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

Gittins Indices for Cost-aware and Freeze-thaw Bayesian Optimization

Ongoing work

Qian Xie (Cornell ORIE)

Admission to Candidacy Exam ("A Exam")

Collaborators

Cost-aware Bayesian Optimization

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Committee member

Ziv Scully
Advisor

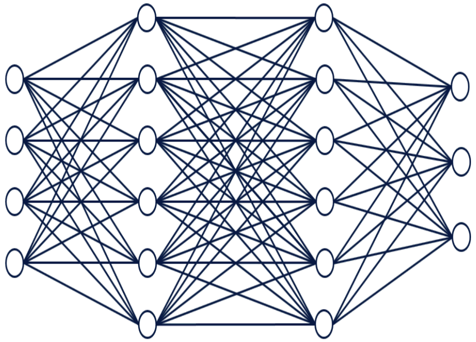
Alexander Terenin
Cornell RAP

Theo Brown
UCL PhD

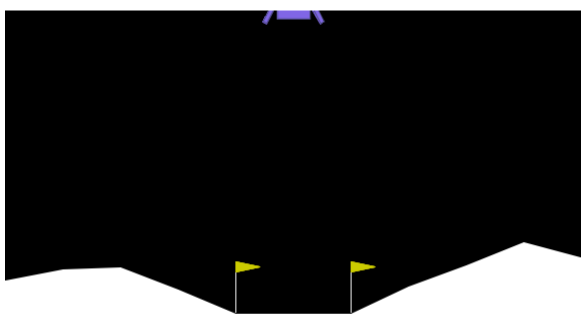
Freeze-thaw Bayesian Optimization

World of Parameter Optimization

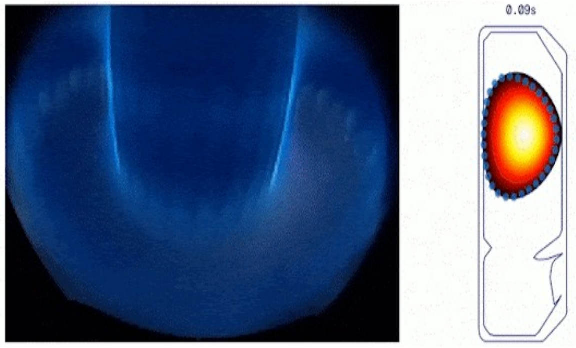
Hyperparameter tuning:

Training parameters →  → Accuracy

Control optimization:

Control variables →  → Reward

Plasma physics:

Reactor parameters → 

→ Stability

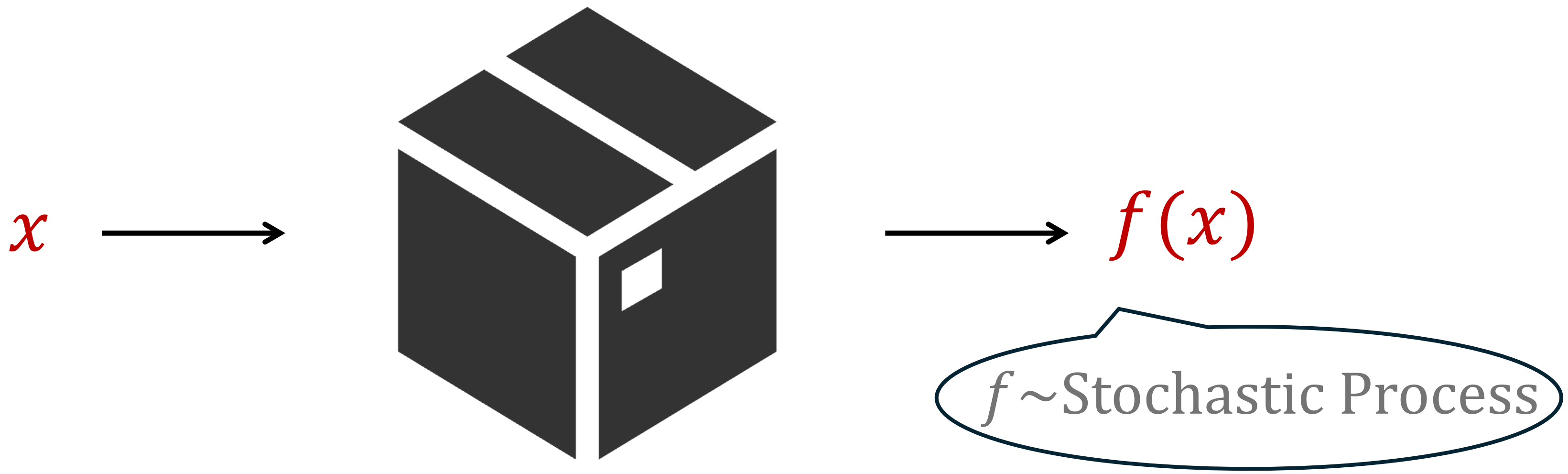
World of Parameter Optimization

Black-box optimization:

Input parameters ⟶  ⟶ Performance metric

World of Parameter Optimization

Black-box function:



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

$x \longrightarrow$

$\longrightarrow f(x)$

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

$f \sim$Stochastic Process

Grid Search? Random search?

Optimizing Black-box Functions

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

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: $\sup\limits_{\text{policy}} \mathbb{E} \max\limits_{t=1,2,\ldots,T} f(x_t)$

f ~Stochastic Process

Grid Search? Random search?

Optimizing Black-box Functions

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

limited #evaluations

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

$f \sim$Stochastic Process

More efficient: Bayesian optimization!

Bayesian Optimization

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

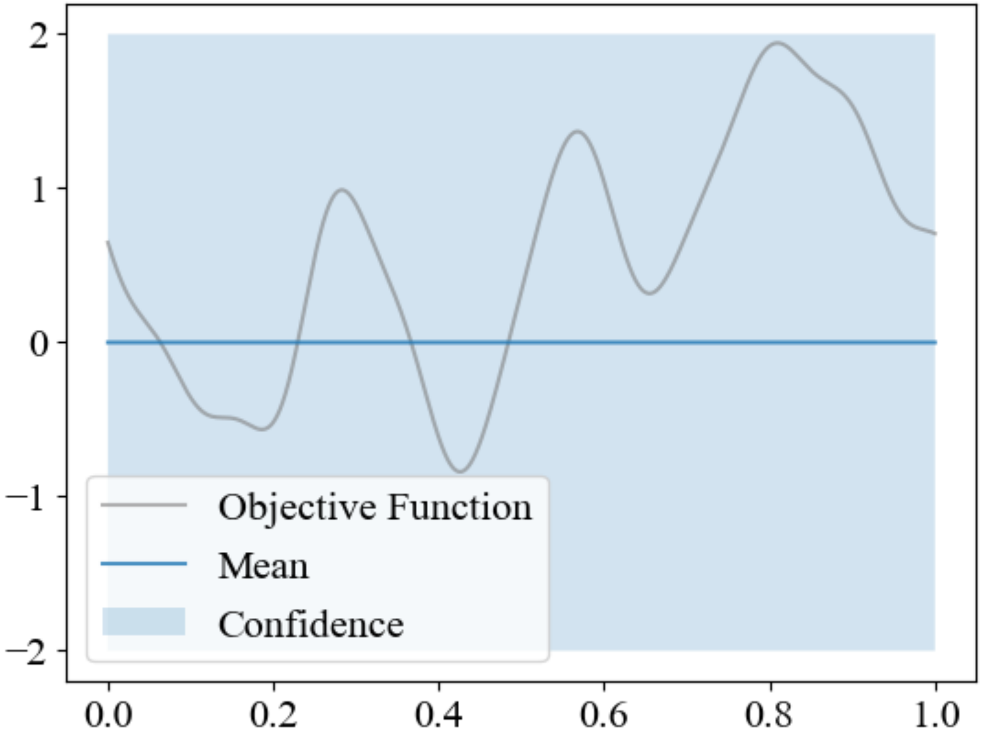
limited #evaluations

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

$f \sim$Gaussian Process

Key idea: maintain posterior belief about f

Bayesian Optimization



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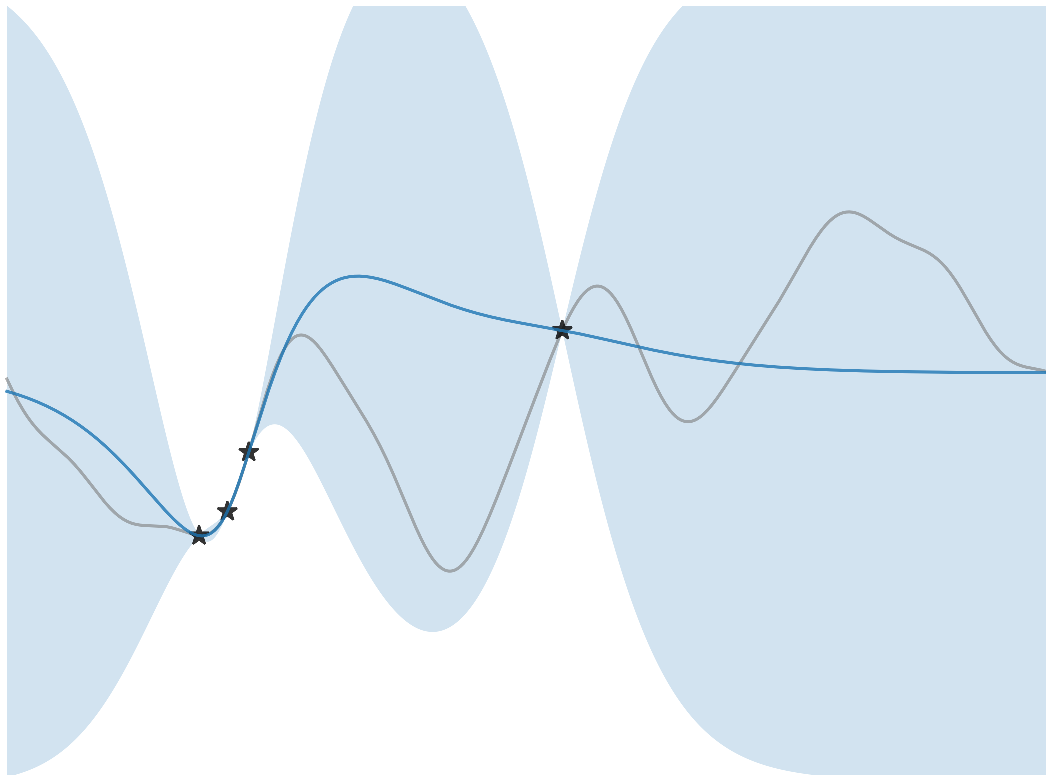

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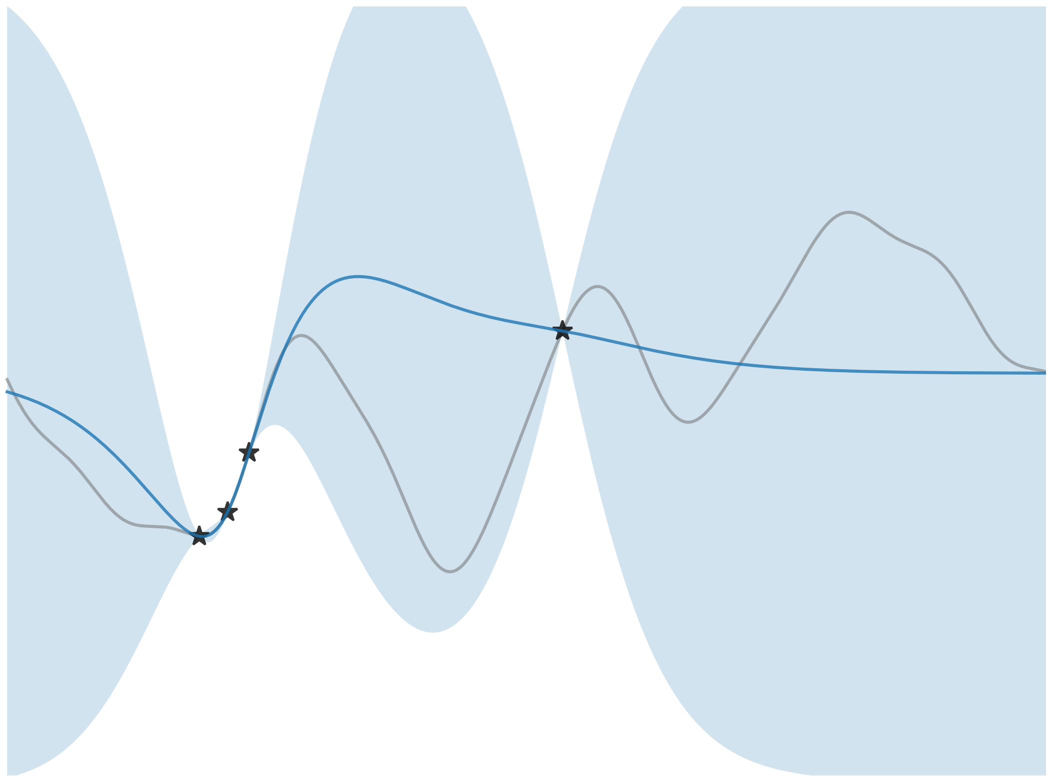
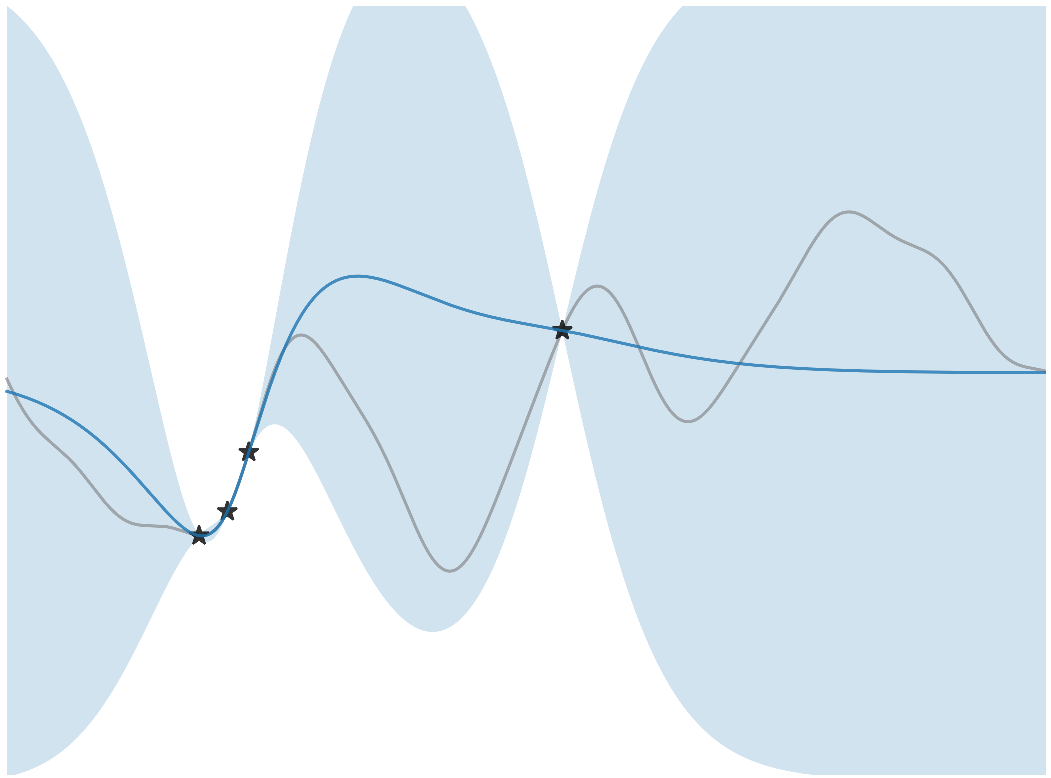
Bayesian Optimization



What to evaluate next?

