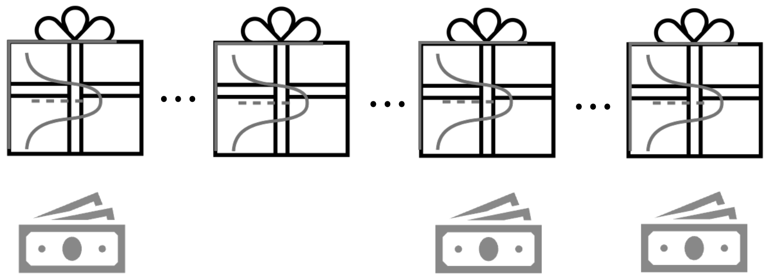
How to translate?

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

Pandora's Box

[Weitzman'79]

$\Longleftarrow$



$f(x)$

$c(x)$

How to convert?

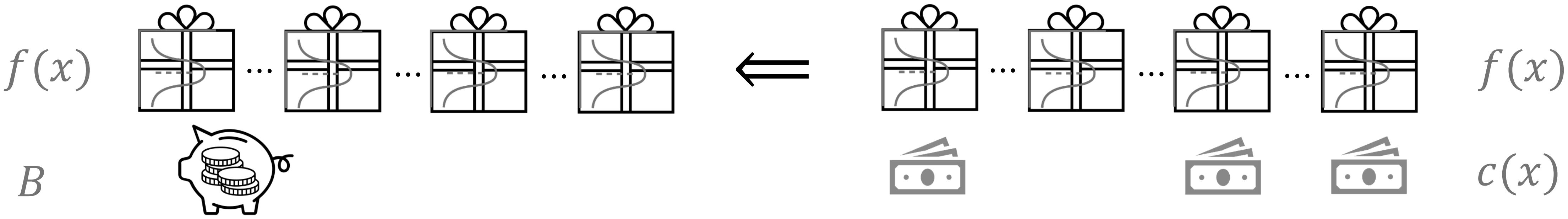
Expected-budget-constrained $\Longleftarrow$ Cost-per-sample

Budgeted Pandora's Box

[Aminian, Manshadi, Niazadeh'24]

Pandora's Box

[Weitzman'79]



Expected-budget-constrained

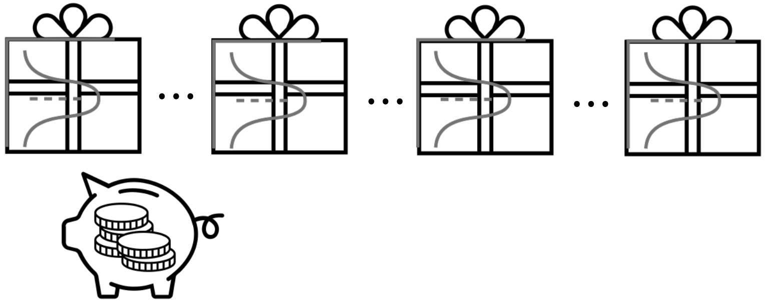
Cost-per-sample

Budgeted Pandora's Box

[Aminian, Manshadi, Niazadeh'24]

$f(x)$

B



$$\sup_{\text{policy}} \mathbb{E} \max_{t=1,2,\ldots,T} f(x_t)$$

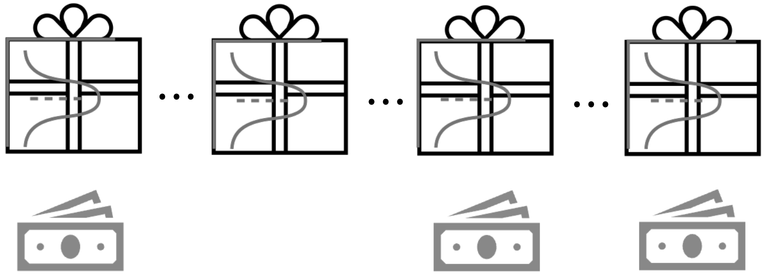
$$\textbf{s.t. } \mathbb{E} \textstyle\sum_{t=1}^{T} c(x_t) \leq B$$

Expected-budget-constrained

$\Leftarrow$

Pandora's Box

[Weitzman'79]



$f(x)$

$c(x)$

$$\sup_{\text{policy}} \mathbb{E} \left(\max_{t=1,2,\ldots,T} f(x_t) - \sum_{t=1}^{T} c(x_t) \right)$$

Cost-per-sample

Budgeted Pandora's Box

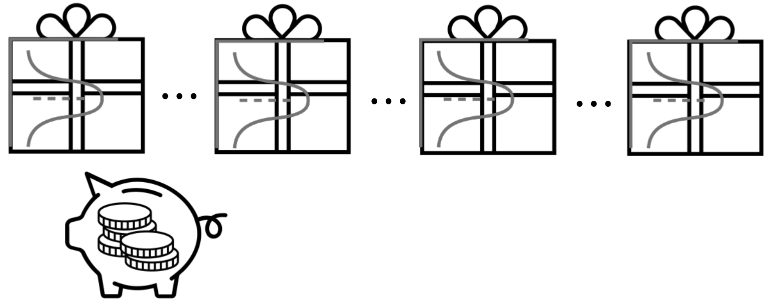
[Aminian, Manshadi, Niazadeh'24]

Pandora's Box

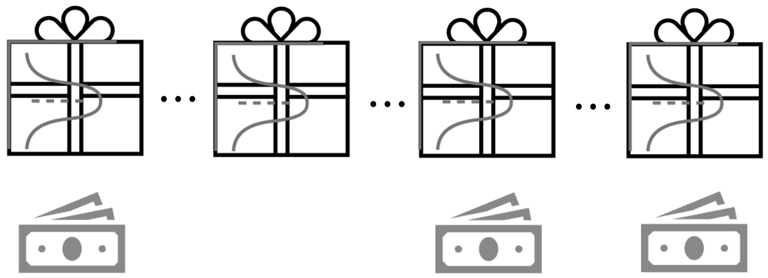
[Weitzman'79]

$f(x)$

B



$\Longleftarrow$



$f(x)$

$c(x)$

$$\sup_{\text{policy}} \mathbb{E} \max_{t=1,2,\ldots,T} f(x_t)$$
$$\textbf{s.t. } \mathbb{E}\textstyle\sum_{t=1}^{T} c(x_t) \leq B$$

scaling factor

$$\sup_{\text{policy}} \mathbb{E}\left(\max_{t=1,2,\ldots,T} f(x_t) - \lambda_B \sum_{t=1}^{T} c(x_t)\right)$$

Lagrangian relaxation

Expected-budget-constrained $\Longleftrightarrow$ Cost-per-sample

Budgeted Pandora's Box

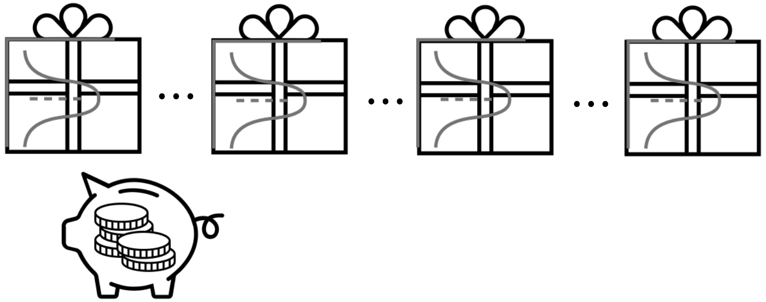
[Aminian, Manshadi, Niazadeh'24]

Pandora's Box

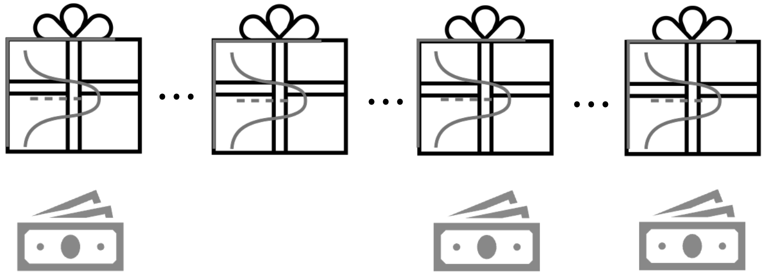
[Weitzman'79]

$f(x)$

B



$\Longleftarrow$



$f(x)$

$c(x)$

$$\sup_{\text{policy}} \mathbb{E} \max_{t=1,2,\ldots,T} f(x_t)$$
$$\text{s.t. } \mathbb{E} \textstyle\sum_{t=1}^{T} c(x_t) \leq B$$

$$\sup_{\text{policy}} \mathbb{E}\left(\max_{t=1,2,\ldots,T} f(x_t) - \sum_{t=1}^{T} c(x_t) \right)$$

Expected-budget-constrained $\Longleftrightarrow$ Cost-per-sample

How to translate?

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

Budgeted Pandora's Box

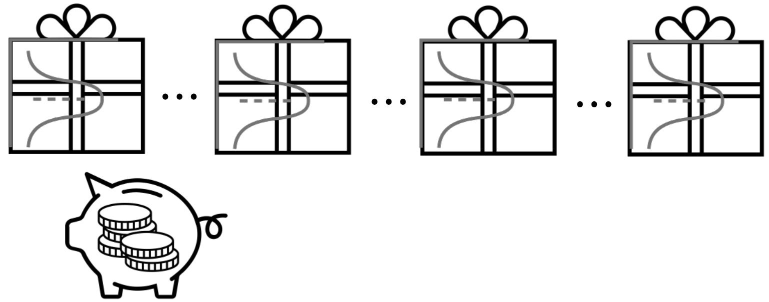
[Aminian, Manshadi, Niazadeh'24]

Pandora's Box

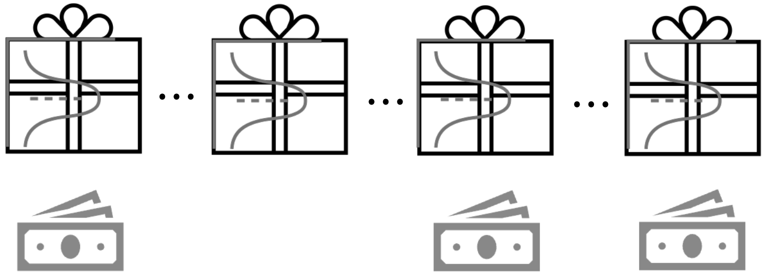
[Weitzman'79]

$f(x)$

B



$\Longleftarrow$



$f(x)$

$c(x)$

$$\sup_{\text{policy}} \mathbb{E} \max_{t=1,2,\ldots,T} f(x_t)$$
$$\textbf{s.t. } \mathbb{E} \sum_{t=1}^{T} c(x_t) \leq B$$

$$\sup_{\text{policy}} \mathbb{E}\left(\max_{t=1,2,\ldots,T} f(x_t) - \sum_{t=1}^{T} c(x_t) \right)$$