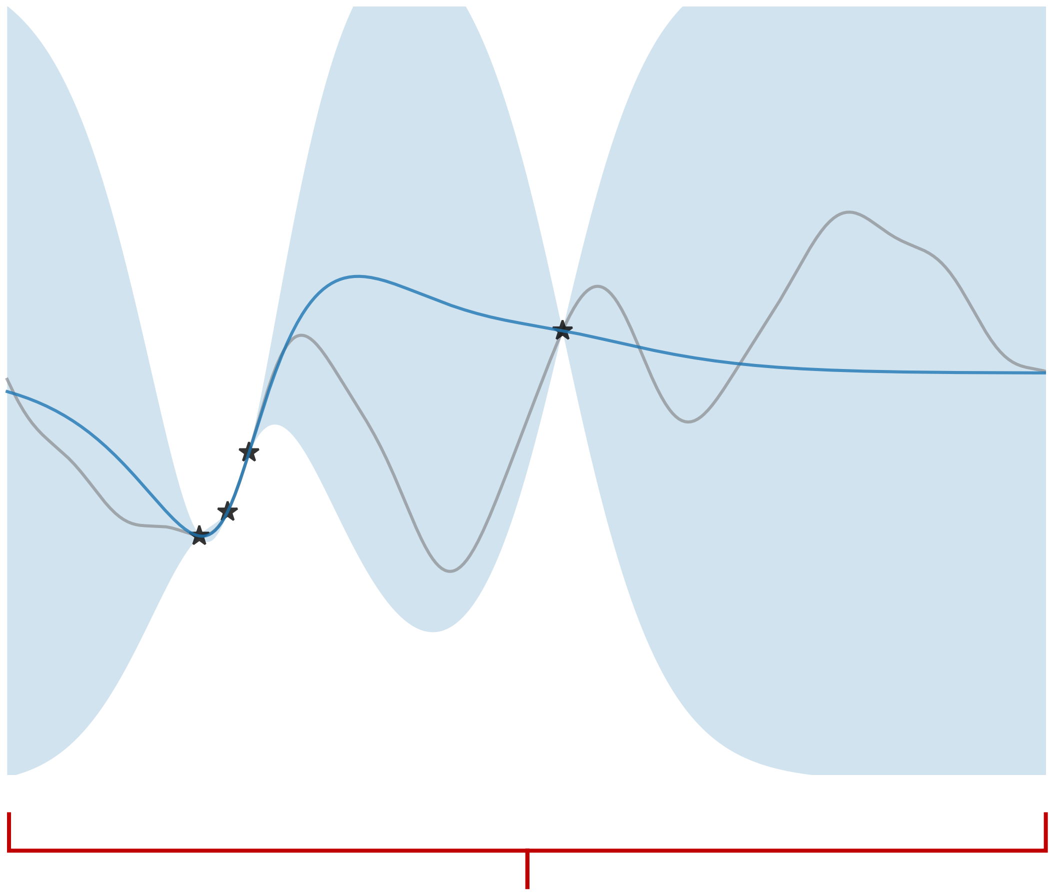
Bayesian Optimization



What to evaluate next?

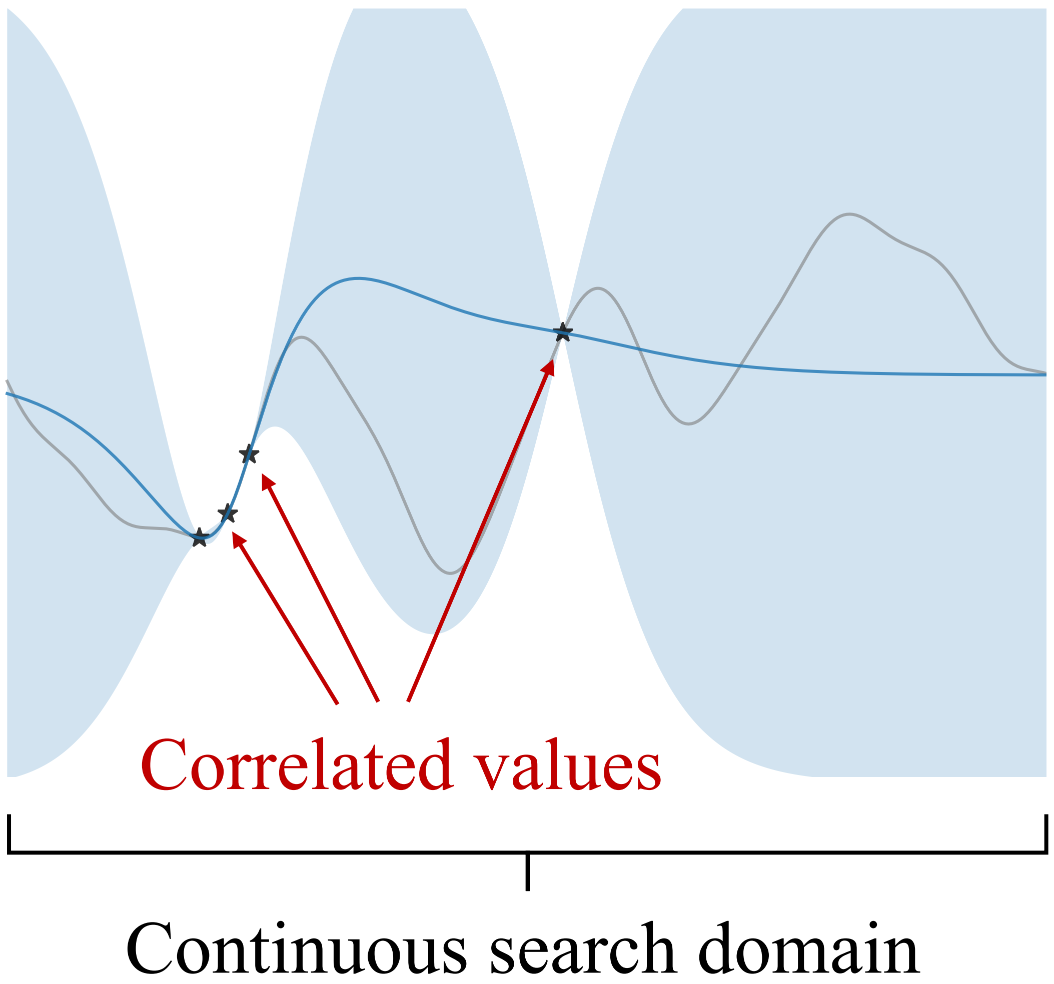
Optimal policy?

Properties of Bayesian Optimization

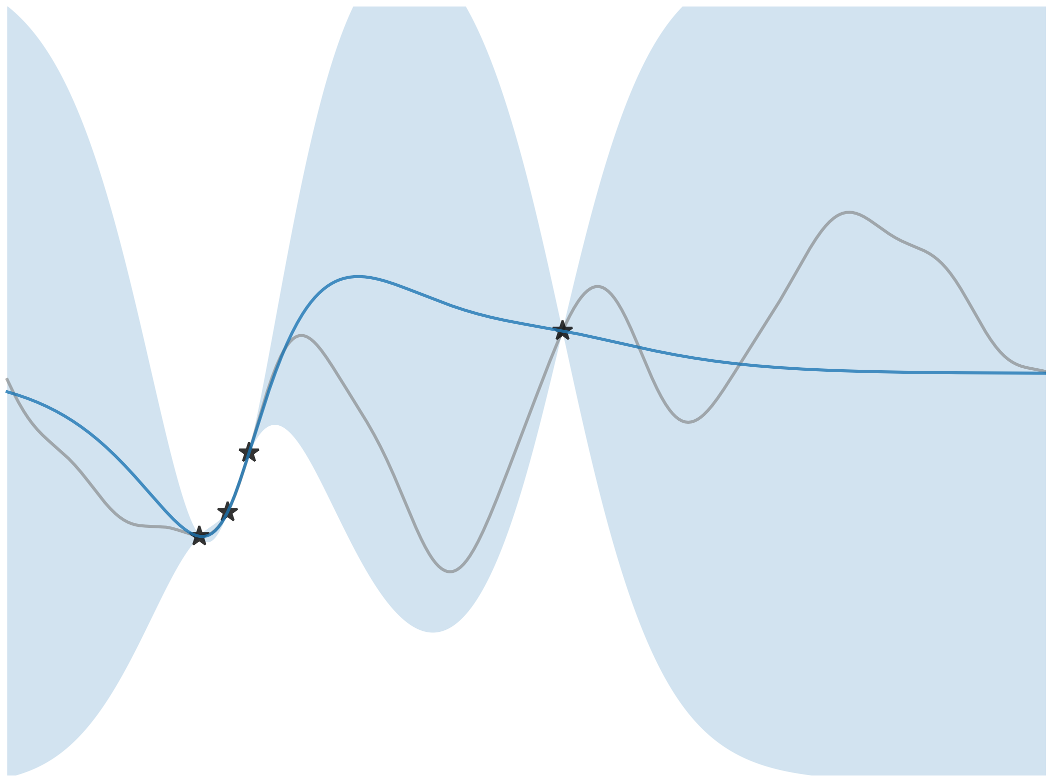


Continuous search domain

Properties of Bayesian Optimization

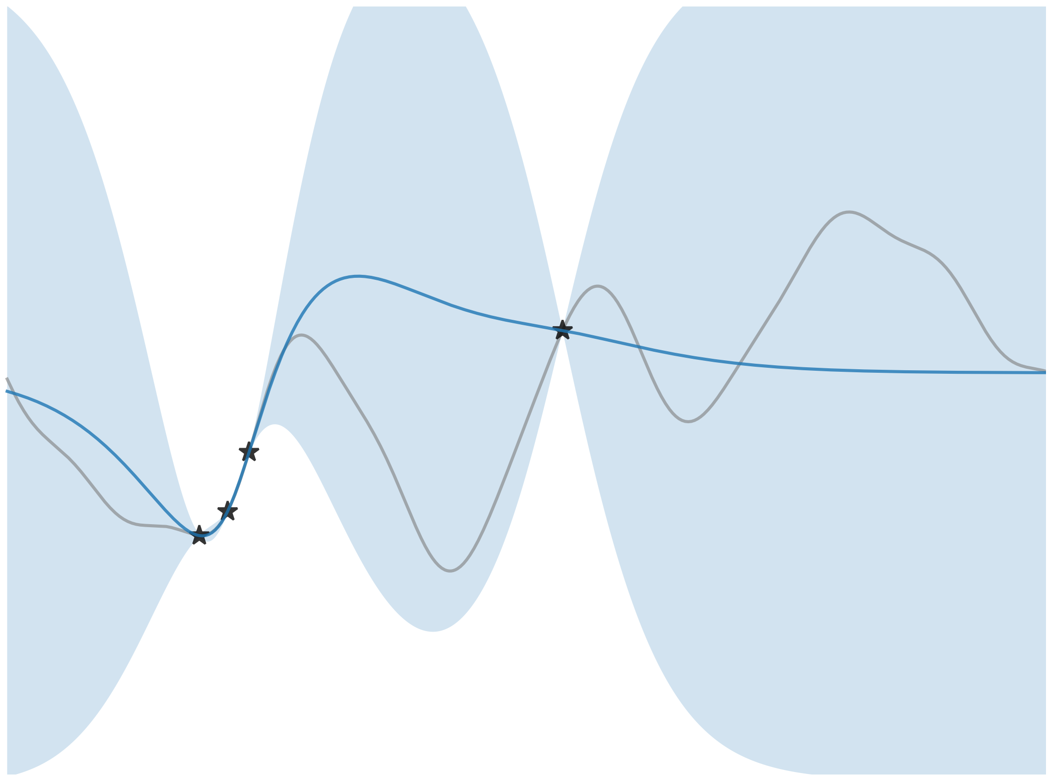


Properties of Bayesian Optimization



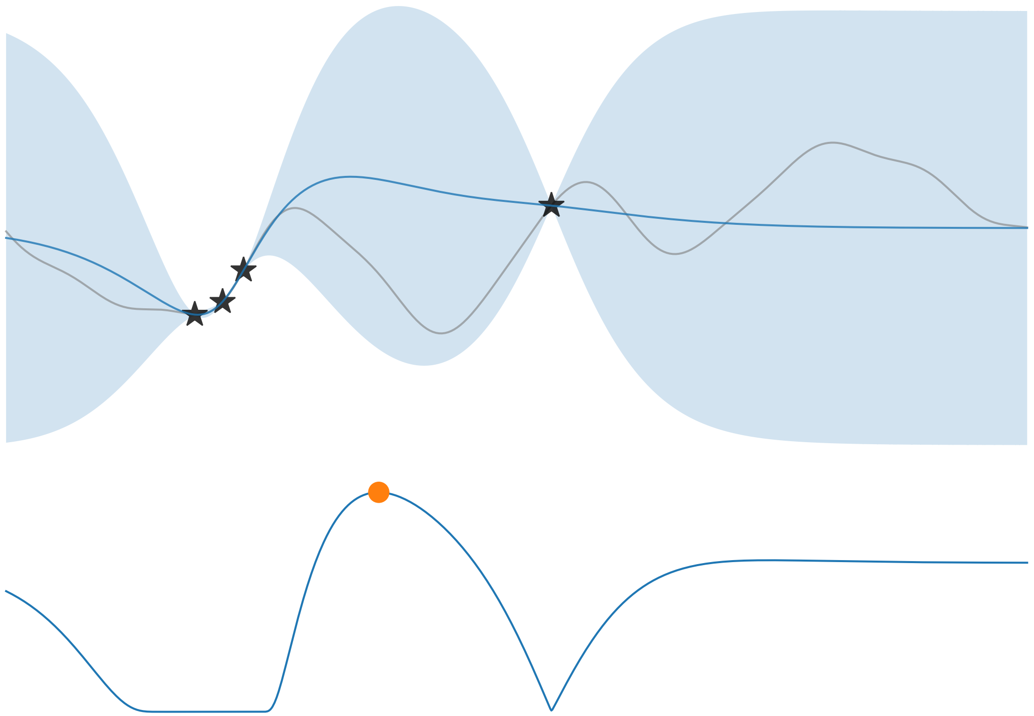
Correlation & continuity $\Longrightarrow$ Intractable MDP

Properties of Bayesian Optimization



Intractable MDP $\Longrightarrow$ Optimal policy unknown

Popular Policy: Expected Improvement



current best observed

data

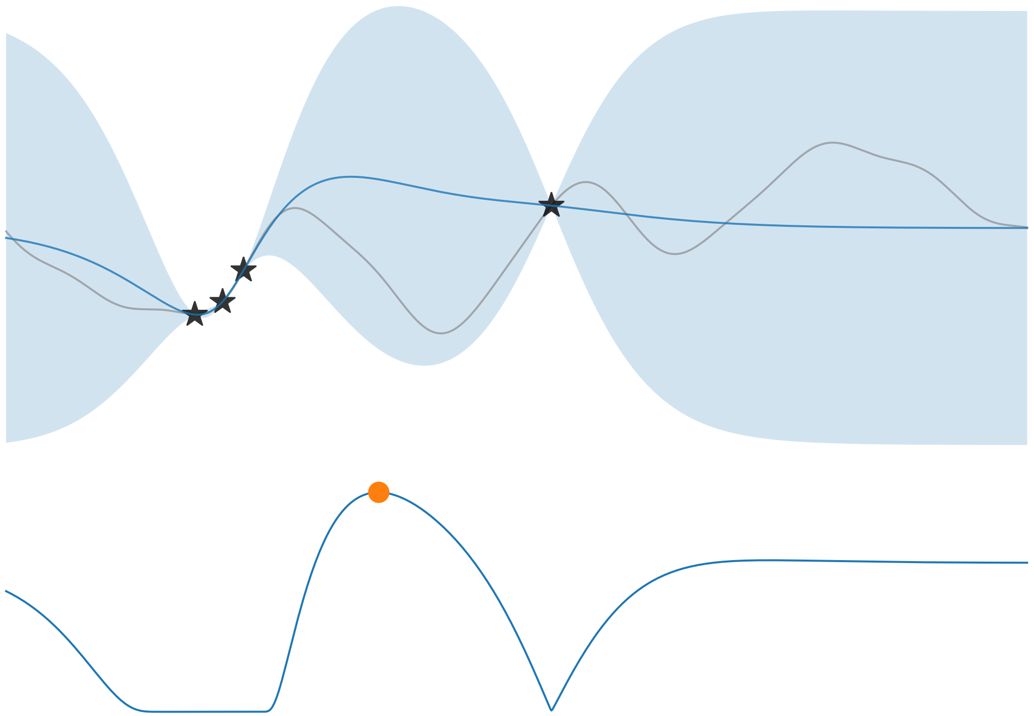
$$\mathrm{EI}(x) = \mathbb{E}[\underbrace{\max(f(x) - y_{\text{best}}, 0)}_{\text{“improvement”}} \mid D]$$

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

posterior distribution

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

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Approaches to Bayesian Optimization

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Why another approach?

Approaches to Bayesian Optimization

- Improvement-based
- Entropy-based
- Upper Confidence Bound
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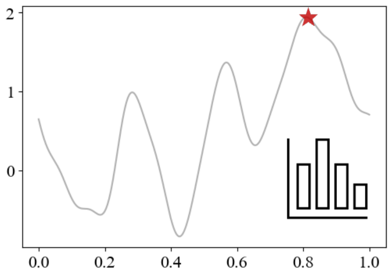
Why another approach?

Less-explored Practical Factors!

Outline: Two Less-explored Practical Factors

Part I: Varying Evaluation Costs

- Cost-aware Bayesian Optimization



Outline: Two Less-explored Practical Factors

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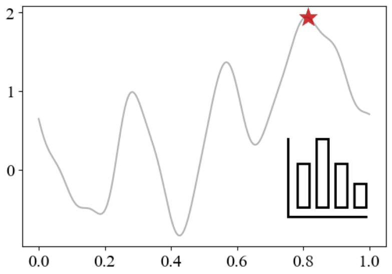

Part II: Observable Partial Feedback

- Freeze-thaw Bayesian Optimization

Outline: Two Less-explored Practical Factors

Part I: Varying Evaluation Costs

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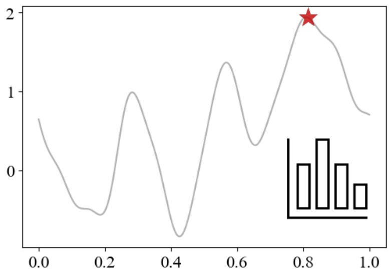

Part II: Observable Partial Feedback

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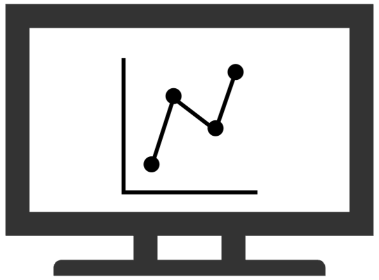
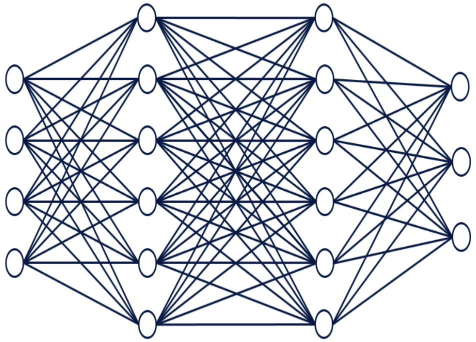


New design principle:
Gittins index

Part I: Varying Evaluation Costs

Hyperparameter tuning:

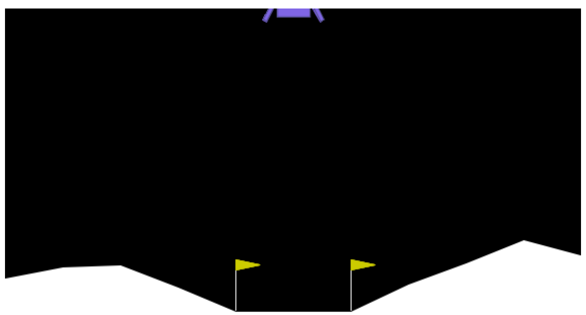
Training parameters →



→ Accuracy

Control optimization:

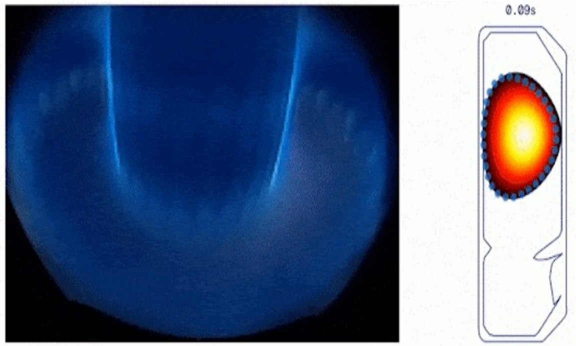
Control variables →



→ Reward

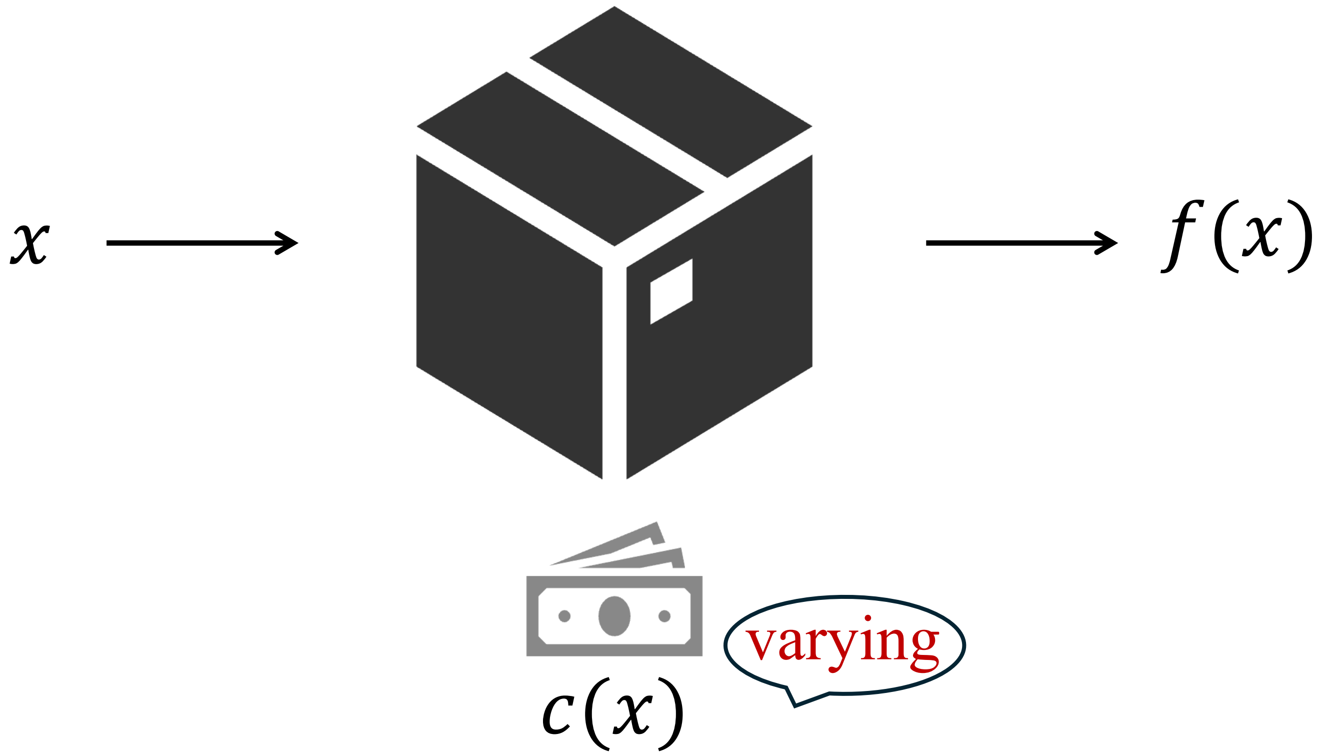
Plasma physics:

Reactor parameters →



→ Stability

Practical Factor: Varying Evaluation Costs



Cost-aware Bayesian Optimization

[Lee, Perrone, Archambeau, Seeger'21]

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

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

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

Cost-aware Bayesian Optimization

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

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

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

Cost-aware Bayesian Optimization

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

Cost-aware Bayesian Optimization

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

Cost-aware Bayesian Optimization

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

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	?
	Thompson Sampling	?
	⋮	⋮

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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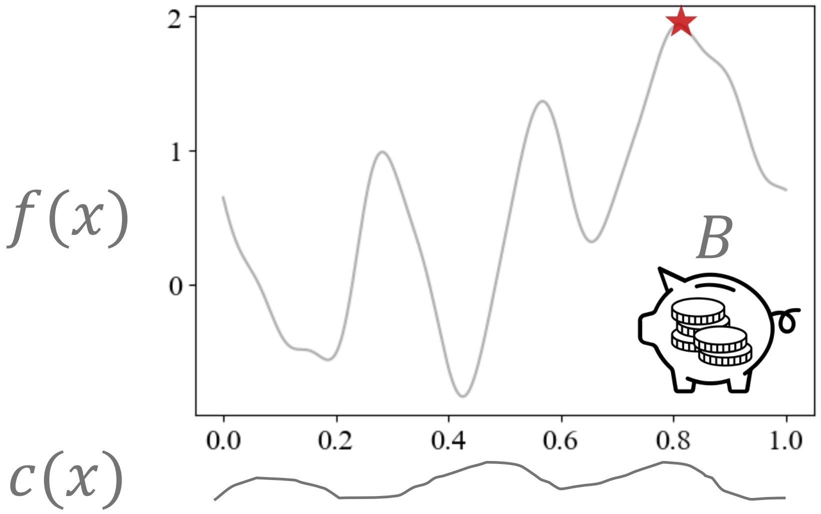
	⋮	⋮

New design principle: Gittins Index

inherently cost-aware

Cost-aware Bayesian Optimization



Continuous

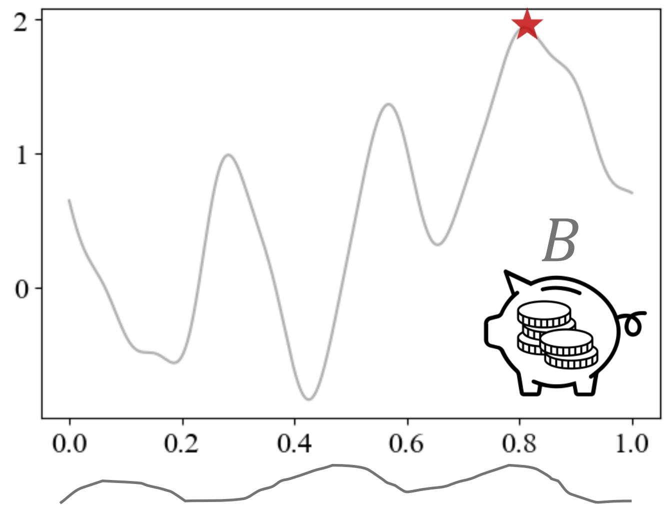
Correlated

Cost-aware Bayesian Optimization

Pandora's Box

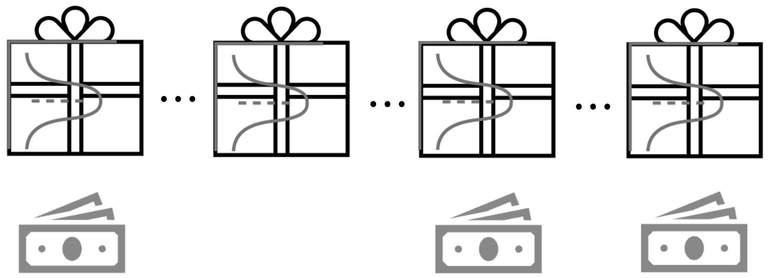
[Weitzman'79]