Expected-budget-constrained $\Longleftrightarrow$ Cost-per-sample

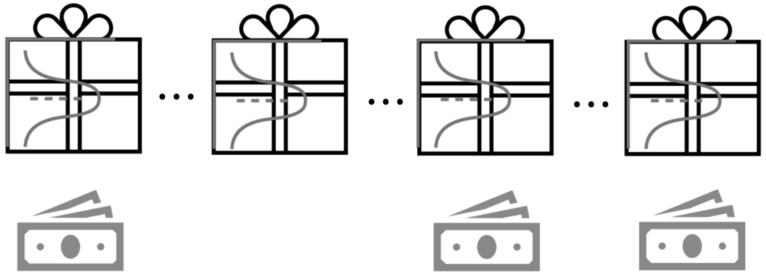
Optimal policy: $\mathrm{GI}_f(x; \lambda_B c(x))$ $\overset{\text{scale costs}}{\Longleftarrow}$ Optimal policy: $\mathrm{GI}_f(x; c(x))$

Budgeted Pandora's Box

[Aminian, Manshadi, Niazadeh'24]

Pandora's Box

[Weitzman'79]

$f(x)$  $\Longleftarrow$  $f(x)$

B $\qquad\qquad$ $c(x)$

Our work: extension to general reward distribution

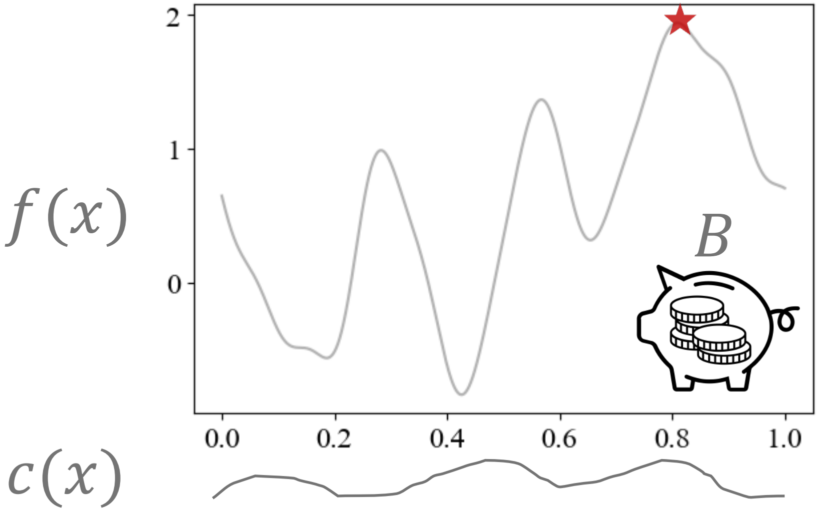
$$\sup_{\text{policy}} \mathbb{E} \max_{t=1,2,\ldots,T} f(x_t)$$
$$\textbf{s.t. } \mathbb{E} \textstyle\sum_{t=1}^{T} c(x_t) \leq B$$

$$\sup_{\text{policy}} \mathbb{E} \left(\max_{t=1,2,\ldots,T} f(x_t) - \sum_{t=1}^{T} c(x_t) \right)$$

Expected-budget-constrained $\Longleftrightarrow$ Cost-per-sample

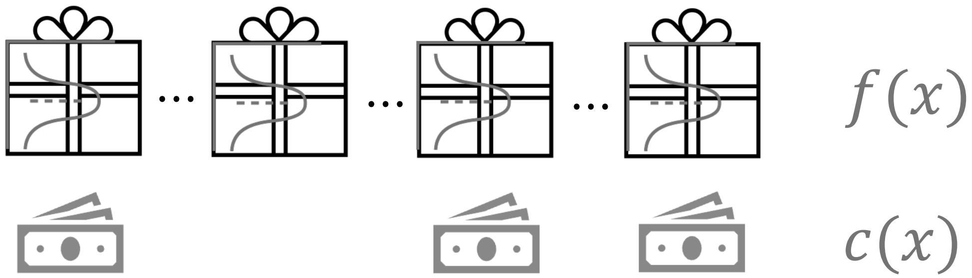
Optimal policy: $\mathrm{GI}_f(x; \lambda_B c(x))$ $\overset{\text{scale costs}}{\Longleftarrow}$ Optimal policy: $\mathrm{GI}_f(x; c(x))$

Cost-aware Bayesian Optimization



Pandora's Box

[Weitzman'79]



Continuous — Discrete

Correlated — Independent

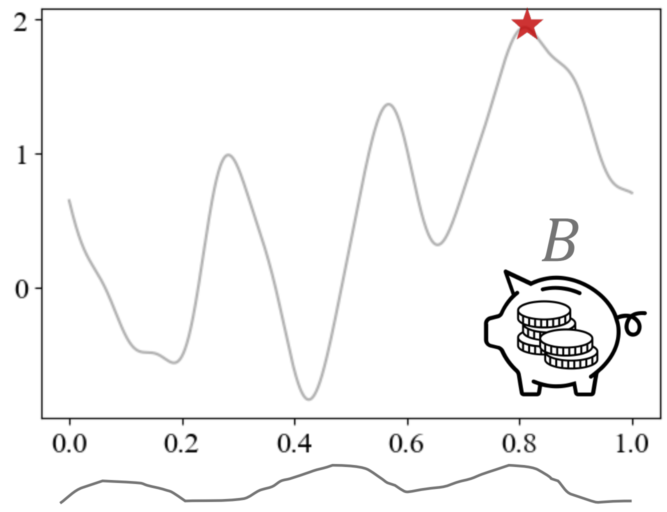
Expected-budget-constrained $\Longleftarrow$ Cost-per-sample ✓

How to translate?

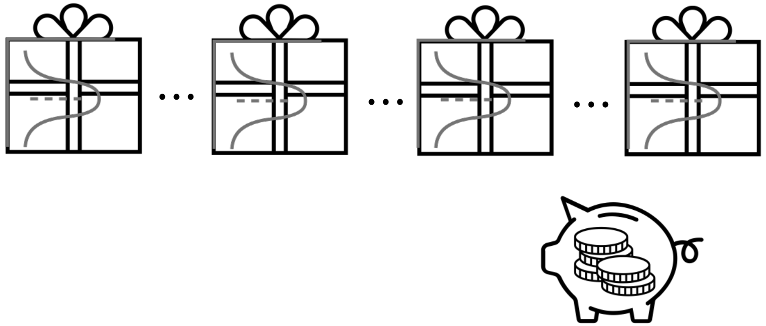
$\Longleftarrow$ Optimal policy: $\mathrm{GI}_f(x; c(x))$

Cost-aware Bayesian Optimization   Budgeted Pandora's Box

$f(x)$



$c(x)$



$f(x)$

B

Continuous

Correlated

Discrete

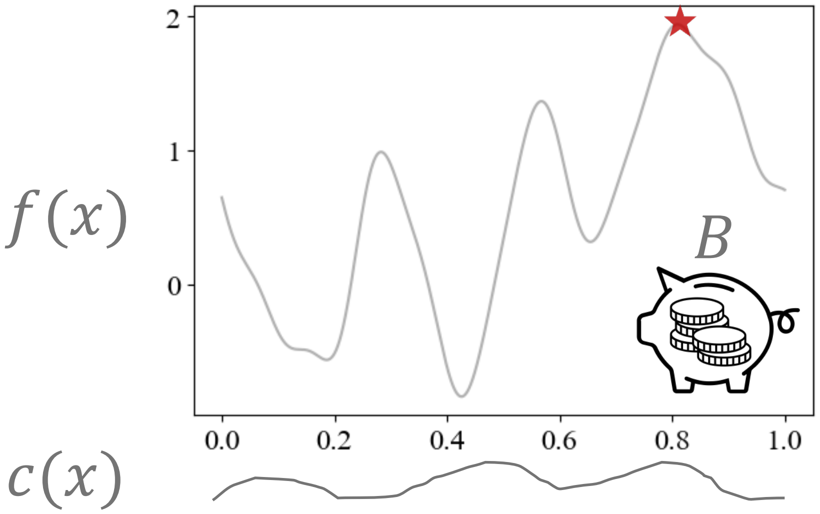
Independent

scaling factor

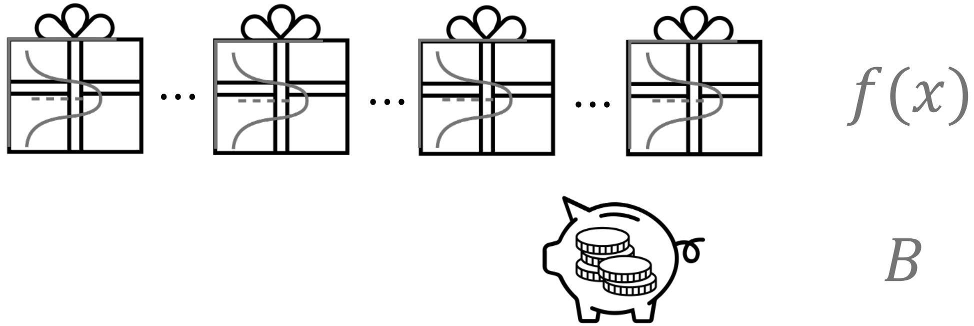
How to translate?

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

Cost-aware Bayesian Optimization Budgeted Pandora's Box



$\Longleftarrow$



Continuous $\Longleftarrow$ Discrete

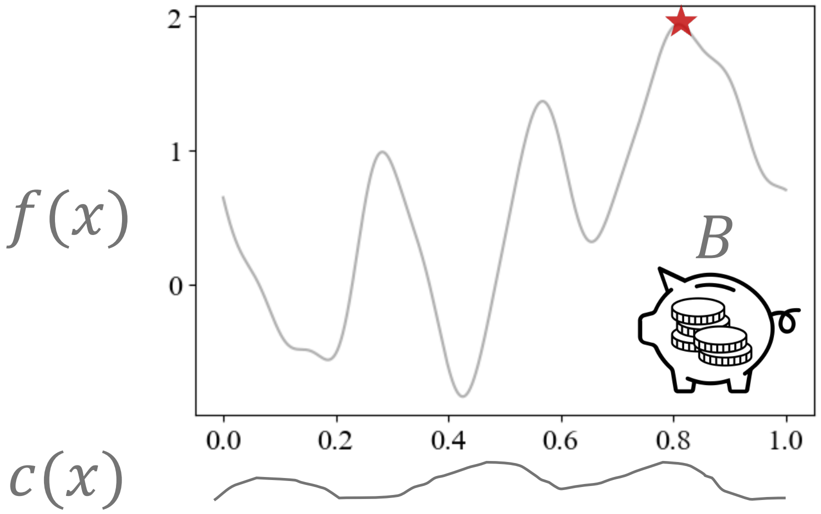
Correlated $\Longleftarrow$ Independent

scaling factor

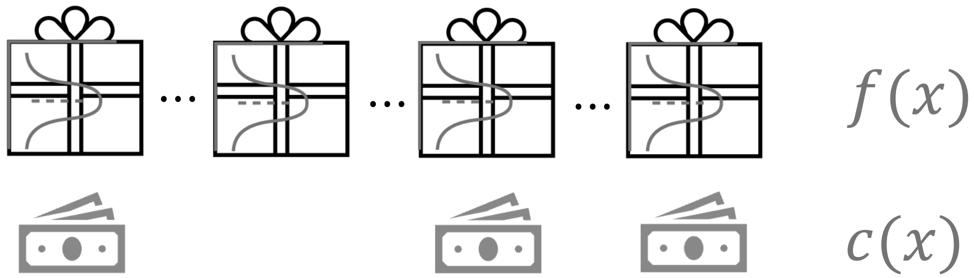
incorporate posterior

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

Cost-aware Bayesian Optimization   Pandora's Box



$\Leftarrow$

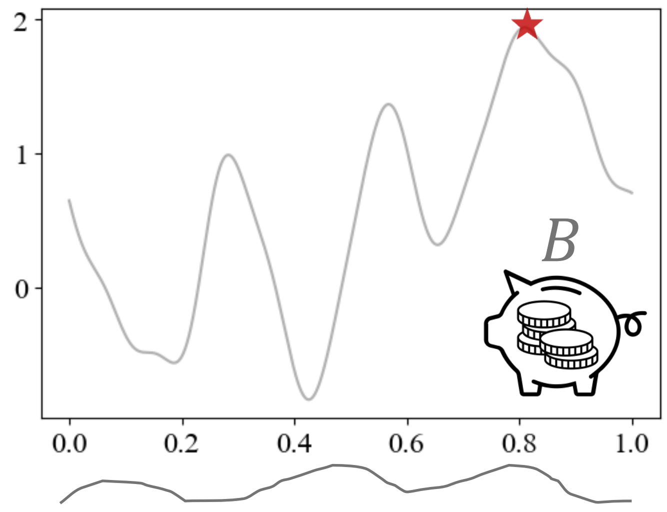


Continuous	$\Leftarrow$	Discrete	✓
Correlated	$\Leftarrow$	Independent	✓
Expected-budget-constrained	$\Leftarrow$	Cost-per-sample	✓

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

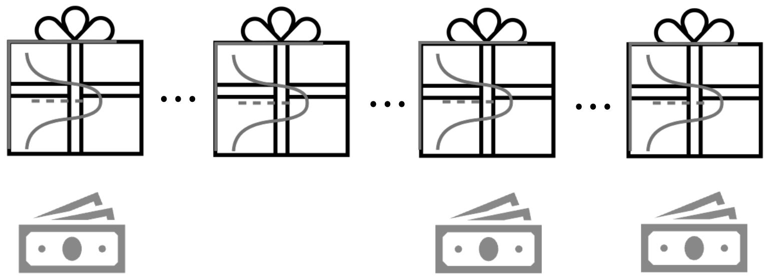
Cost-aware Bayesian Optimization $\quad$ Pandora's Box

$f(x)$



$c(x)$

$\Longleftarrow$



$f(x)$

$c(x)$

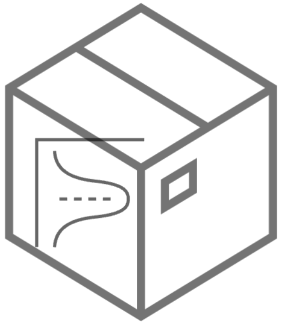
Cost-aware Bayesian Optimization	Pandora's Box
Continuous	Discrete
Correlated	Independent
Expected-budget-constrained	Cost-per-sample

Our policy: $\mathrm{GI}_{f|D}(x; \lambda c(x))$ $\underset{\text{scale costs}}{\overset{\text{incorporate posterior}}{\Longleftarrow}}$ Optimal policy: $\mathrm{GI}_f(x; c(x))$

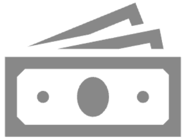
How to compute?

How to compute Gittins index?

$f(x)$

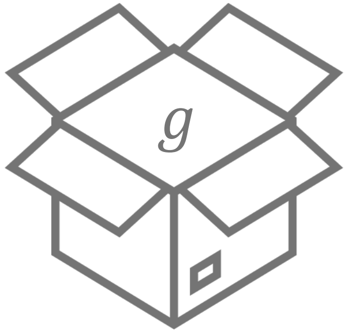


$c(x)$



$\downarrow$?

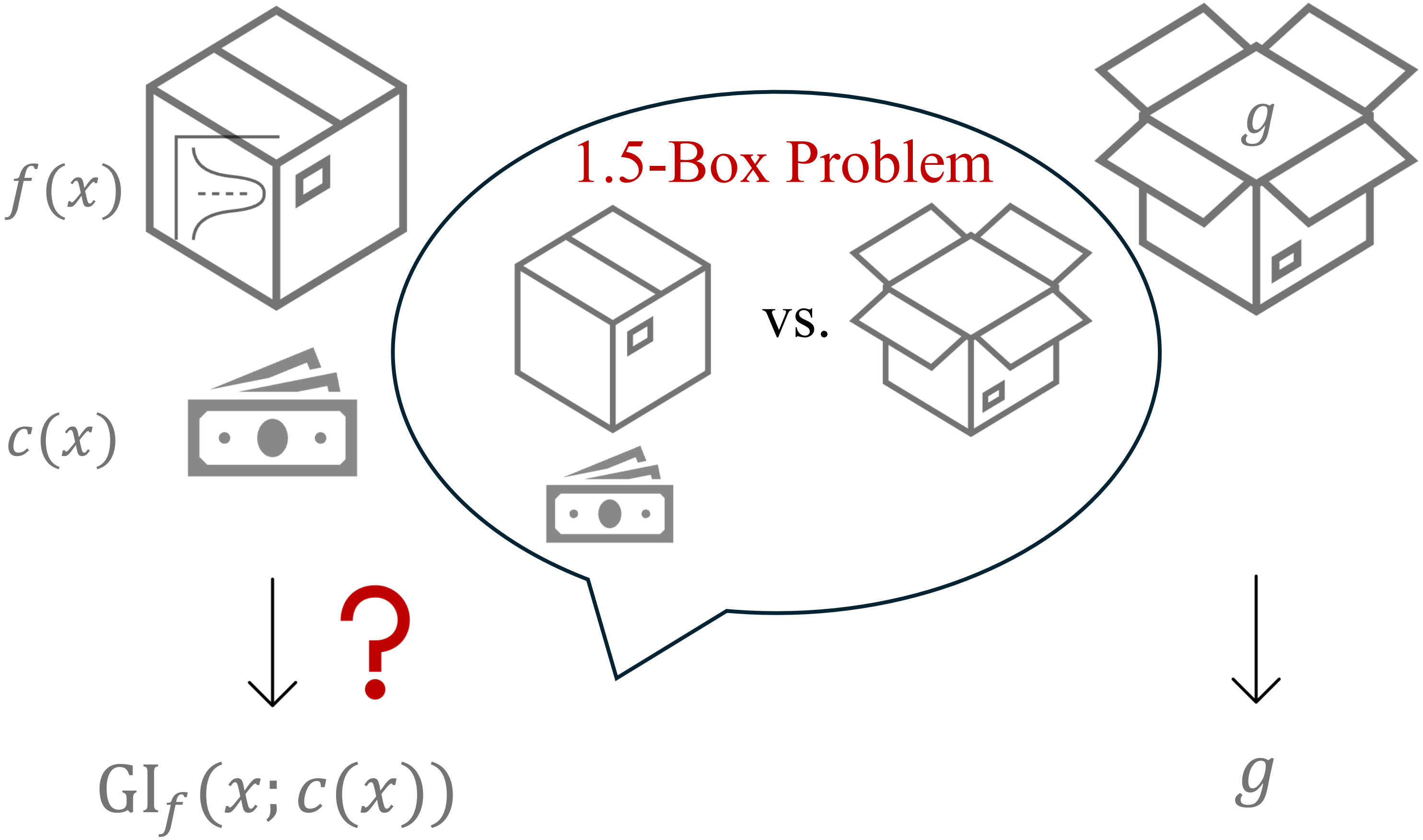
$\mathrm{GI}_f(x; c(x))$



$\downarrow$

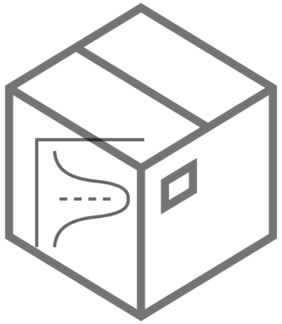
g

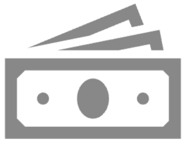
How to compute Gittins index?



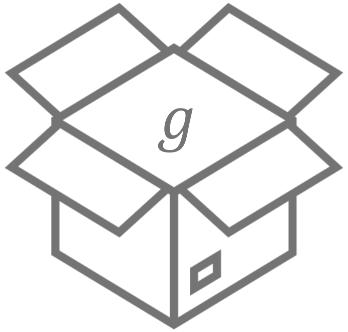
Whether to open a new box or take current best?

Gittins Index Computation: 1.5-Box Problem

$f(x)$ 

$c(x)$ 

vs.

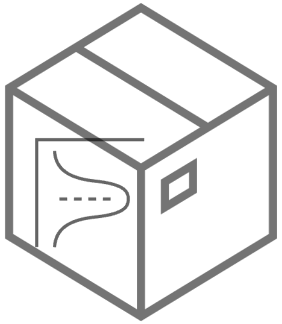


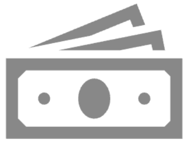
Open closed box

Take opened box

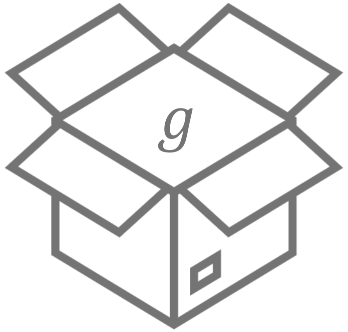
Whether to open a new box or take current best?

Gittins Index Computation: 1.5-Box Problem

$f(x)$ 

$c(x)$ 

vs.