$f(x)$



$c(x)$

$\Longrightarrow$



$f(x)$

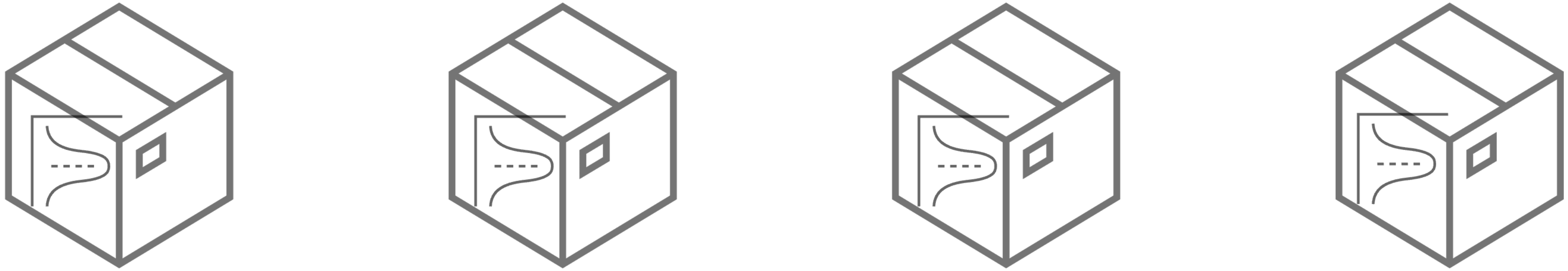
$c(x)$

Continuous $\Longrightarrow$ Discrete

Correlated $\Longrightarrow$ Independent

Pandora's Box

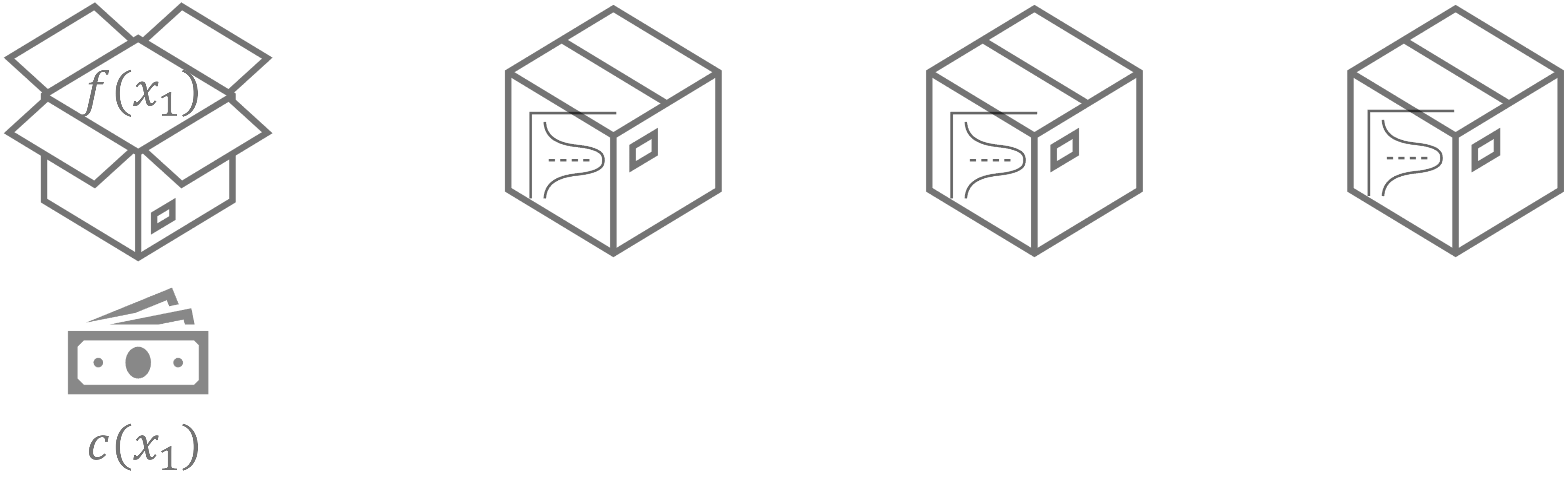
$t = 0$



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

Pandora's Box

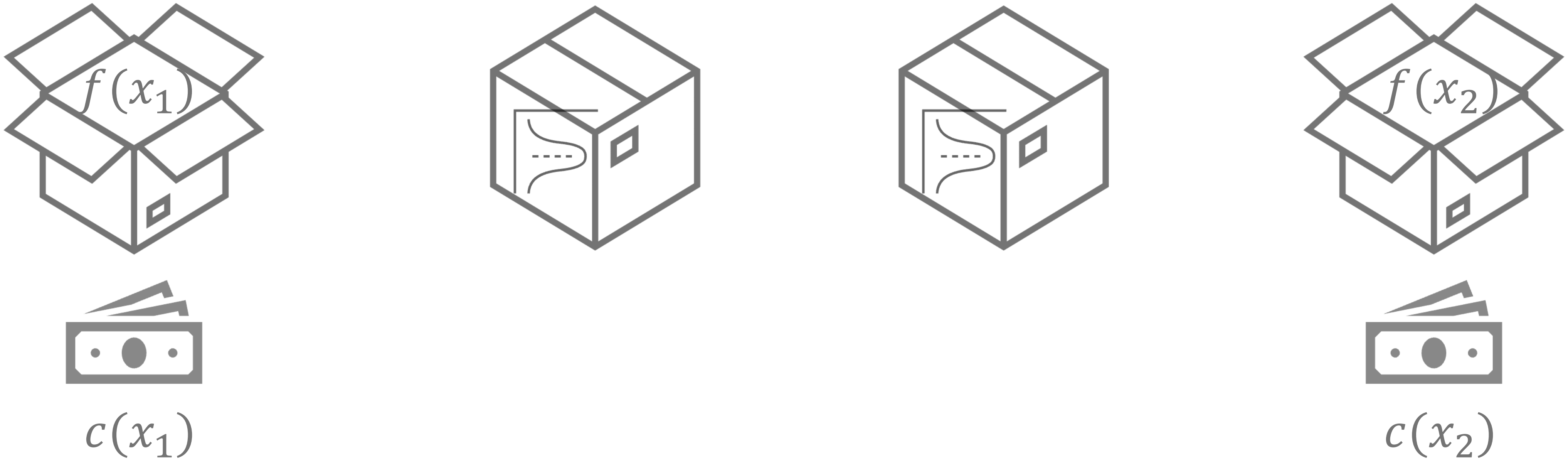
$t = 1$



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

Pandora's Box

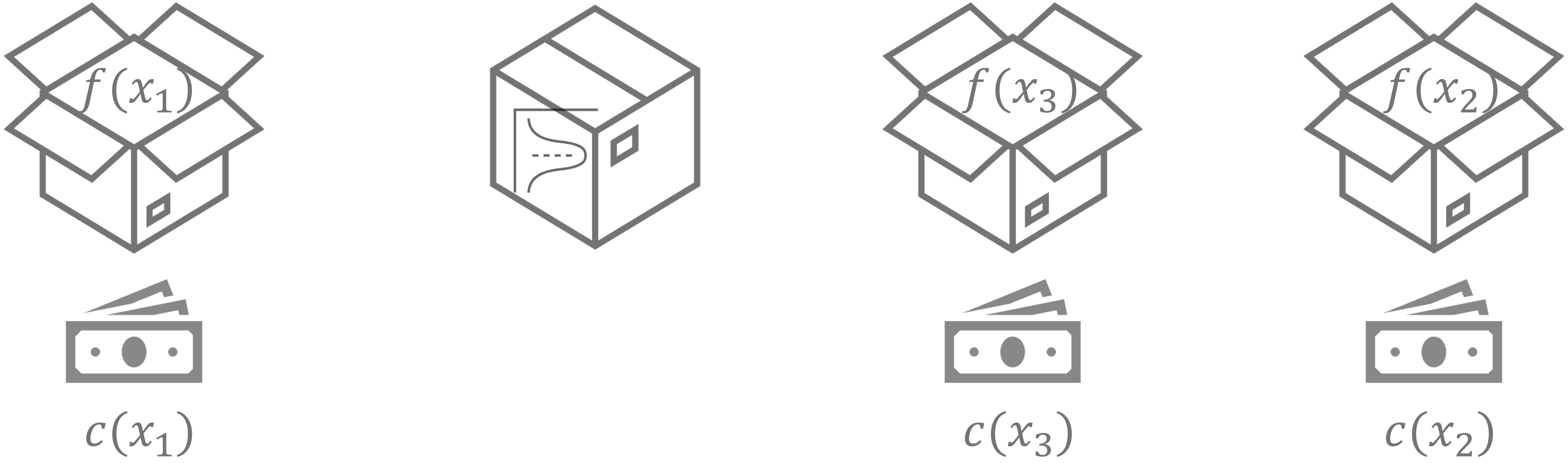
$t = 2$



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

Pandora's Box

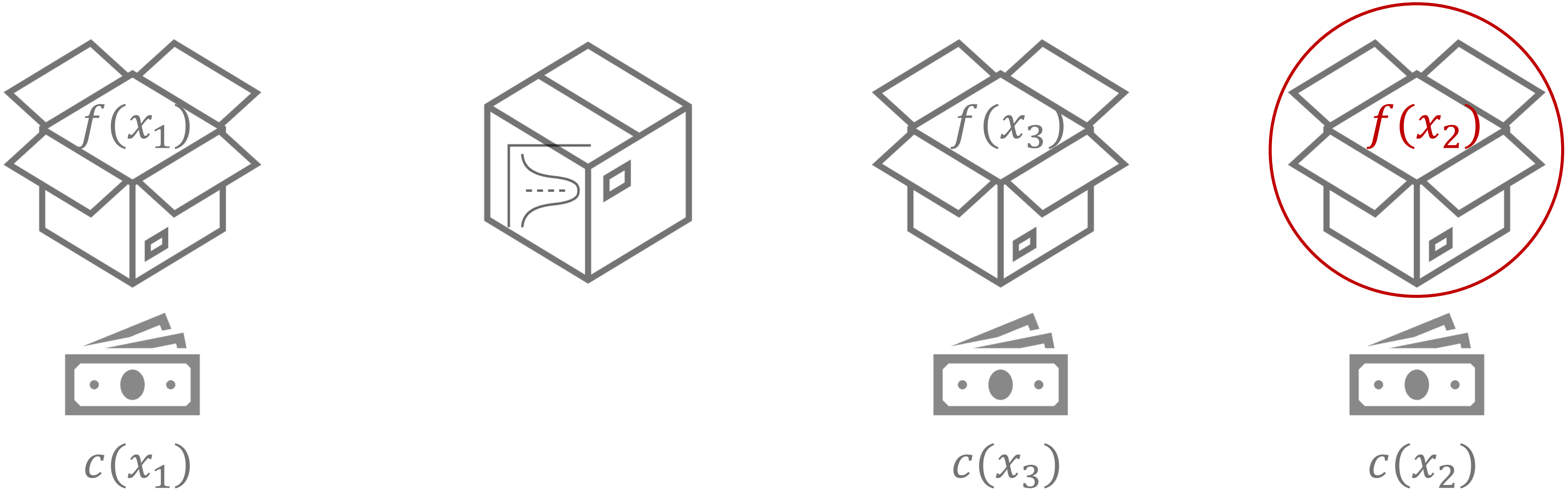
$t = 3$



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

Pandora's Box

$t = T$, stop



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

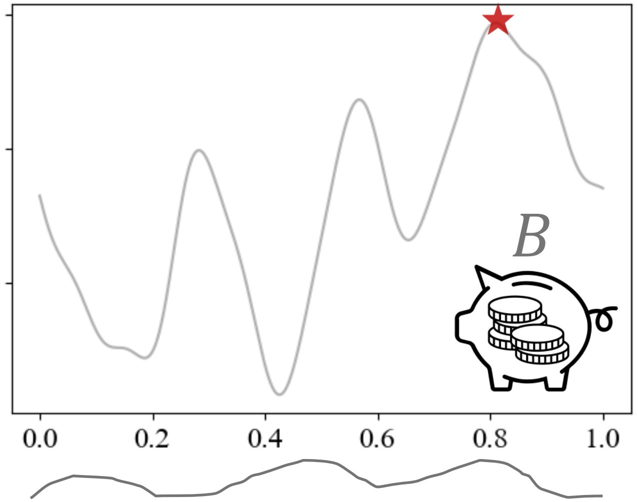
Cost-aware Bayesian Optimization

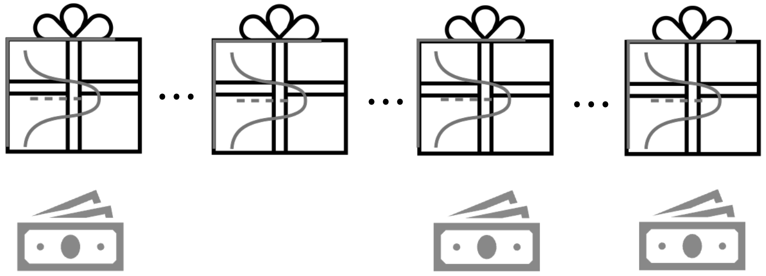
Pandora's Box

[Weitzman'79]

$f(x)$

$c(x)$





$f(x)$

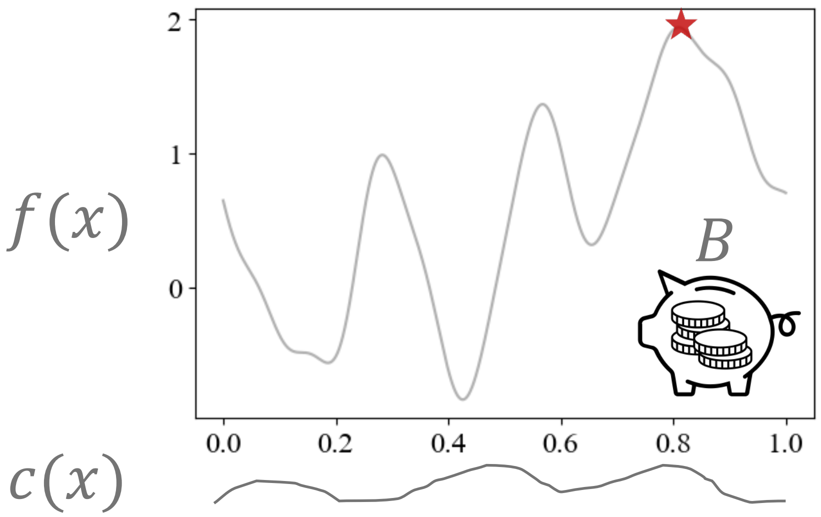
$c(x)$

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

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

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

Cost-aware Bayesian Optimization



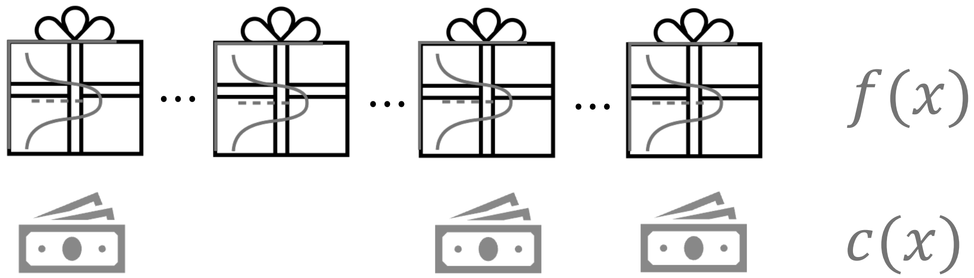
Continuous

Correlated

Expected-budget-constrained

Pandora's Box

[Weitzman'79]