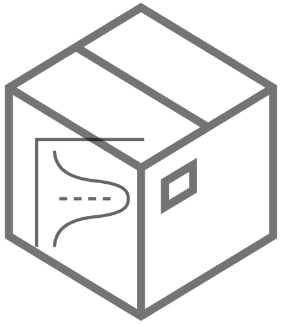
Open closed box — Take opened box — g

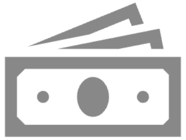
Profit:

$$\begin{cases} \text{take inside value}, & f(x) > g \\ \text{take outside option}, & f(x) \leq g \end{cases}$$

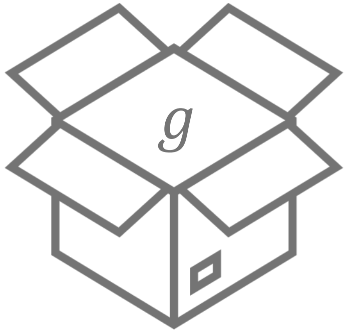
Profit:

Gittins Index Computation: 1.5-Box Problem

$f(x)$ 

$c(x)$ 

vs.



Open closed box | Take opened box → g

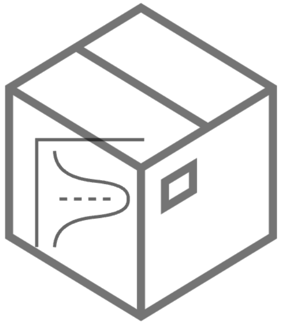
Profit: $\mathbb{E}[\underbrace{\max(f(x), g)}]-c(x)$

$\begin{cases} \text{take inside value}, & f(x) > g \\ \text{take outside option}, & f(x) \leq g \end{cases}$

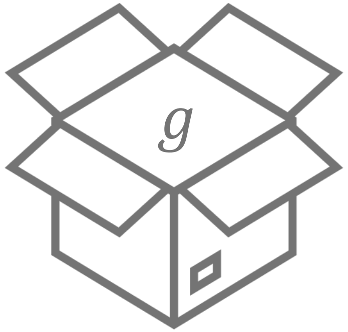
Profit: g

Gittins Index Computation: 1.5-Box Problem

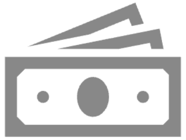
$f(x)$

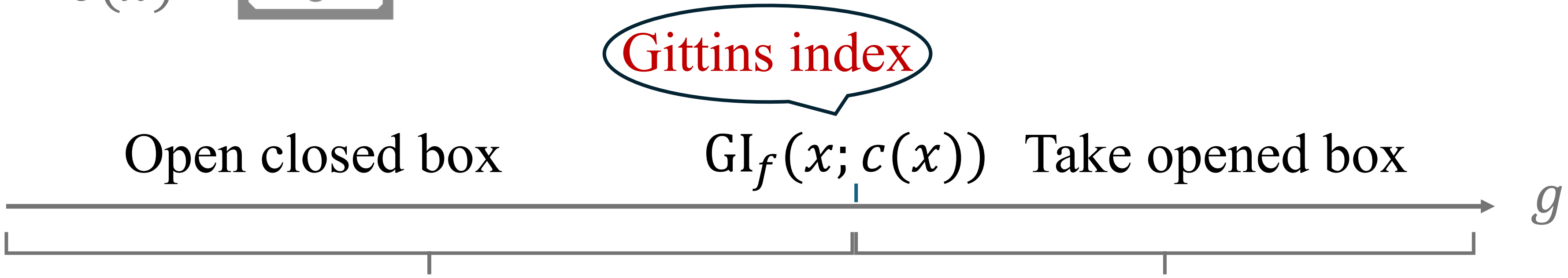


vs.



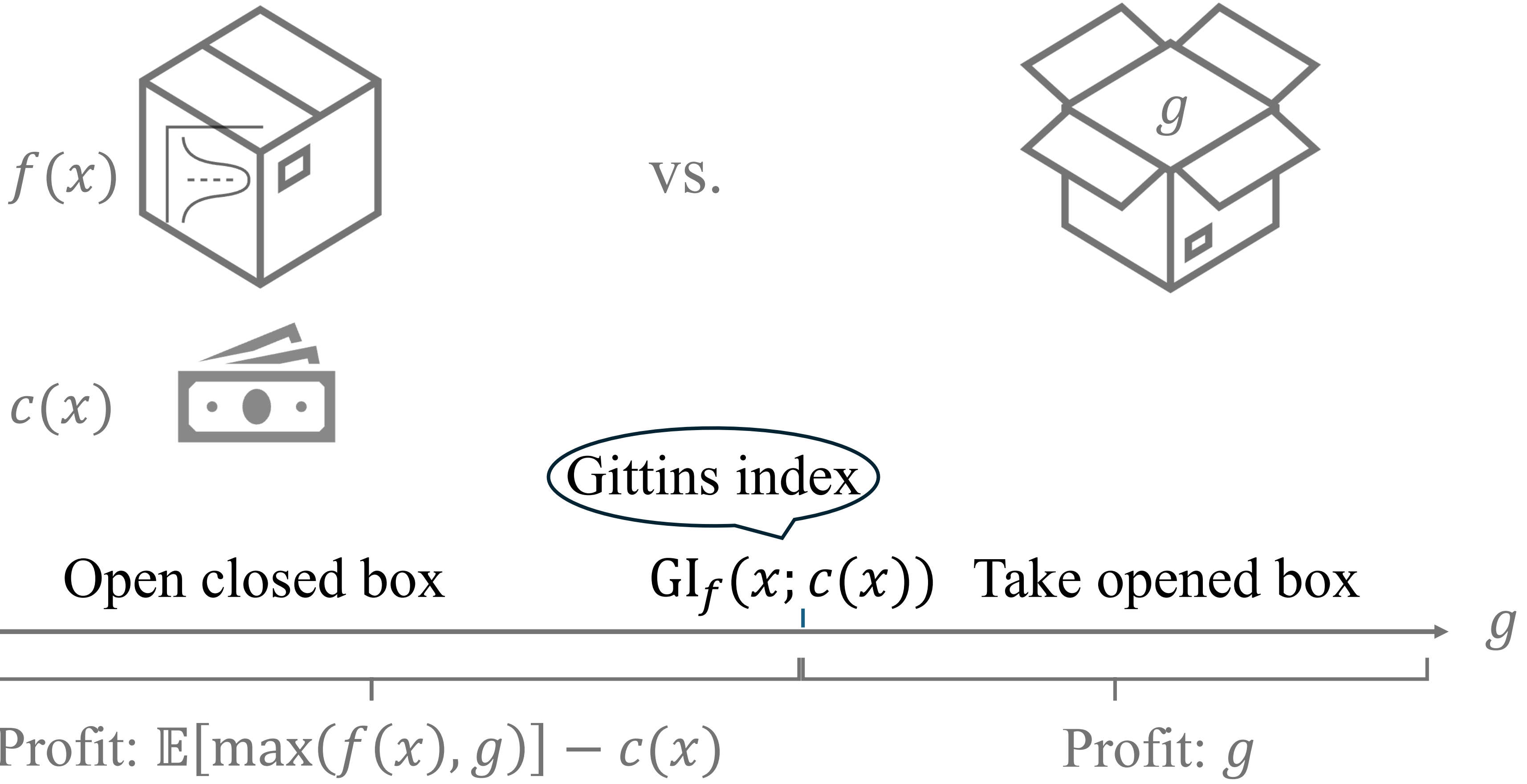
$c(x)$





$\mathrm{GI}_f(x; c(x))$: solution g to $\mathbb{E}[\max(f(x), g)] - c(x) = g$

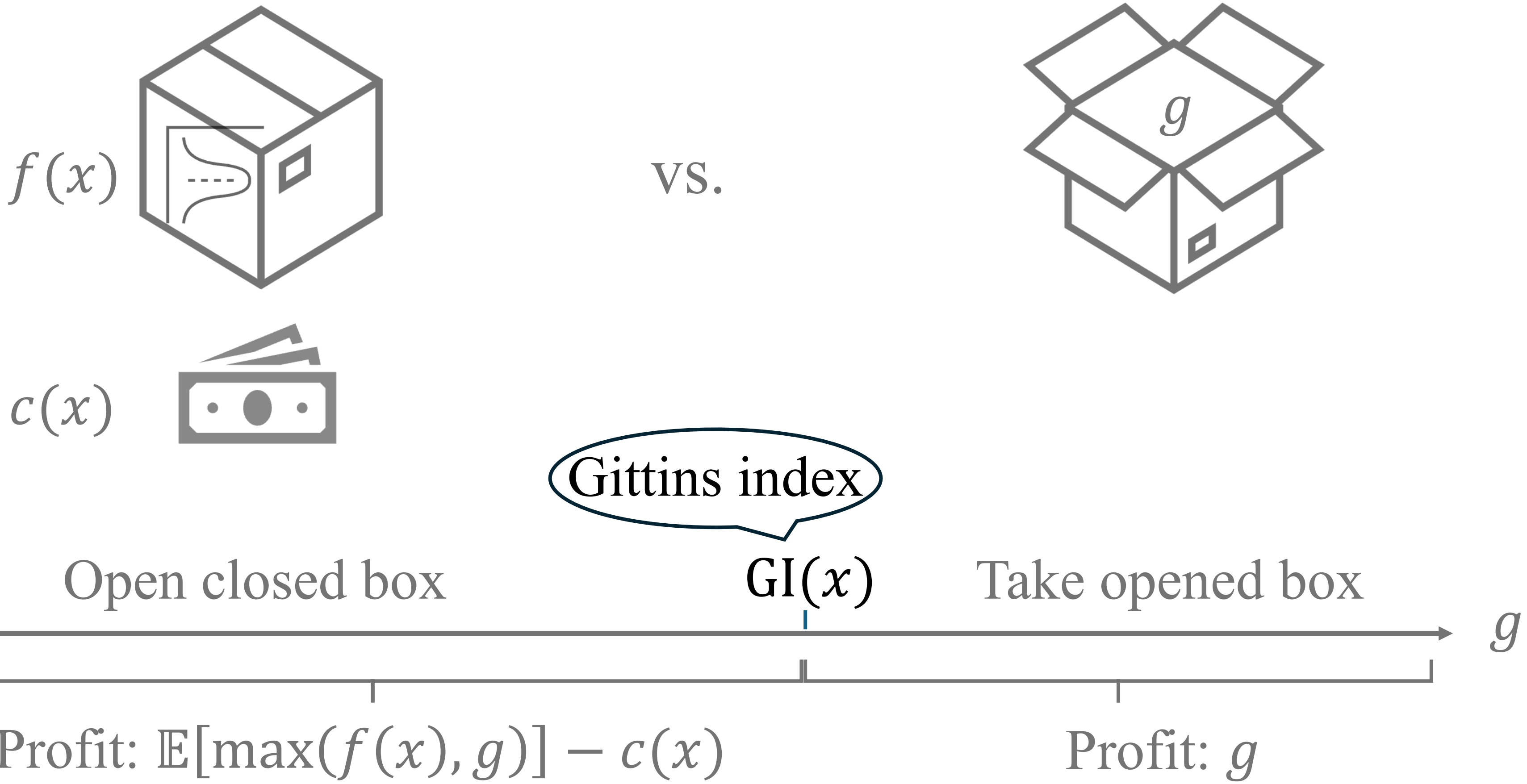
Gittins Index Computation: 1.5-Box Problem