Discrete

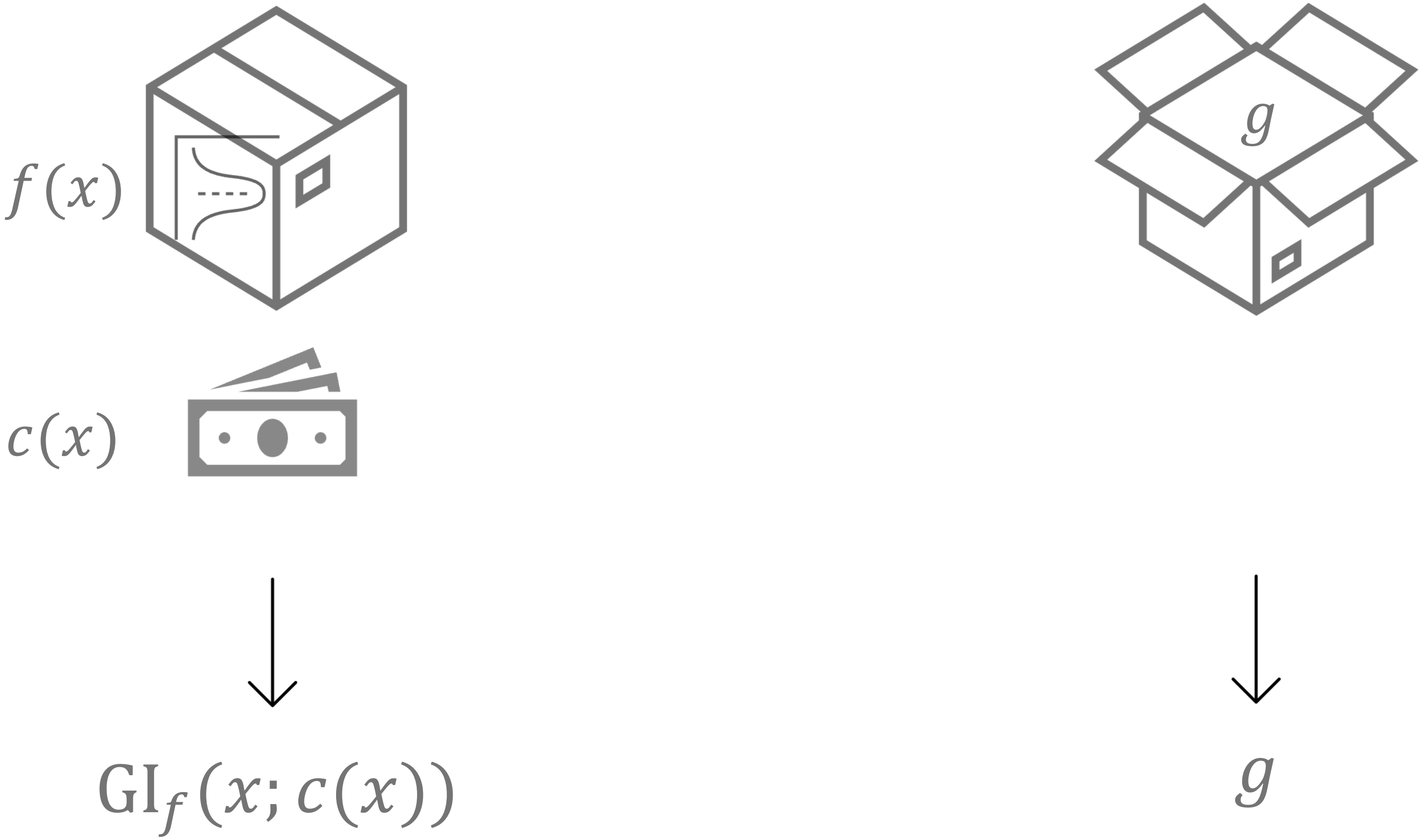
Independent

Cost-per-sample

Optimal policy: Gittins index

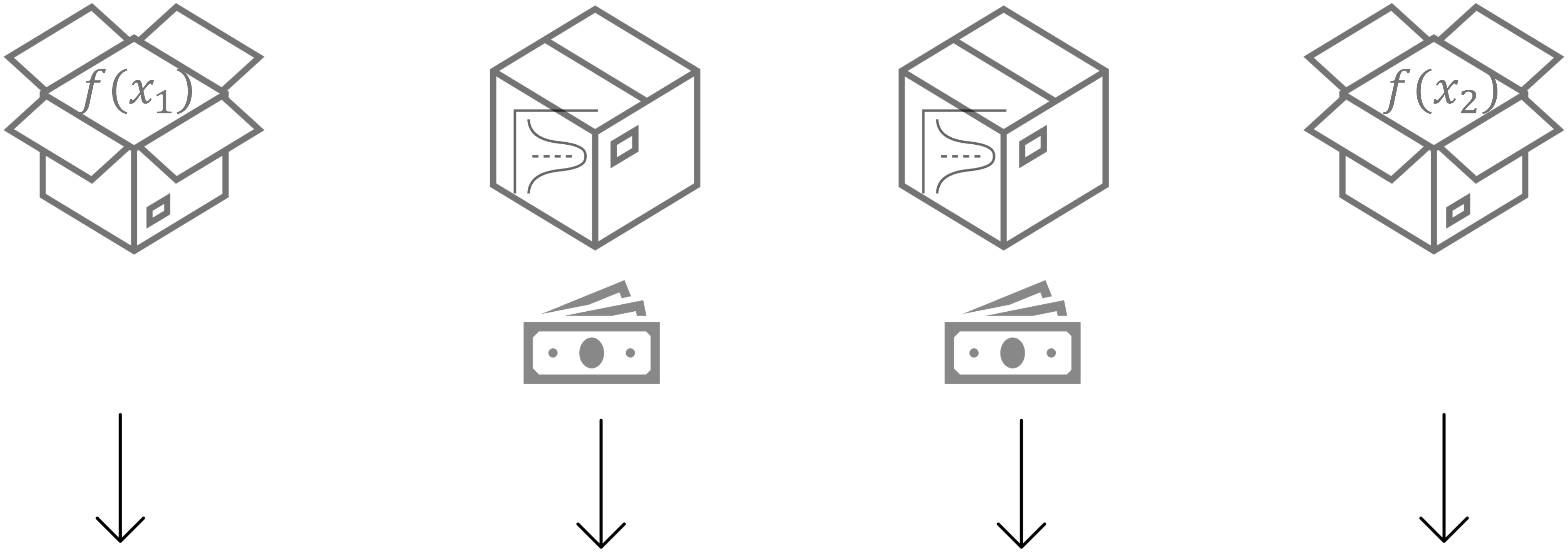
Optimal Policy: Gittins Index

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



Optimal Policy: Gittins Index

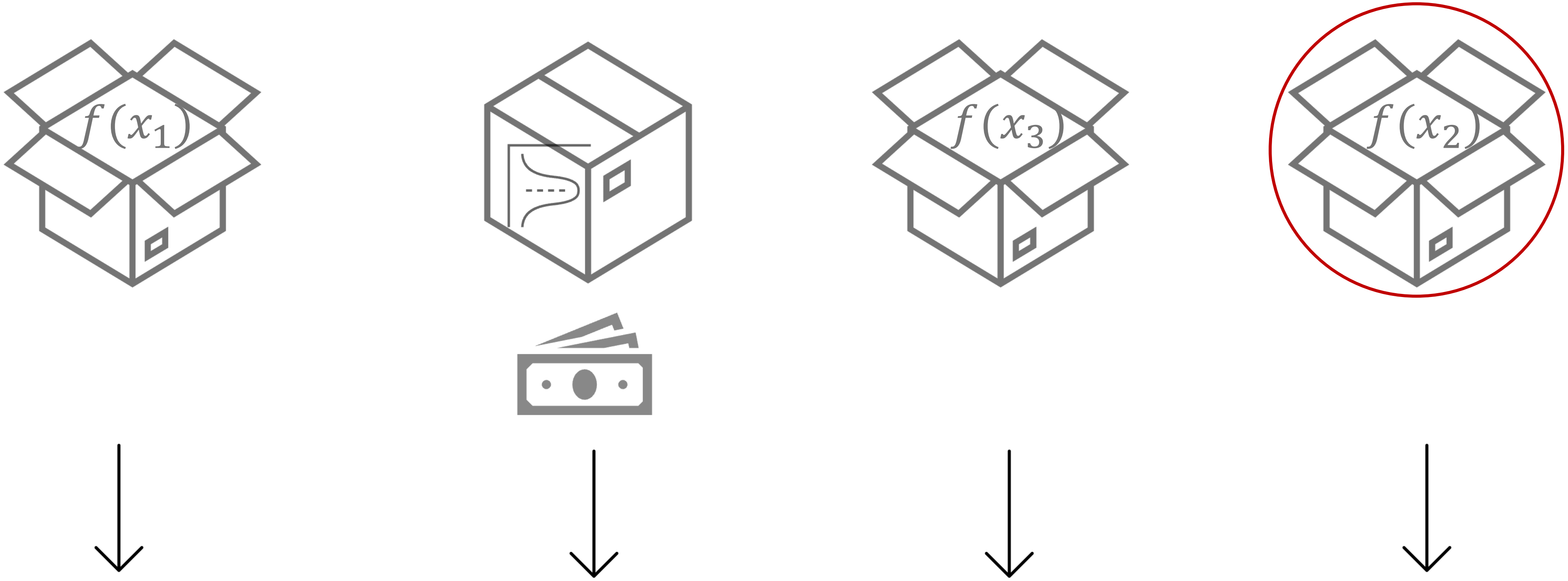
Step 2: Open the box with highest index if it is closed



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

Optimal Policy: Gittins Index

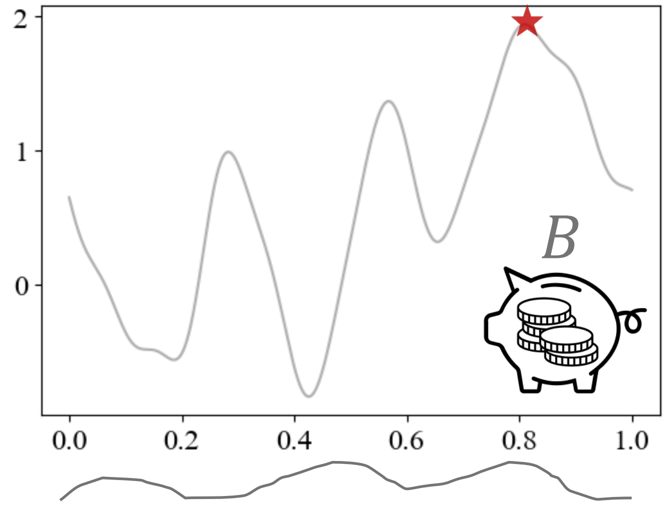
Step 2’: Select the box with highest index if it is opened and stop



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

Cost-aware Bayesian Optimization

$f(x)$



$c(x)$

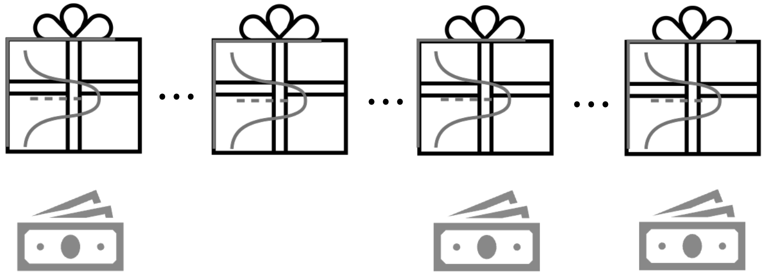
Continuous

Correlated

Expected-budget-constrained

Pandora's Box

[Weitzman'79]



$f(x)$

$c(x)$

Discrete

Independent

Cost-per-sample

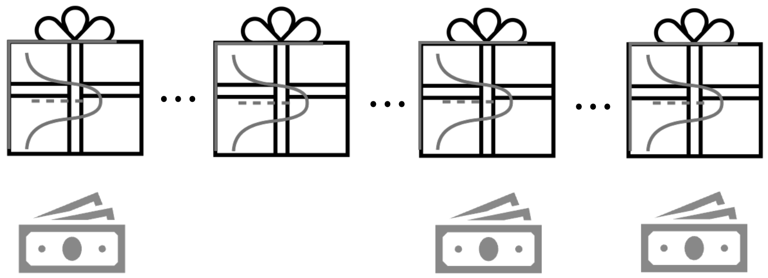
How to translate?

$\Longleftarrow$ 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

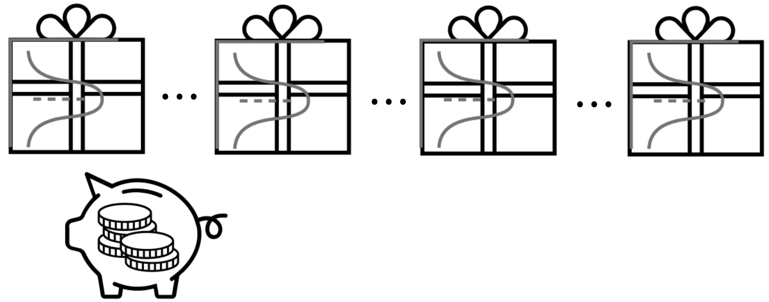
[Aminian, Manshadi, Niazadeh’24]

Pandora’s Box

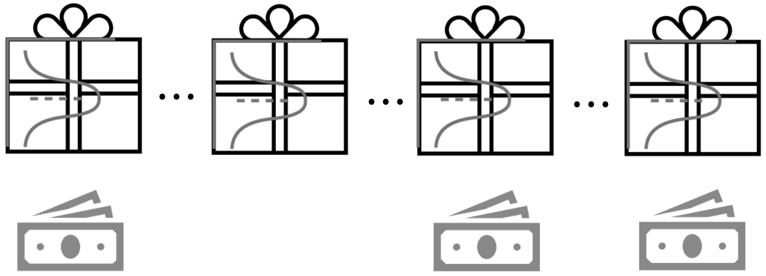
[Weitzman’79]

$f(x)$

B



$\Longleftarrow$



$f(x)$

$c(x)$

Expected-budget-constrained

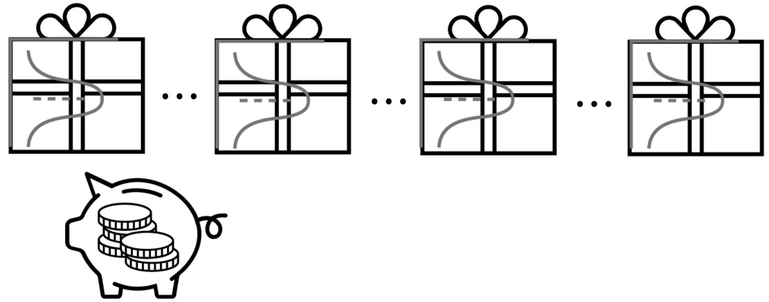
Cost-per-sample

Budgeted Pandora's Box

[Aminian, Manshadi, Niazadeh'24]

$f(x)$

B



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

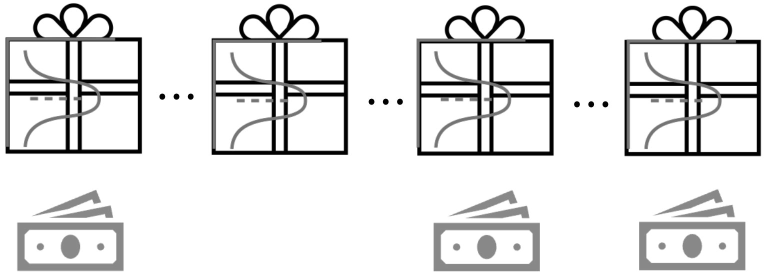
$$\textbf{s.t. } \mathbb{E} \textstyle\sum_{t=1}^{T} c(x_t) \leq B$$

Expected-budget-constrained

$\Longleftarrow$

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

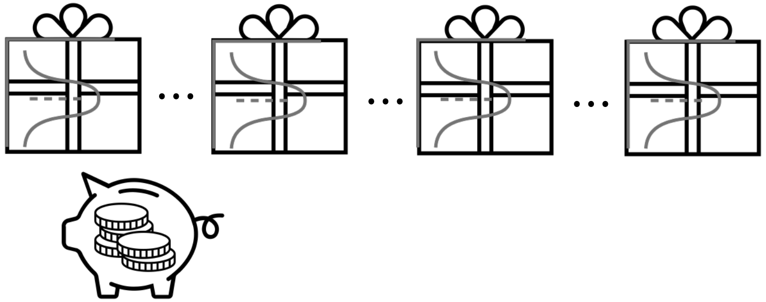
[Aminian, Manshadi, Niazadeh'24]

Pandora's Box

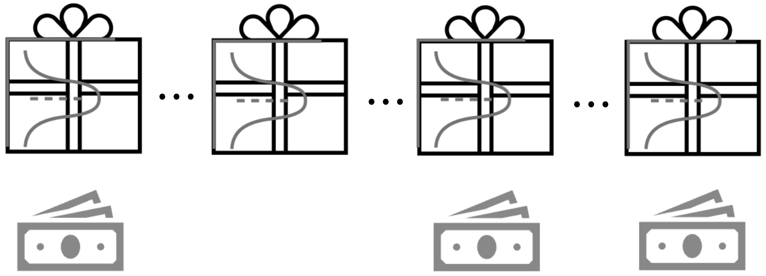
[Weitzman'79]

$f(x)$

B



$\Longleftarrow$



$f(x)$

$c(x)$

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

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

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

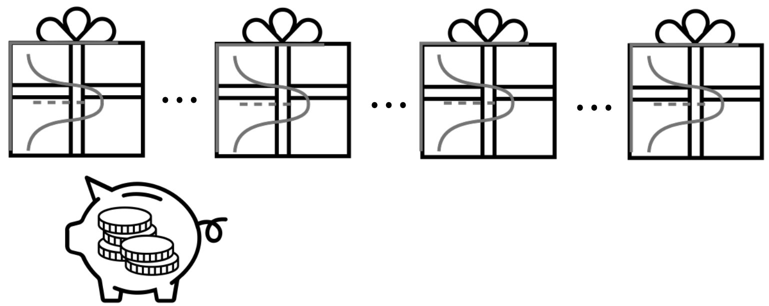
[Aminian, Manshadi, Niazadeh'24]

Pandora's Box

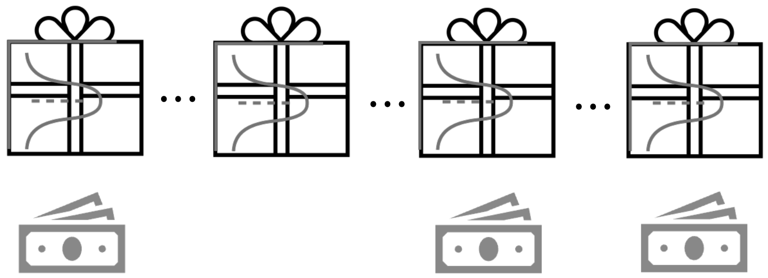
[Weitzman'79]

$f(x)$

B



$\Longleftarrow$



$f(x)$

$c(x)$

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

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

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

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

How to translate?

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

Budgeted Pandora's Box

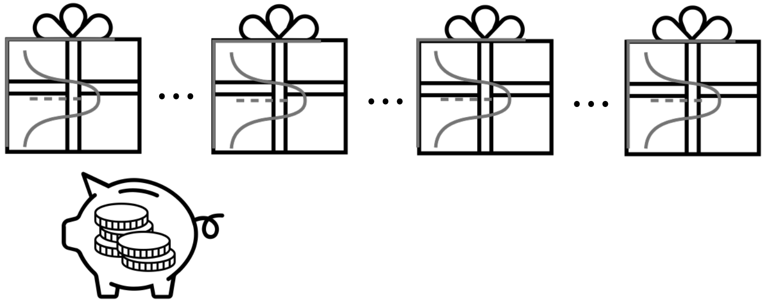
[Aminian, Manshadi, Niazadeh'24]

Pandora's Box

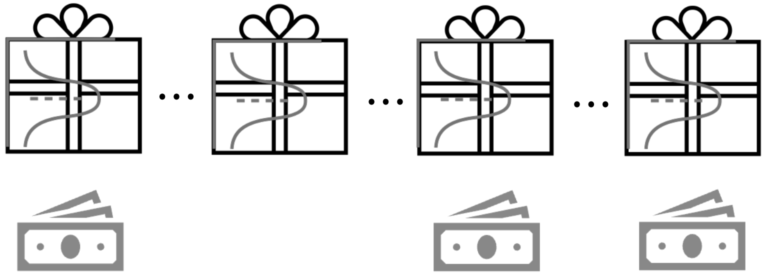
[Weitzman'79]

$f(x)$

B



$\Longleftarrow$



$f(x)$

$c(x)$

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

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

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

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

Budgeted Pandora's Box

[Aminian, Manshadi, Niazadeh'24]

$f(x)$

B

Our work: extension to general reward distribution

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

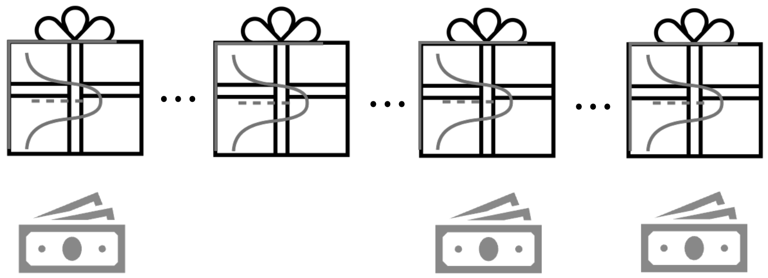
Expected-budget-constrained

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

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

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

$\Leftarrow$

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

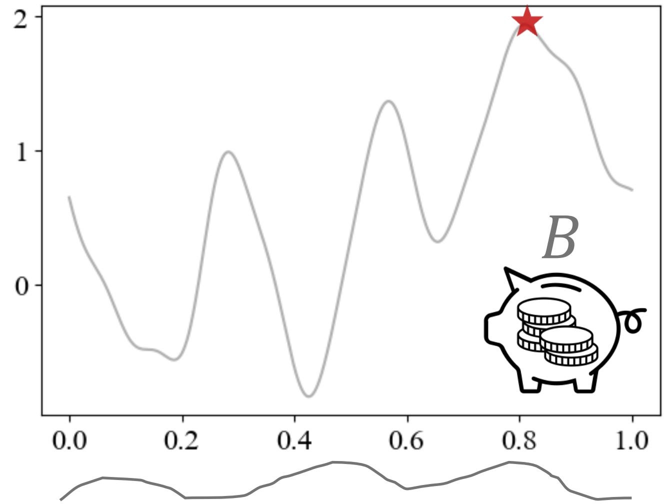
Optimal policy: $\mathrm{GI}_f(x; \lambda_B c(x)) \overset{\text{scale costs}}{\Longleftarrow}$ Optimal policy: $\mathrm{GI}_f(x; c(x))$