$\mathrm{GI}_f(x; c(x))$: solution g to $\mathbb{E}[\max(f(x), g)] - c(x) = g$

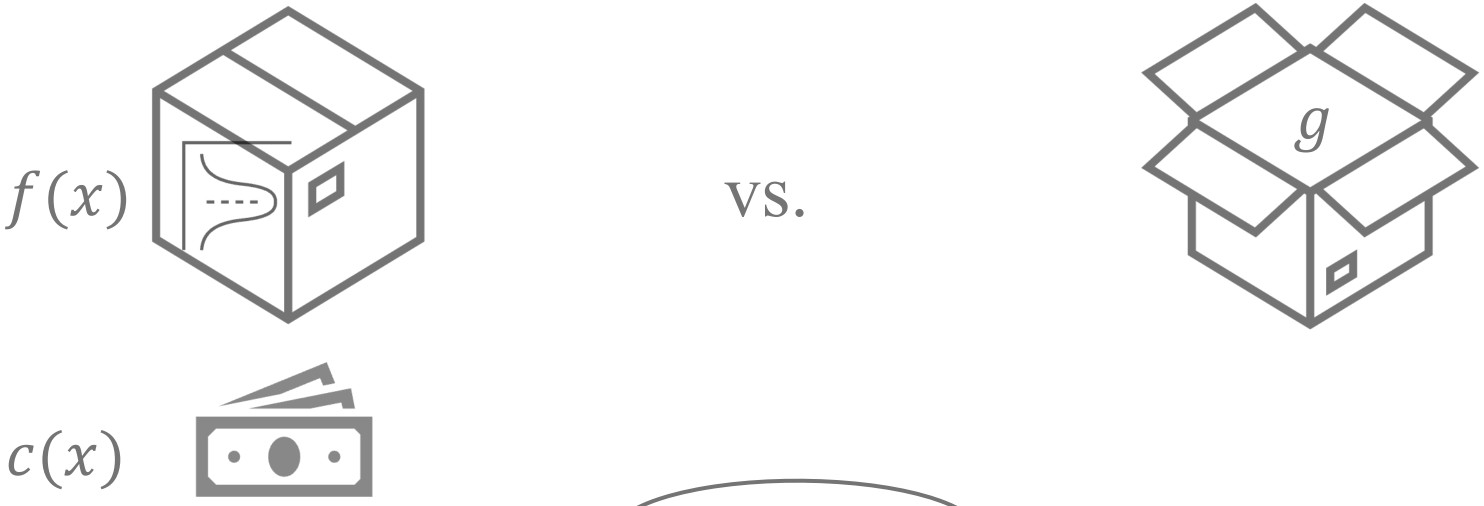
Larger the cost, smaller the Gittins index

Gittins Index Computation: 1.5-Box Problem



$$\mathrm{GI}_f(x; c(x))\text{: solution } g \text{ to } \underbrace{\mathbb{E}[\max(f(x), g)] - c(x) = g}_{\color{red}{\mathbb{E}[\max(f(x) - g, 0)] = c(x)}}$$

Gittins Index Computation: 1.5-Box Problem



Gittins index

$\mathrm{GI}(x)$

Open closed box | Take opened box → g

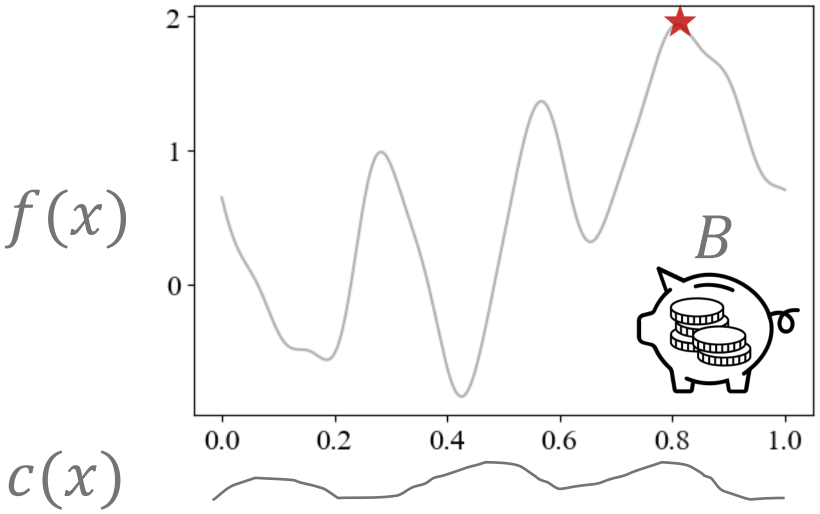
Profit: $\mathbb{E}[\max(f(x), g)] - c(x)$ | Profit: g

$\mathrm{GI}_f(x; c(x))$: solution g to $\underbrace{\mathbb{E}[\max(f(x), g)] - c(x) = g}_{\mathbb{E}[\max(f(x) - g, 0)] = c(x)}$

$\mathrm{EI}_f(x; g)$

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

Cost-aware Bayesian Optimization



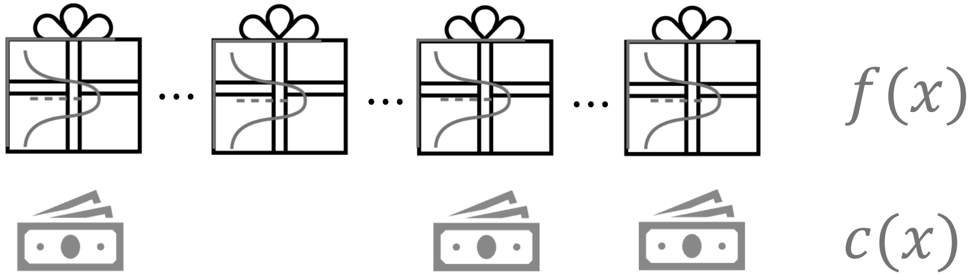
Continuous

Correlated

Expected-budget-constrained

Is Gittins index good?

Pandora's Box



Discrete

Independent

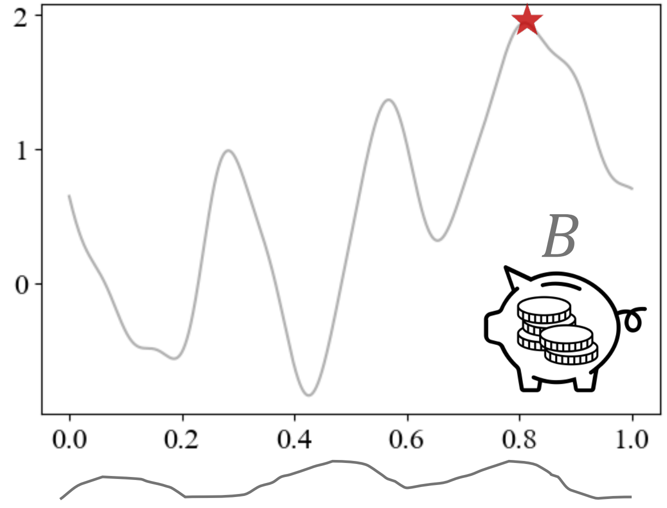
Cost-per-sample

Gittins index is optimal

$\xLeftarrow[\text{scale costs}]{\text{incorporate posterior}}$

Cost-aware Bayesian Optimization

$f(x)$



$c(x)$

Continuous

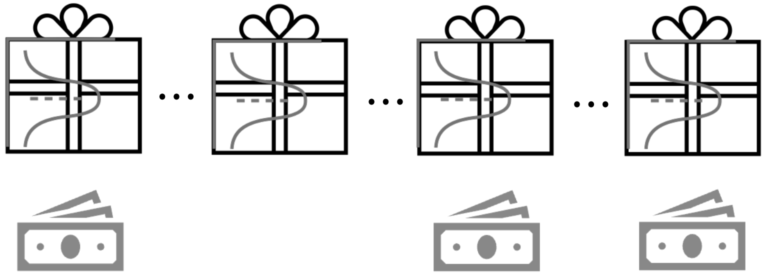
Correlated

Expected-budget-constrained

Is Gittins index empirically good?

this work

Pandora's Box



$f(x)$

$c(x)$

Discrete

Independent

Cost-per-sample

Gittins index is optimal

Experiment Setup: Objective Functions

Synthetic

Samples from prior

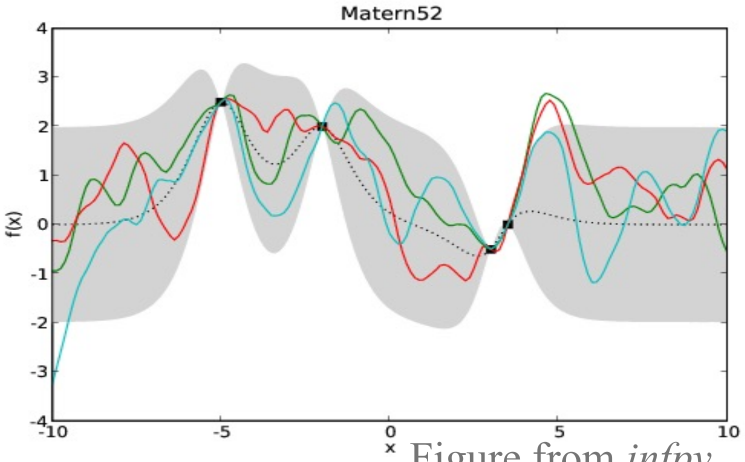


Figure from *infpy*

Ackley function

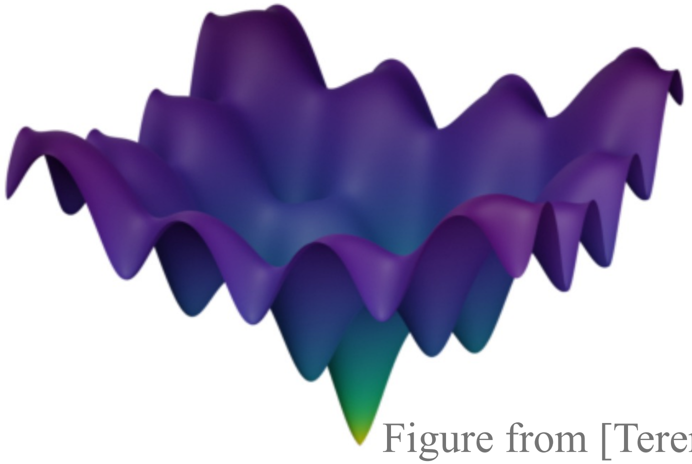


Figure from [Terenin'22]

Empirical

Pest Control

Figure from ChatGPT

Lunar Lander

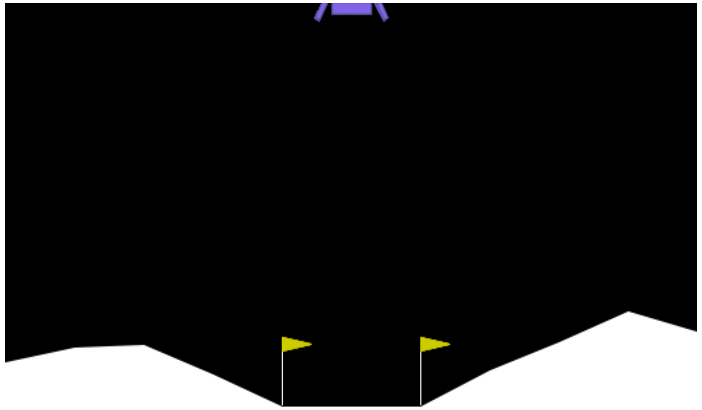
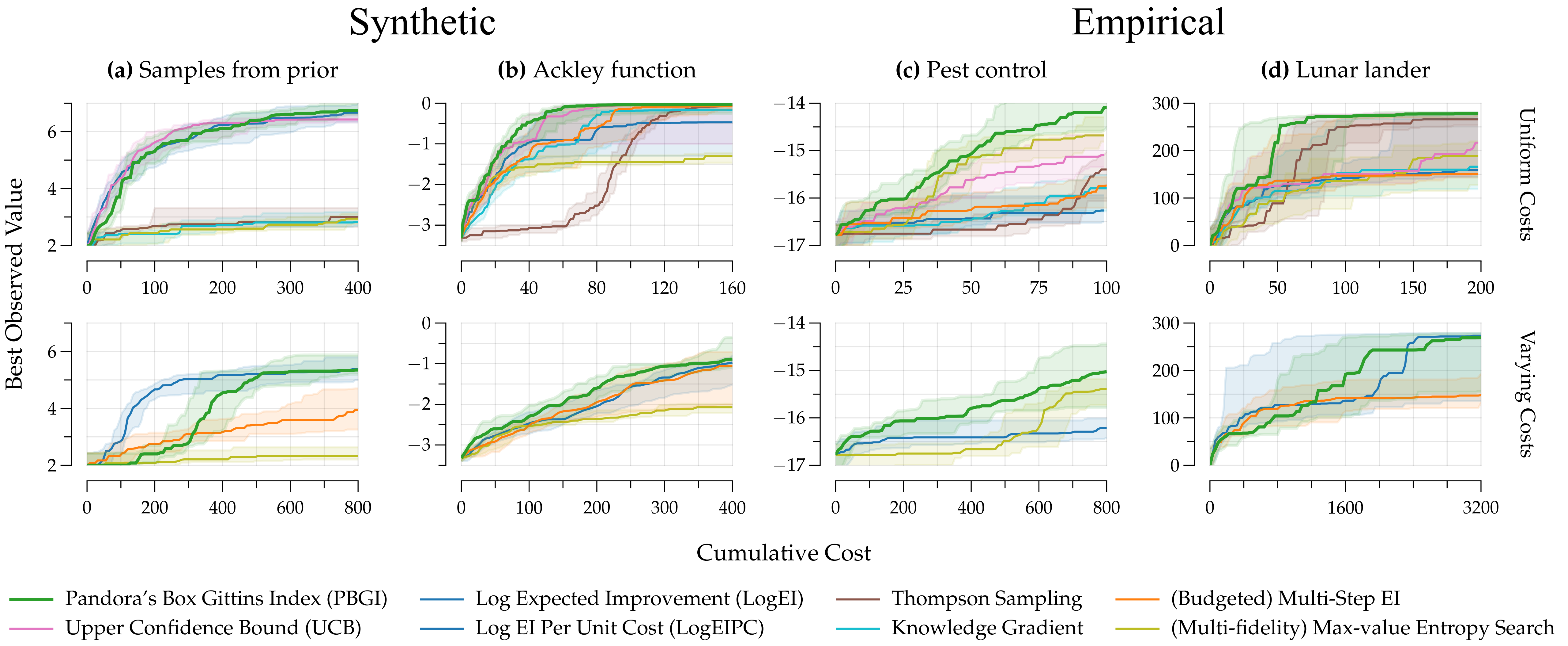


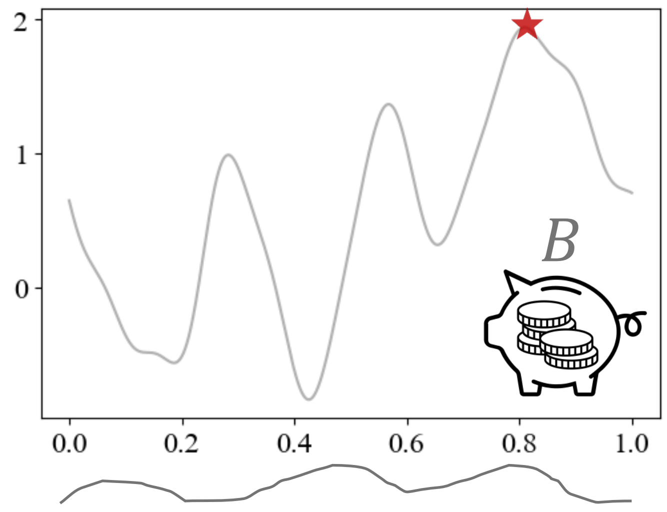
Figure from OpenAI Gym

Experiment Results: Gittins Index vs Baselines



Cost-aware Bayesian Optimization

$f(x)$



$c(x)$

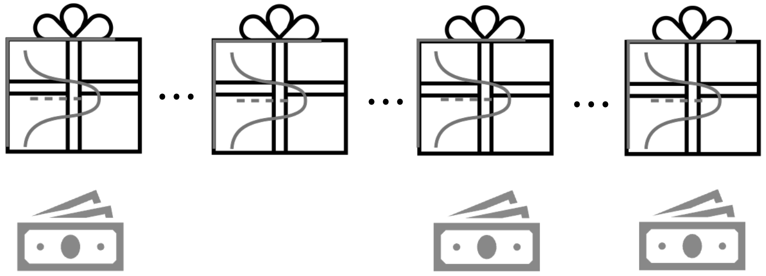
Continuous

Correlated

Expected-budget-constrained

Is Gittins index theoretically good?

Pandora's Box



$f(x)$

$c(x)$

Discrete

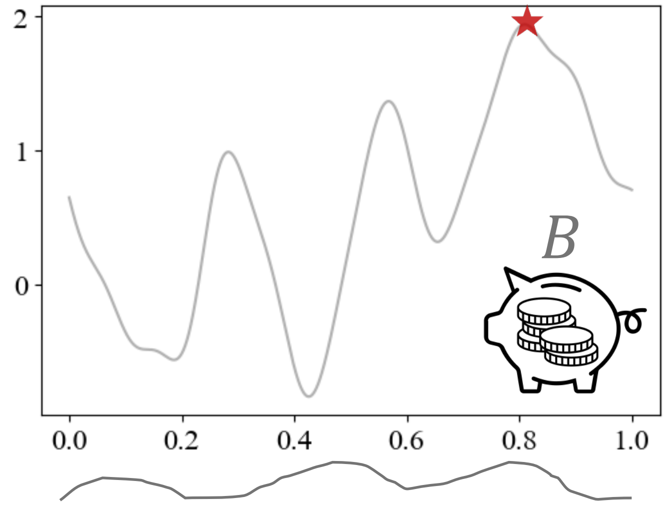
Independent

Cost-per-sample

Gittins index is optimal

Cost-aware Bayesian Optimization

$f(x)$



$c(x)$

Continuous

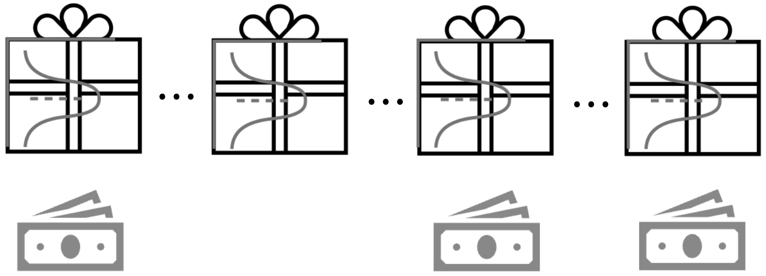
Correlated

Expected-budget-constrained

Is Gittins index theoretically good?