Cost-aware Bayesian Optimization

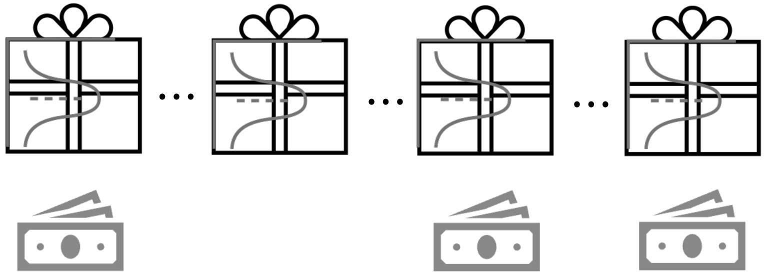
Pandora's Box

[Weitzman'79]

$f(x)$



$c(x)$



$f(x)$

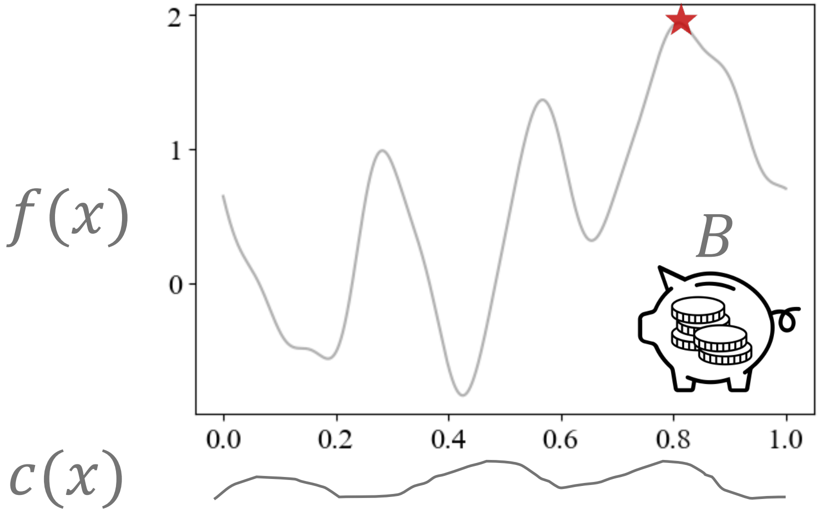
$c(x)$

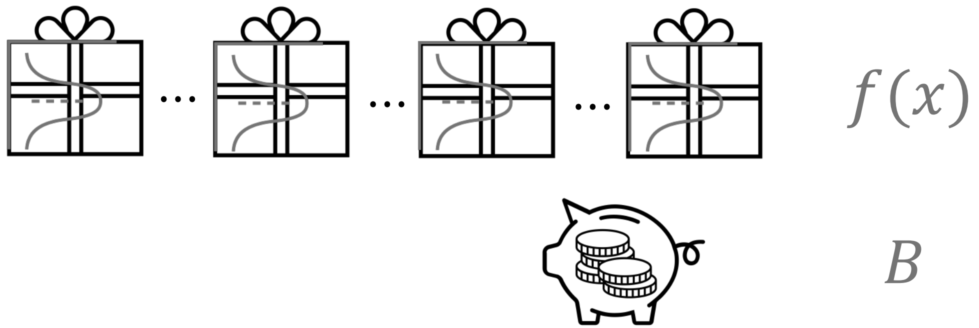
Continuous	Discrete
Correlated	Independent
Expected-budget-constrained $\Longleftarrow$	Cost-per-sample

How to translate?

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

Cost-aware Bayesian Optimization Budgeted Pandora's Box





Continuous Discrete

Correlated Independent

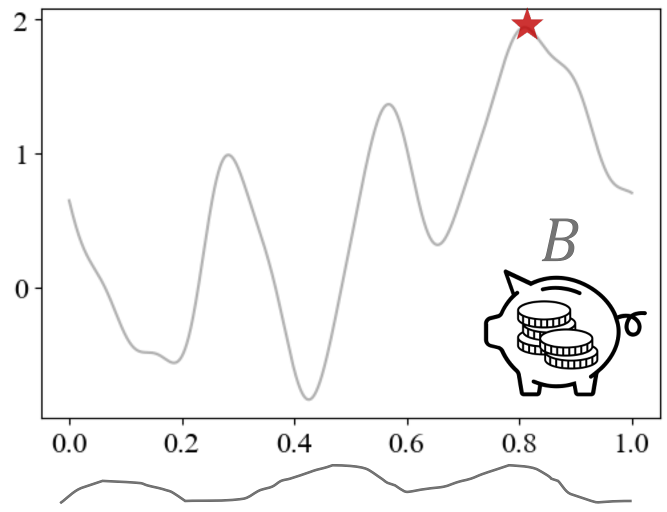
scaling factor

How to translate?

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

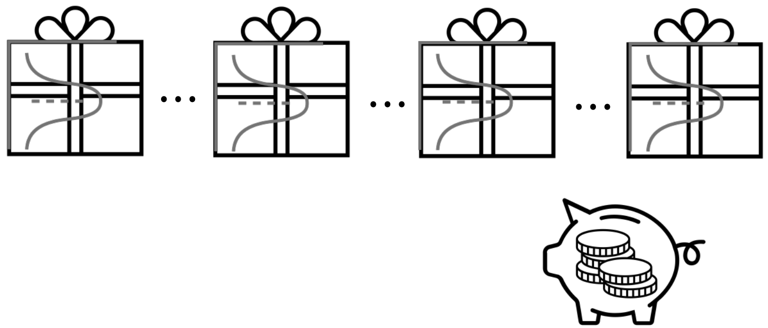
Cost-aware Bayesian Optimization   Budgeted Pandora's Box

$f(x)$



$c(x)$

$\Longleftarrow$



$f(x)$

B

Continuous $\Longleftarrow$ Discrete

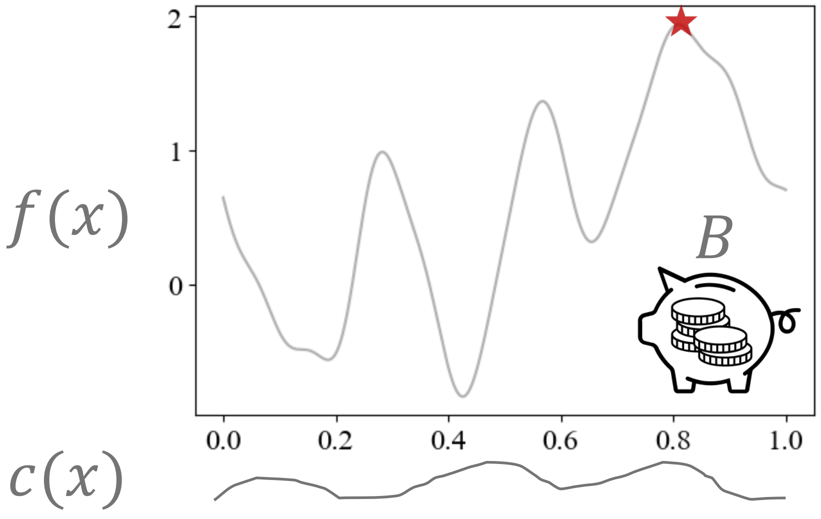
Correlated $\Longleftarrow$ Independent

scaling factor

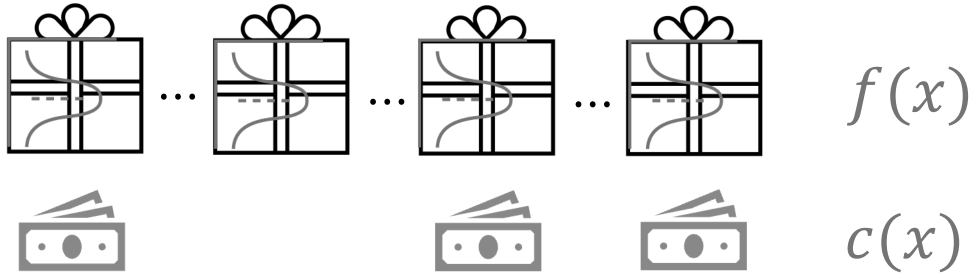
incorporate posterior

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



$\Longleftarrow$



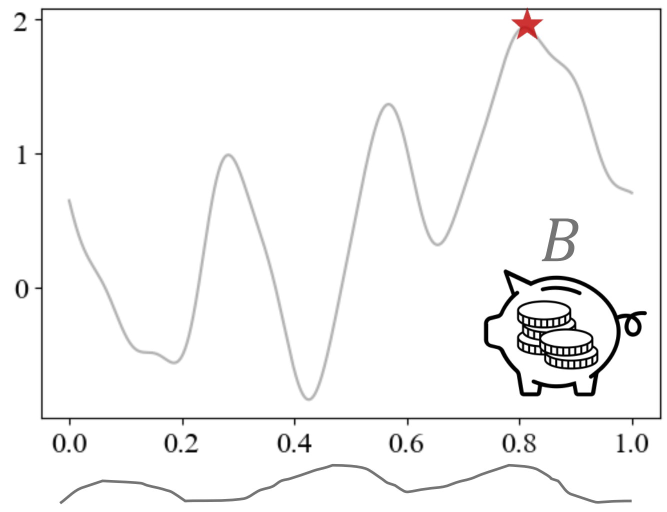
Continuous	$\Longleftarrow$	Discrete	✓
Correlated	$\Longleftarrow$	Independent	✓
Expected-budget-constrained	$\Longleftarrow$	Cost-per-sample	✓

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

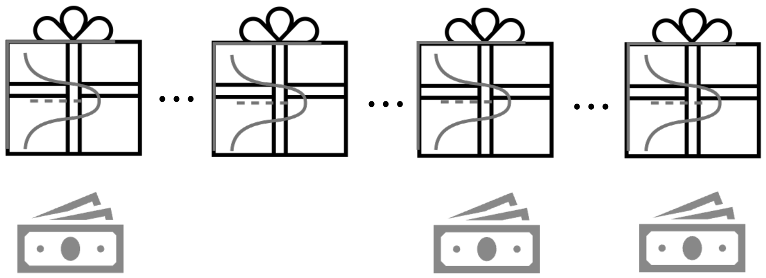
Pandora's Box

$f(x)$



$c(x)$

$\Longleftarrow$



$f(x)$

$c(x)$

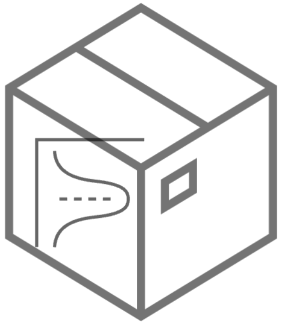
Cost-aware Bayesian Optimization	Pandora's Box
Continuous	Discrete
Correlated	Independent
Expected-budget-constrained	Cost-per-sample

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

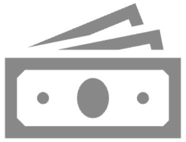
How to compute?

How to compute Gittins index?

$f(x)$

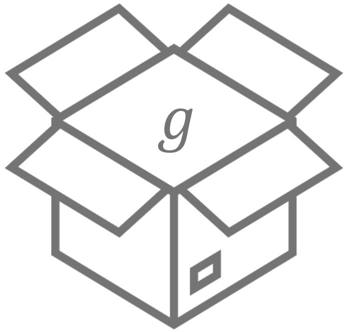


$c(x)$



$\downarrow$?

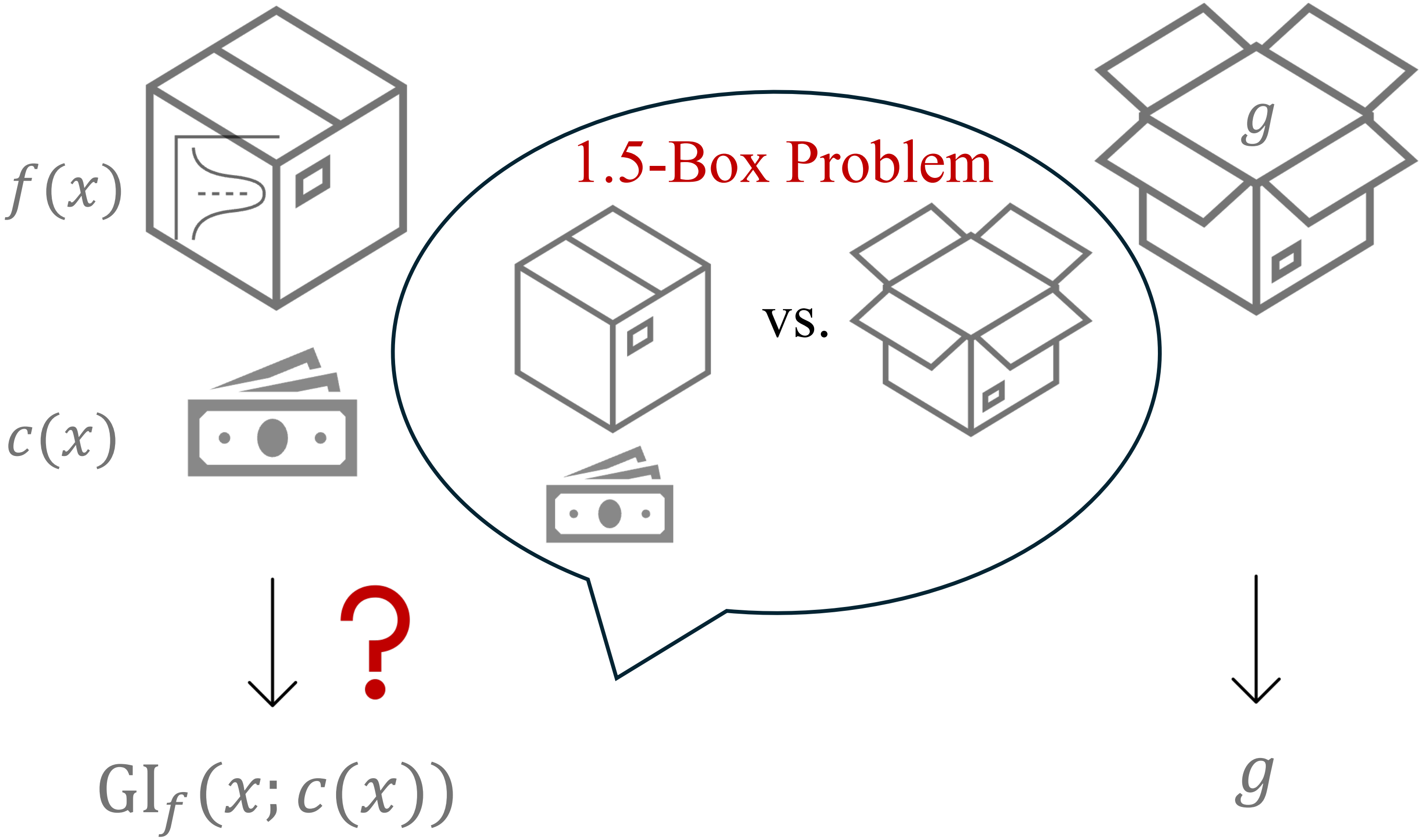
$\mathrm{GI}_f(x; c(x))$



$\downarrow$

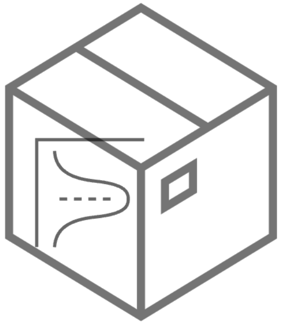
g

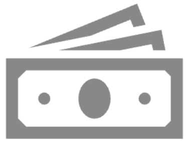
How to compute Gittins index?



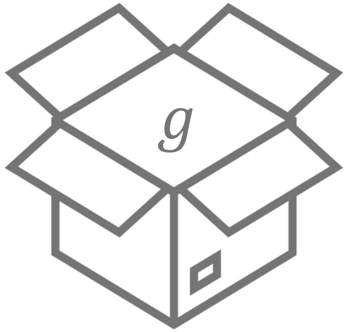
Whether to open a new box or take current best?

Gittins Index Computation: 1.5-Box Problem

$f(x)$ 

$c(x)$ 

vs.