ongoing work

Pandora’s Box



$f(x)$

$c(x)$

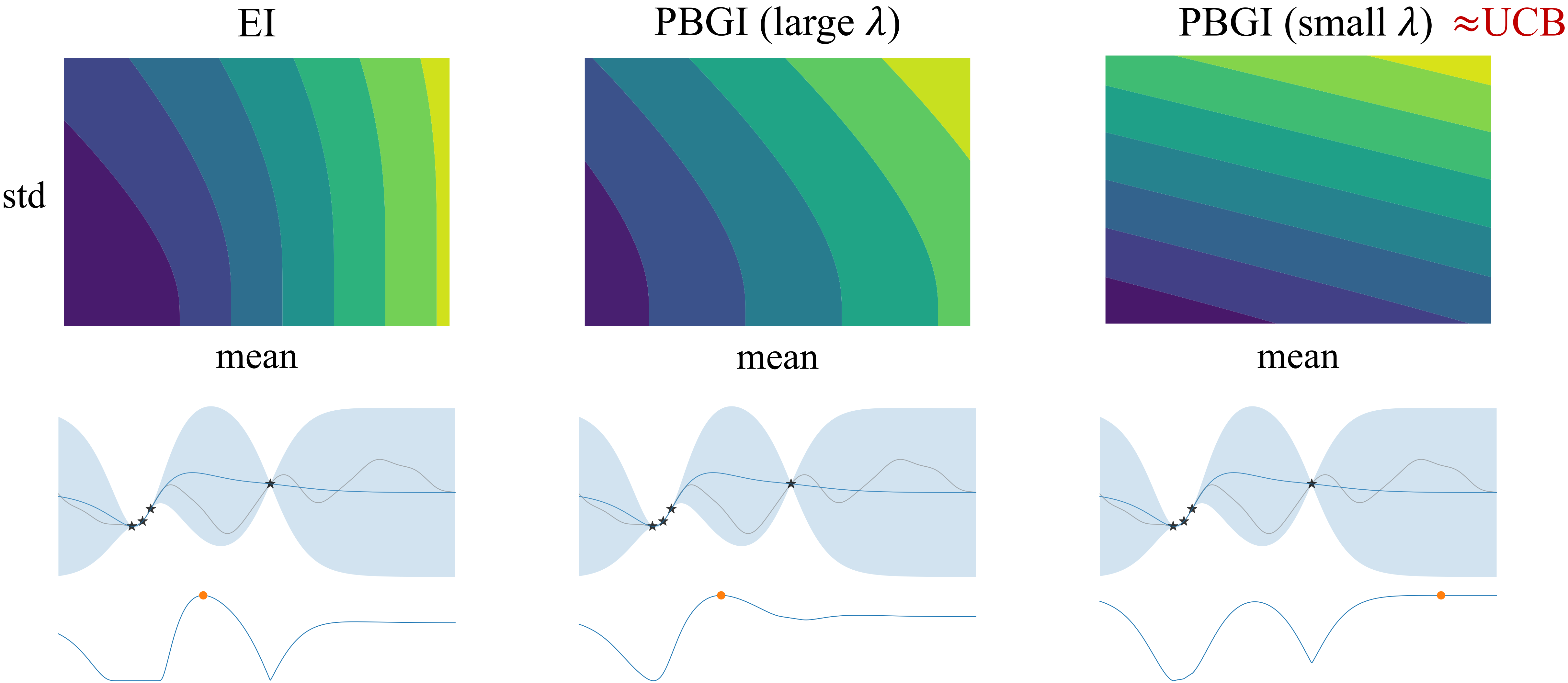
Discrete

Independent

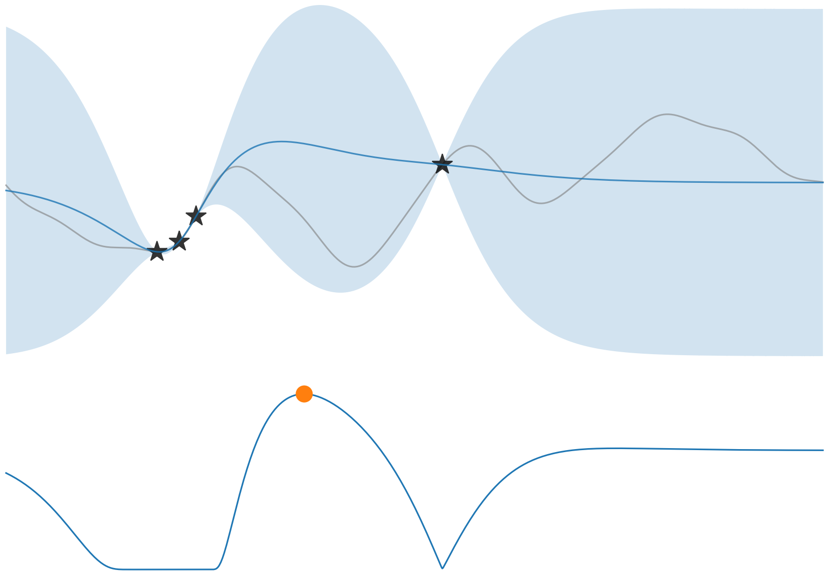
Cost-per-sample

Gittins index is optimal

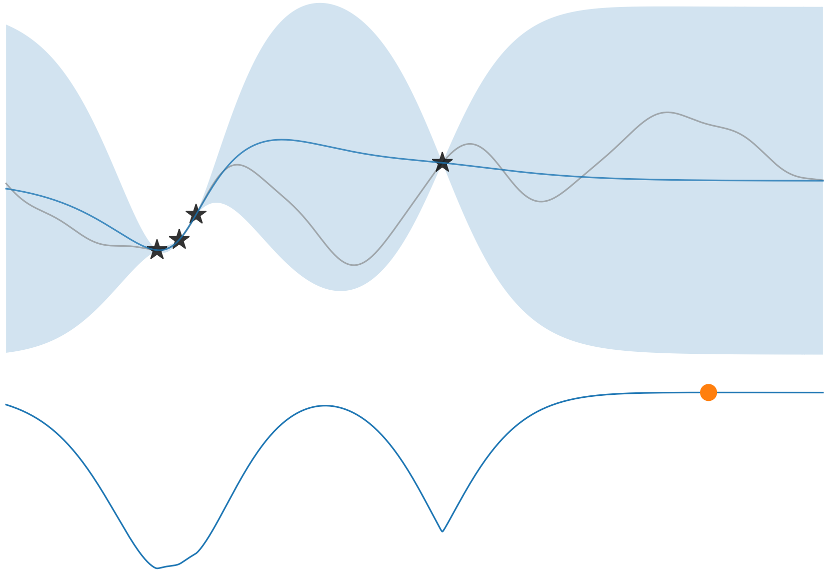
Discussion 1: EI vs PBGI



Expected Improvement



Gittins Index

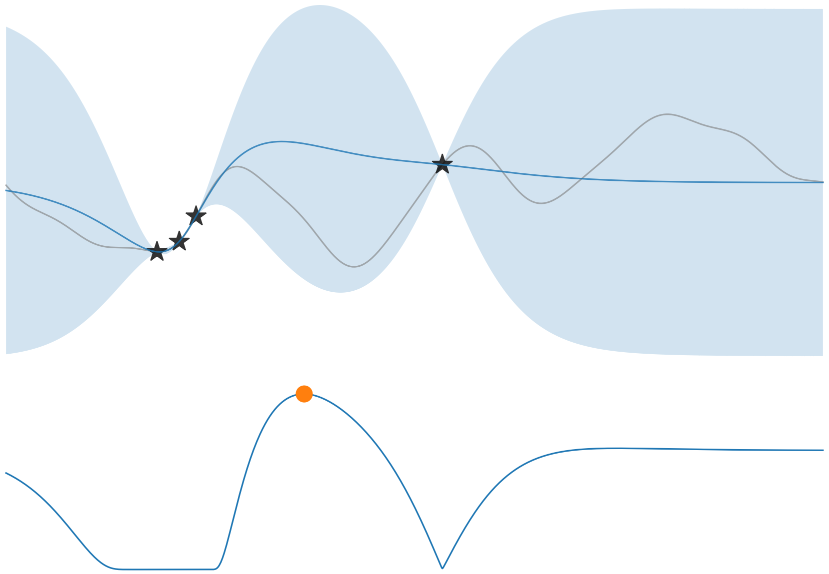


$\mathrm{EI}_{f|D}(x; g) := \mathbb{E}[\max(f(x) - g, 0) \mid D]$

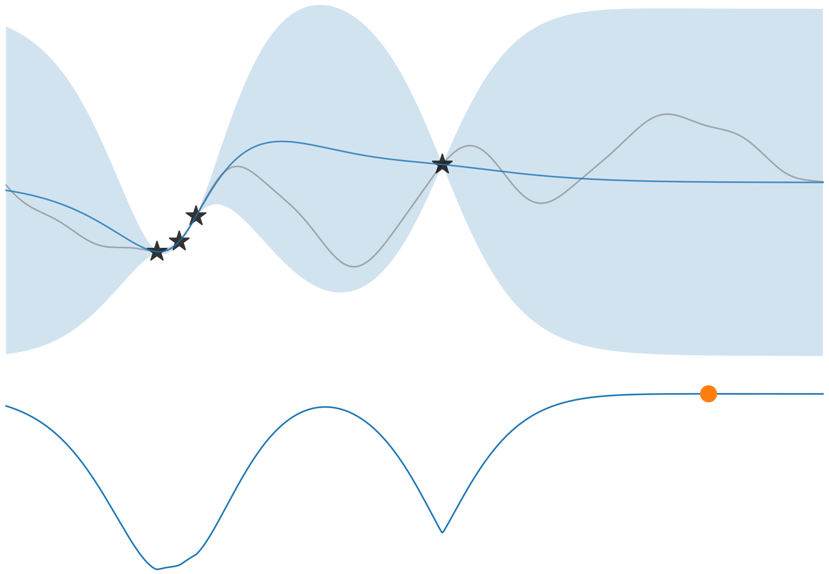
Gaussian distribution

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

Expected Improvement



Gittins Index

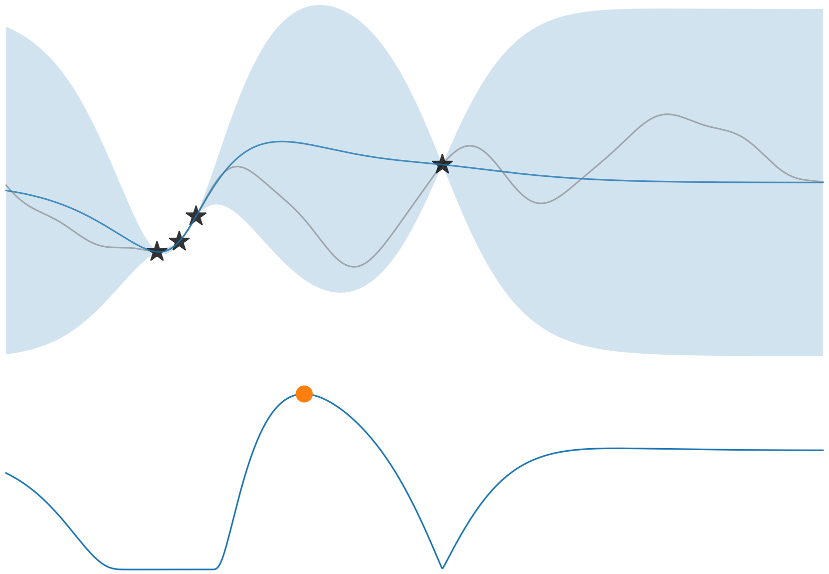


$$\mathrm{EI}_{f|D}(x;g) := \underbrace{\mathbb{E}[\max(f(x)-g,0) \mid D]}_{\text{analytical expression}}$$