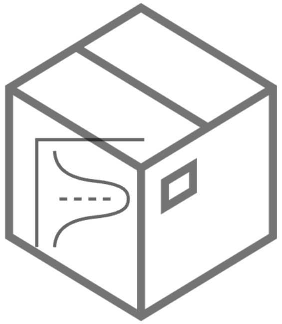


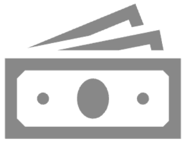
Open closed box

Take opened box

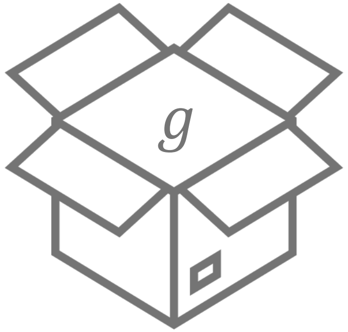
Whether to open a new box or take current best?

Gittins Index Computation:1.5-Box Problem

$f(x)$ 

$c(x)$ 

vs.



Open closed box

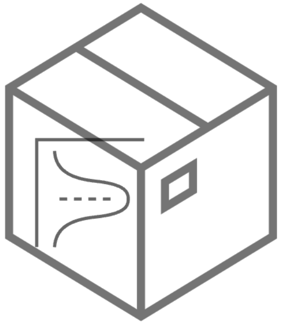
Take opened box

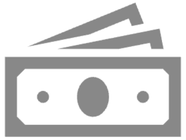
Profit:

Profit:

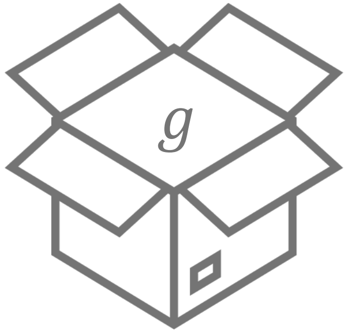
$$\begin{cases} \text{take inside value}, f(x) > g \\ \text{take outside option}, f(x) \le g \end{cases}$$

Gittins Index Computation:1.5-Box Problem

$f(x)$ 

$c(x)$ 

vs.



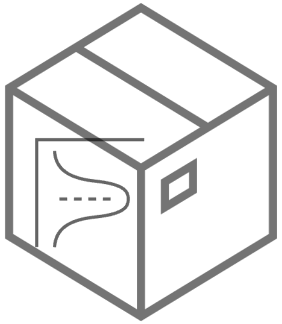
Open closed box | Take opened box

g

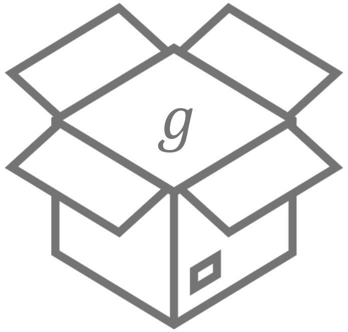
Profit: $\mathbb{E}[\underbrace{\max(f(x), g)}_{\begin{cases} \text{take inside value}, & f(x) > g \\ \text{take outside option}, & f(x) \leq g \end{cases}}] - c(x)$

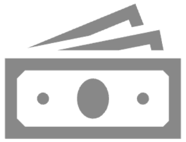
Profit: g

Gittins Index Computation:1.5-Box Problem

$f(x)$ 

vs.



$c(x)$ 

Gittins index

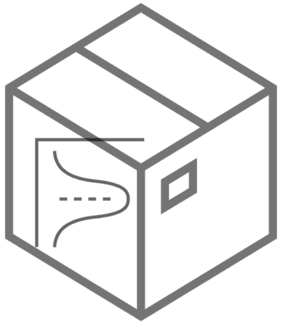
Open closed box $\quad \mathrm{GI}_f(x; c(x)) \quad$ Take opened box $\quad g$

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

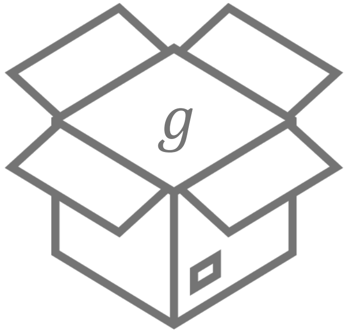
$\mathrm{GI}_f(x; c(x))$: solution g to $\mathbb{E}[\max(f(x), g)] - c(x) = g$

Gittins Index Computation:1.5-Box Problem

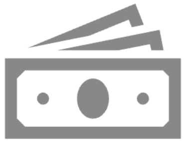
$f(x)$

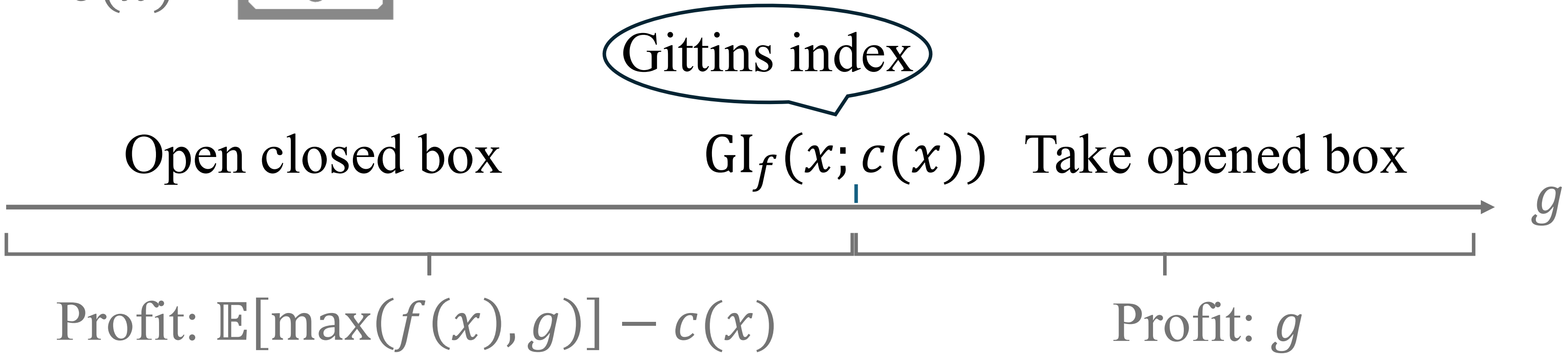


vs.



$c(x)$

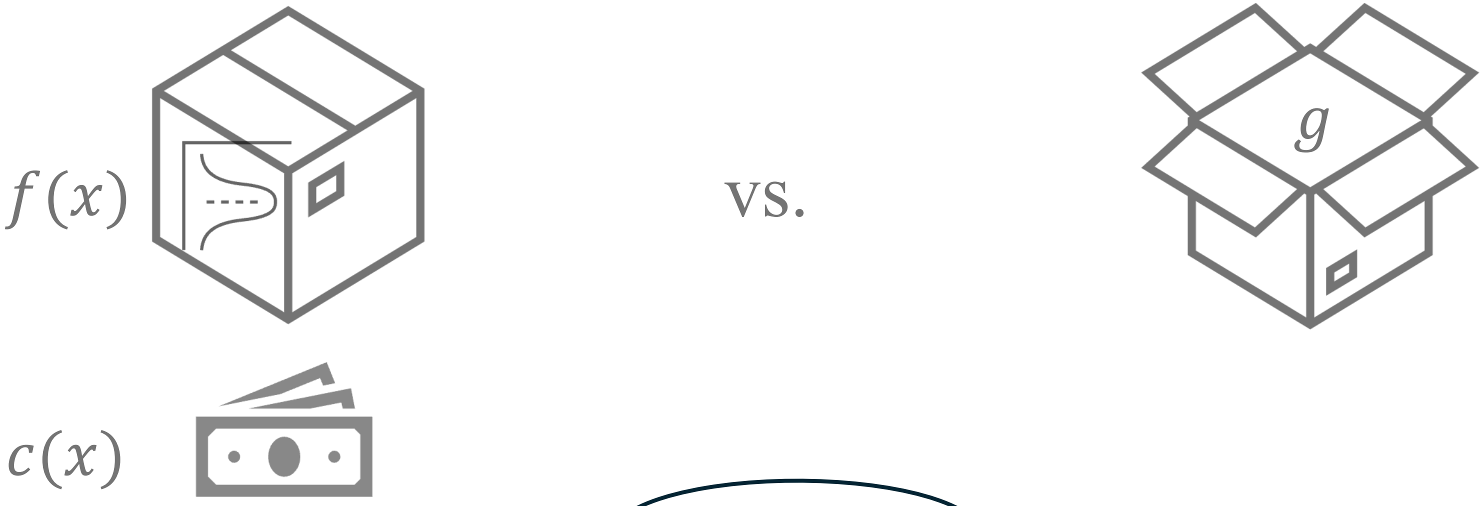


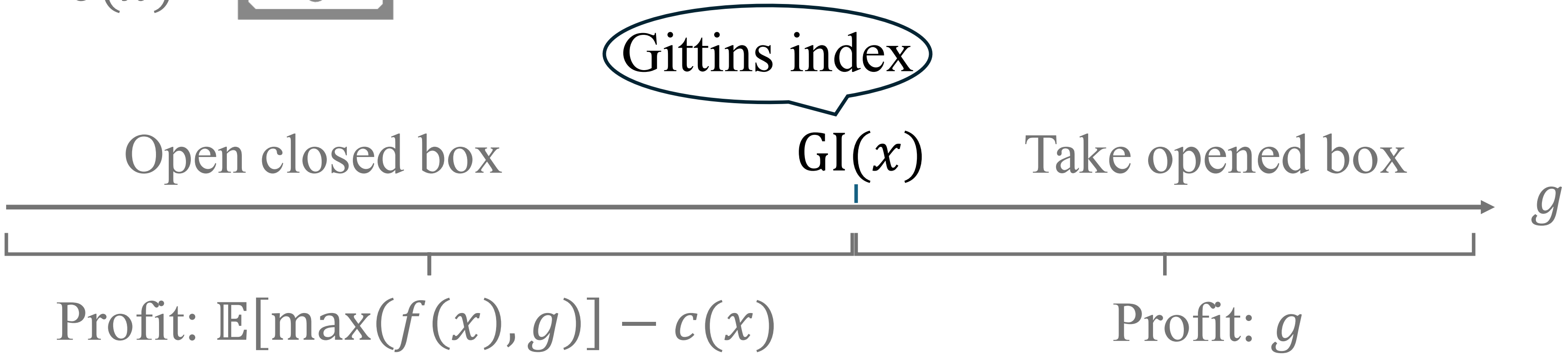


$\mathrm{GI}_f(x; c(x))$: solution g to $\mathbb{E}[\max(f(x), g)] - c(x) = g$

Larger the cost, smaller the Gittins index

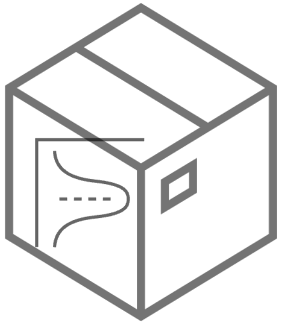
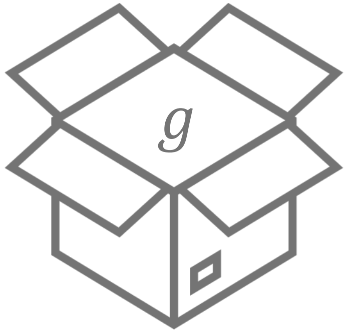
Gittins Index Computation:1.5-Box Problem

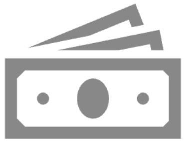




$\mathrm{GI}_f(x; c(x))$: solution g to $\underbrace{\mathbb{E}[\max(f(x), g)] - c(x) = g}_{\mathbb{E}[\max(f(x) - g, 0)] = c(x)}$

Gittins Index Computation: 1.5-Box Problem

$f(x)$  vs. 

$c(x)$ 

Gittins index

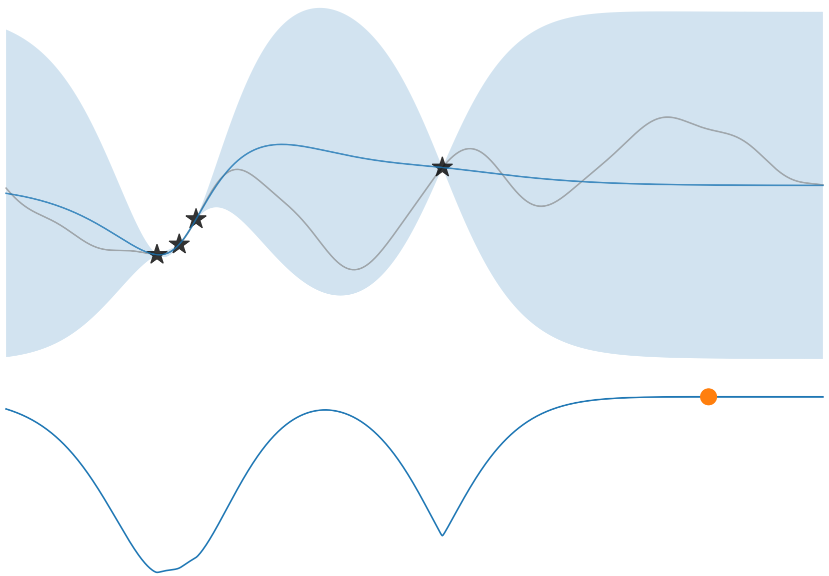
Open closed box | $\mathrm{GI}(x)$ | Take opened box → g