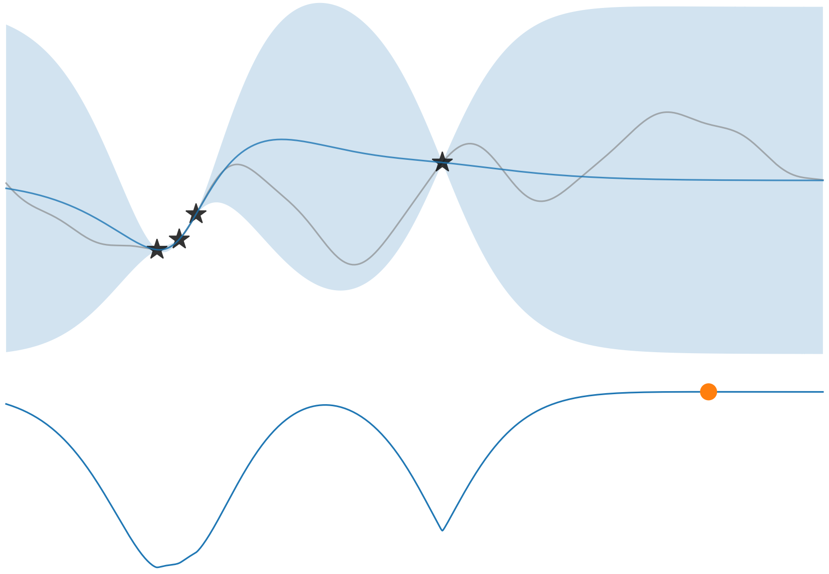
Gaussian distribution

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

Expected Improvement



Gittins Index



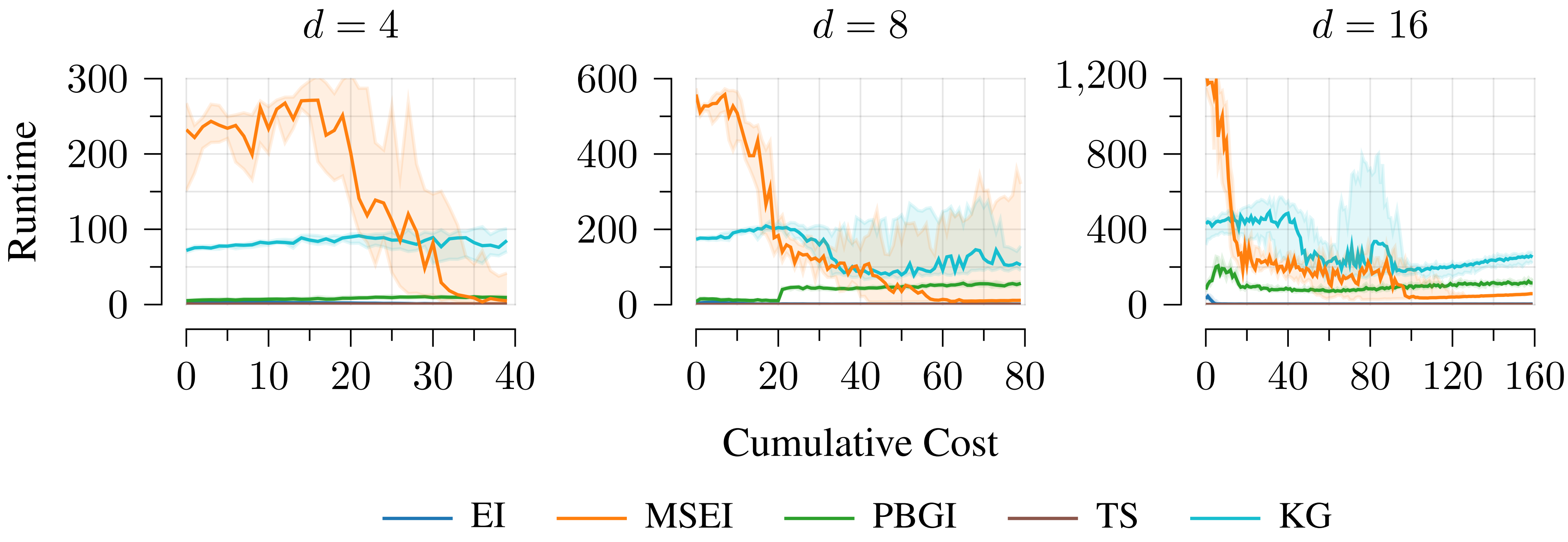
$$\mathrm{EI}_{f|D}(x;g) := \underbrace{\mathbb{E}[\max(f(x)-g,0)\mid D]}_{\text{analytical expression}}$$

Gaussian distribution

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

$\mathrm{GI}_{f|D}$ is easy to compute using $\mathrm{EI}_{f|D}$ + bisection search!

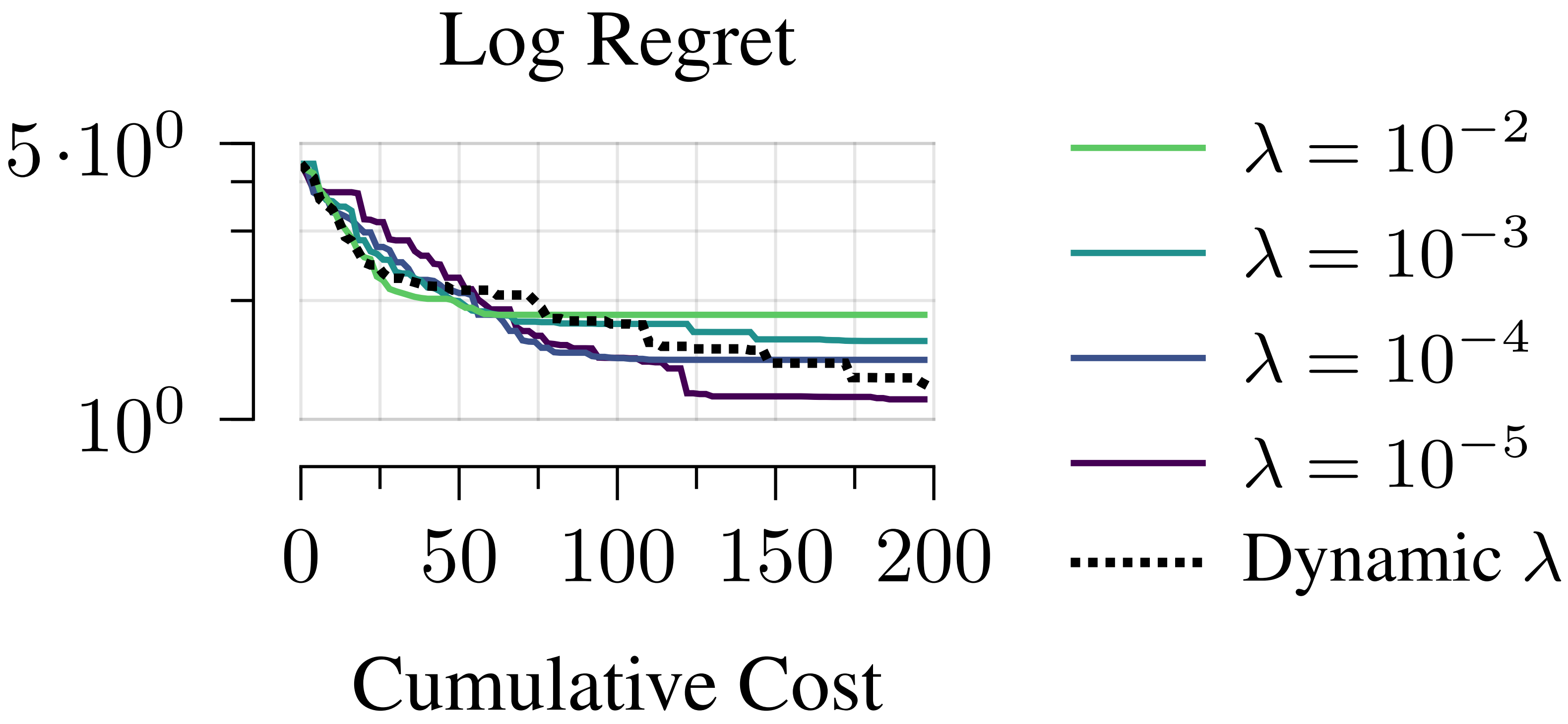
Discussion 2: Timing Experiment



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

PBGI is easy to compute using EI + bisection search!

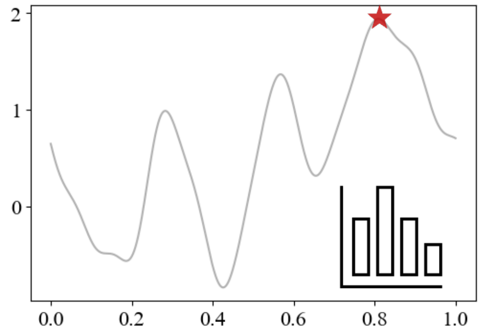
Discussion 3: Effect of λ



Larger budget, smaller λ, higher exploration

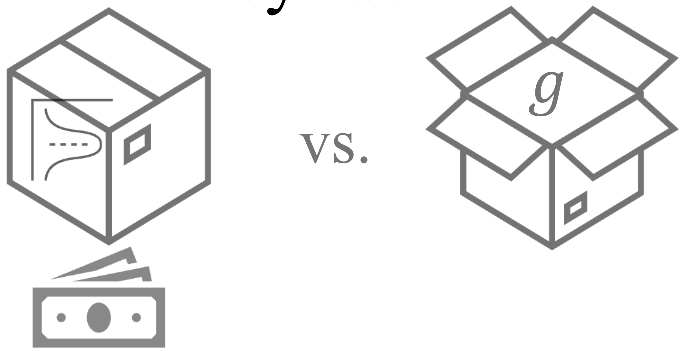
New Design Principle: Gittins Index

Studied Problem



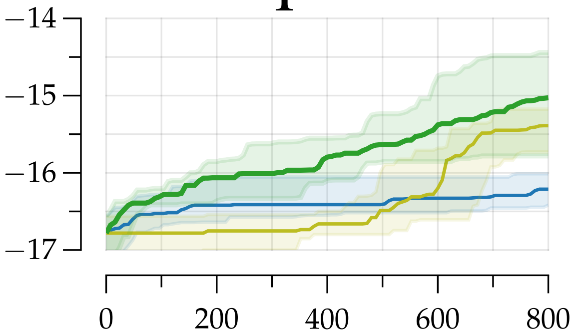
Cost-aware Bayesian optimization

Key idea



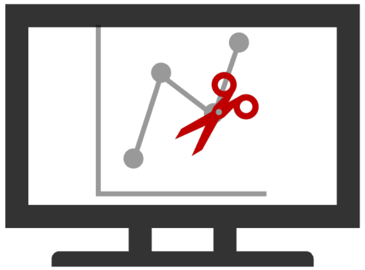
Link to Pandora's box
and Gittins index theory

Impact



Competitive empirical performance

Ongoing work



Cost-aware experiment-level &
trial-level early-stopping

Check our NeurIPS’24 paper on ArXiv!

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