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

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

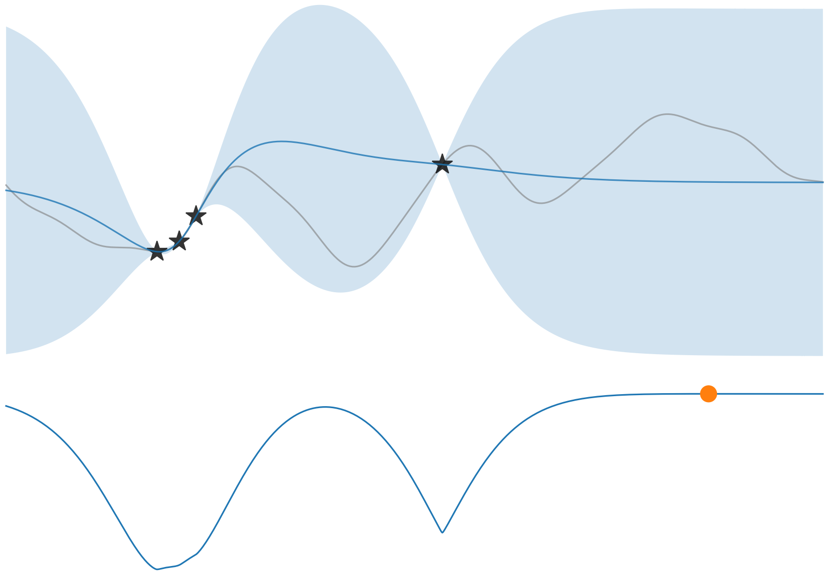
$\mathrm{EI}_f(x; g)$

Gittins Index



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

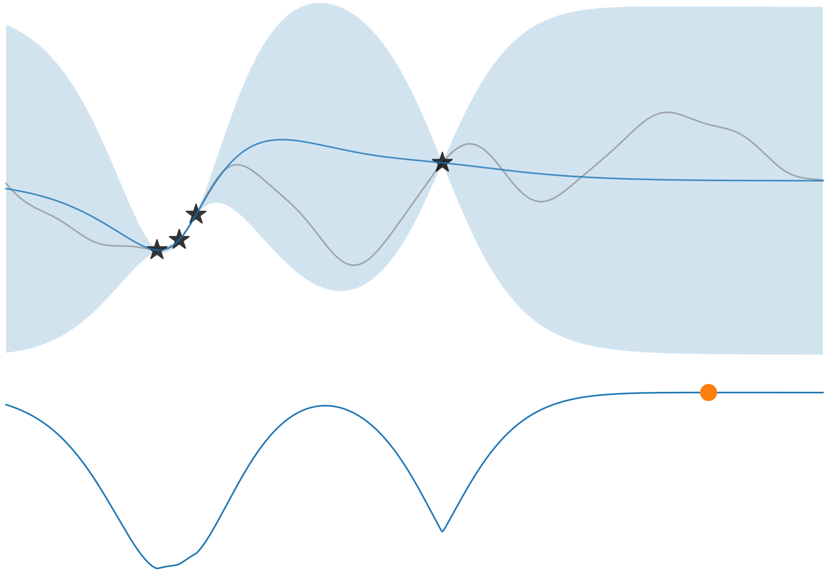
Gittins Index



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

Gaussian distribution

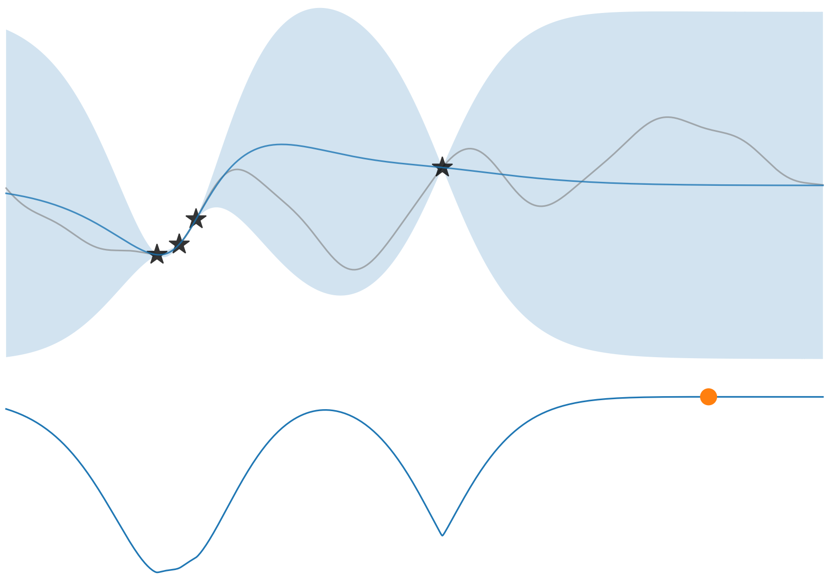
Gittins Index



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

Gaussian distribution

Gittins Index

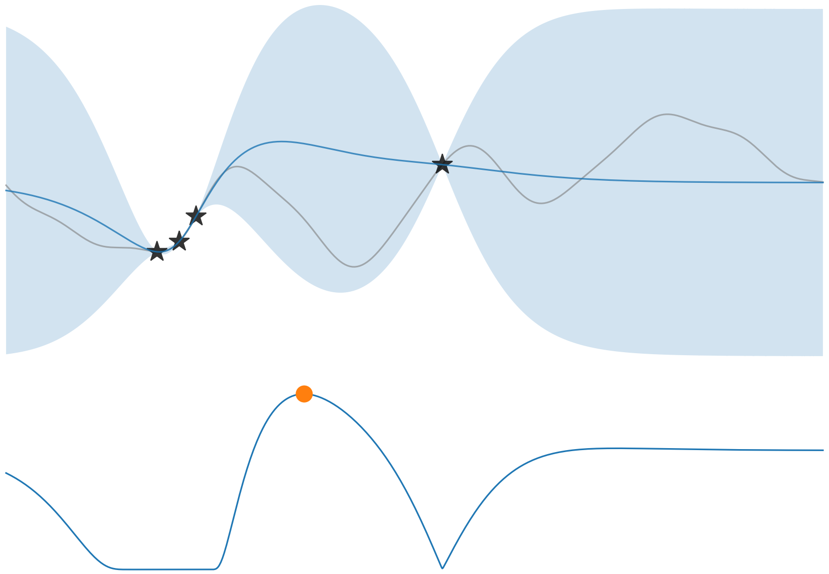


$$\mathrm{EI}_{f|D}(x;g) := \underbrace{\mathbb{E}[\max(f(x) - g, 0) \mid D]}_{\text{analytical expression}} \qquad \mathrm{GI}_{f|D}(x) = g \text{ s.t. } \mathrm{EI}_{f|D}(x;g) = \lambda c(x)$$

Gaussian distribution

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

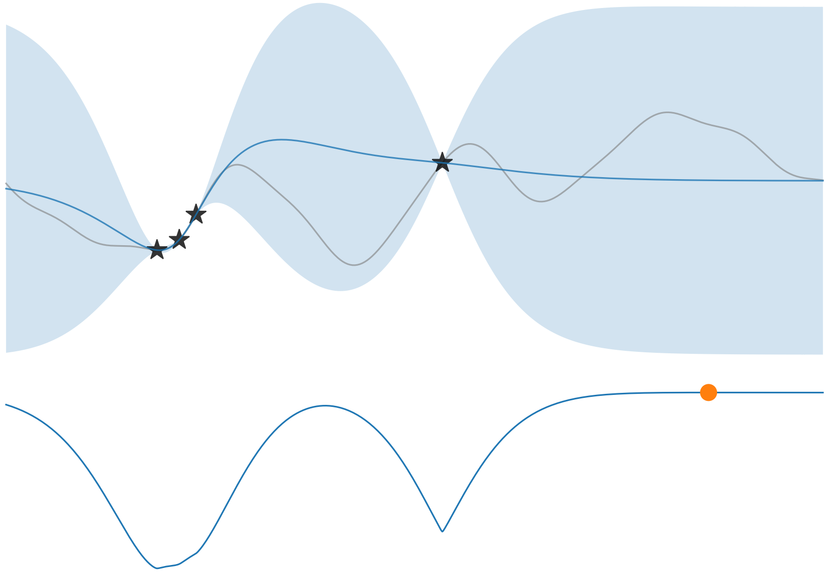
Expected Improvement



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

$$\max_x \mathrm{EI}_{f|D}(x; y_{\mathrm{best}})$$

Gittins Index



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

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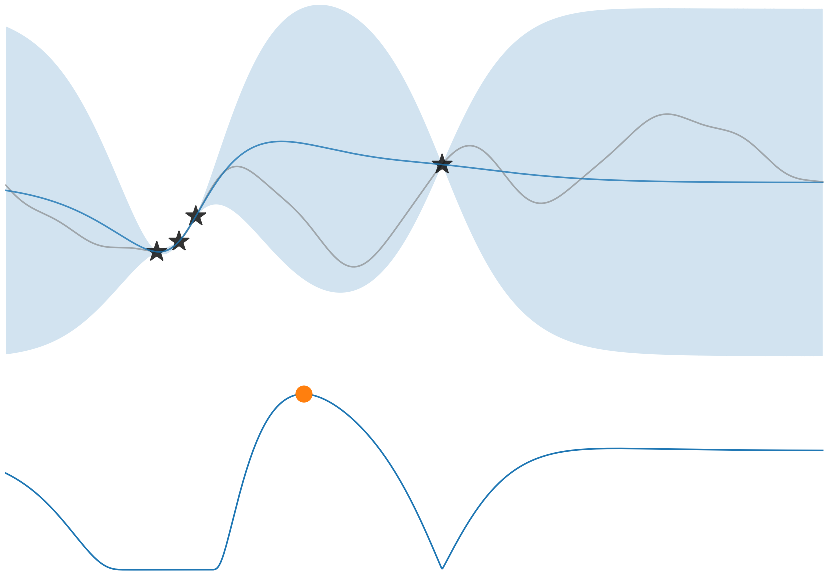
Expected Improvement



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

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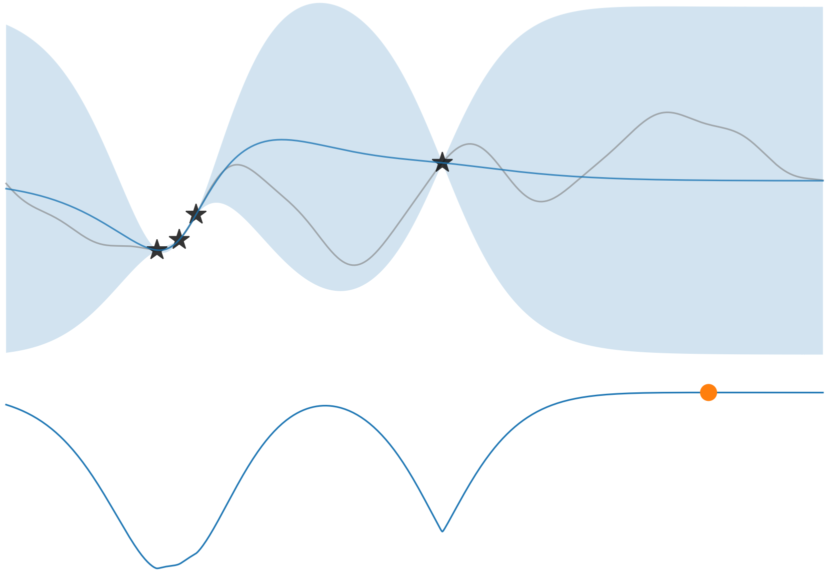
Cost-unaware

Gittins Index



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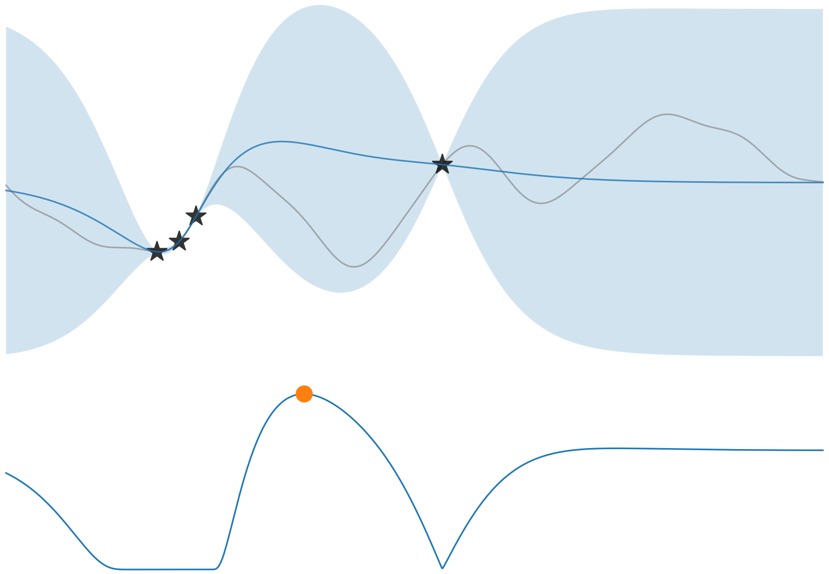
Cost-aware

Expected Improvement



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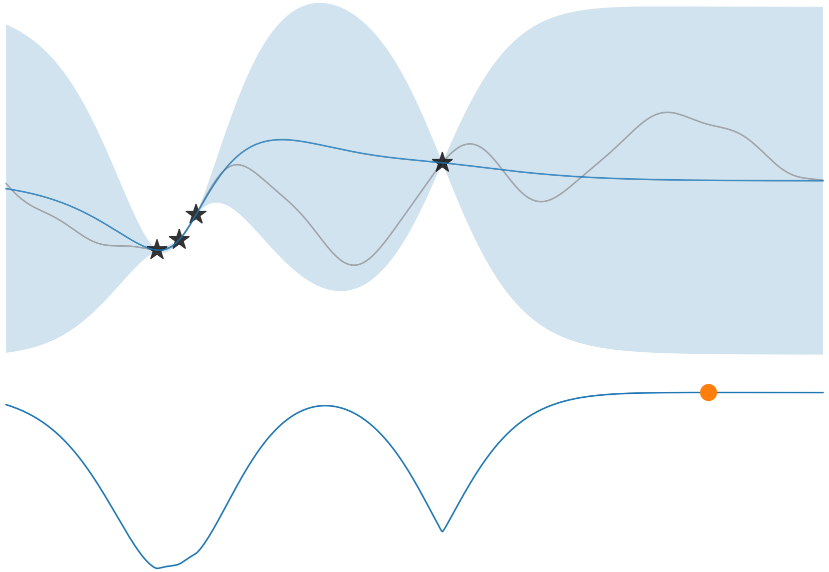
Cost-unaware

One-step approximation to MDP

Gittins Index



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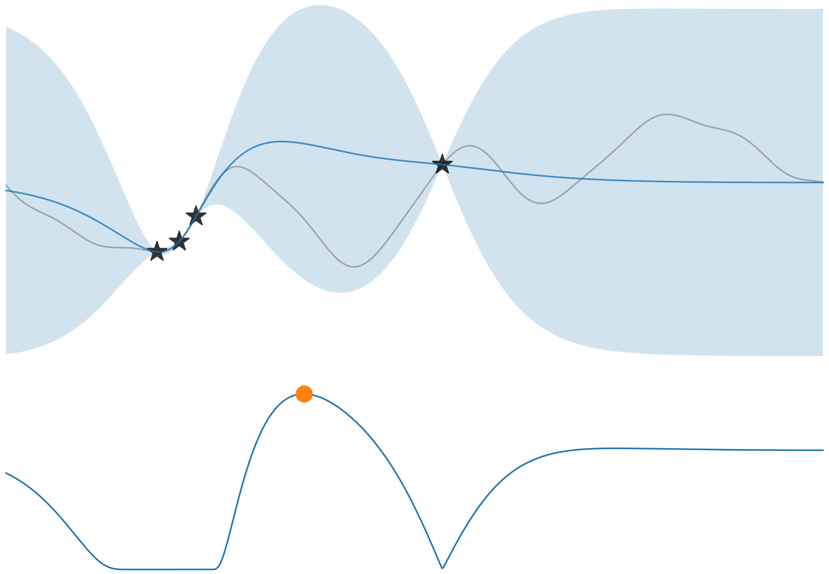
$$\max_x \mathrm{GI}_{f|D}(x; \lambda c(x))$$

Cost-aware

Anytime-lookahead

Expected Improvement



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

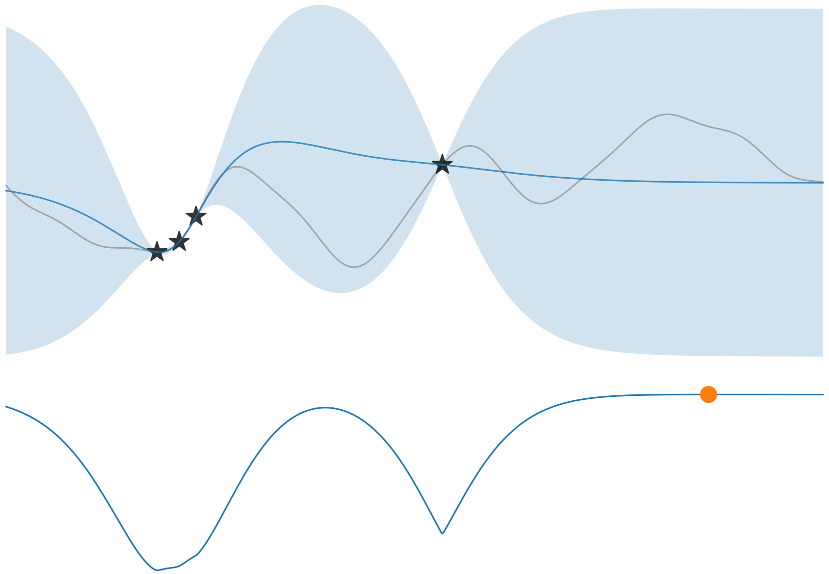
$\max_x \mathrm{EI}_{f|D}(x; y_{\mathrm{best}})$

Cost-unaware

One-step approximation to MDP

Temporal simplification to MDP

Gittins Index



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

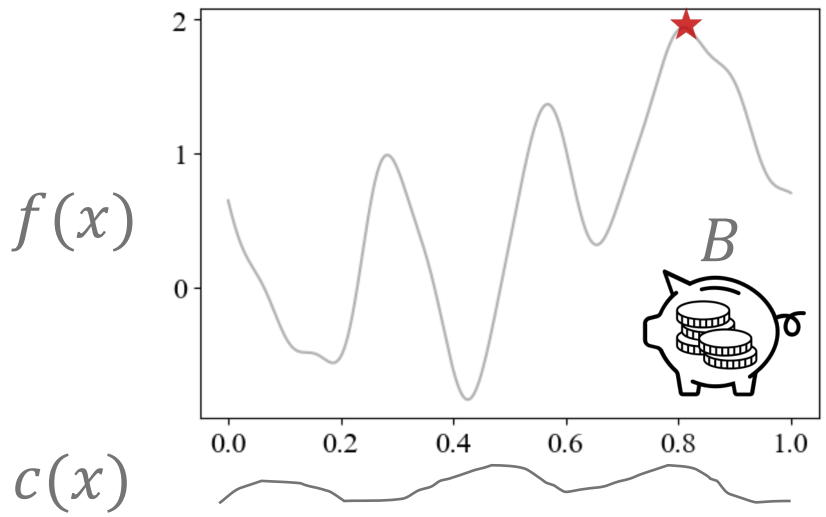
$\max_x \mathrm{GI}_{f|D}(x; \lambda c(x))$

Cost-aware

Anytime-lookahead

Spatial simplification to MDP

Cost-aware Bayesian Optimization

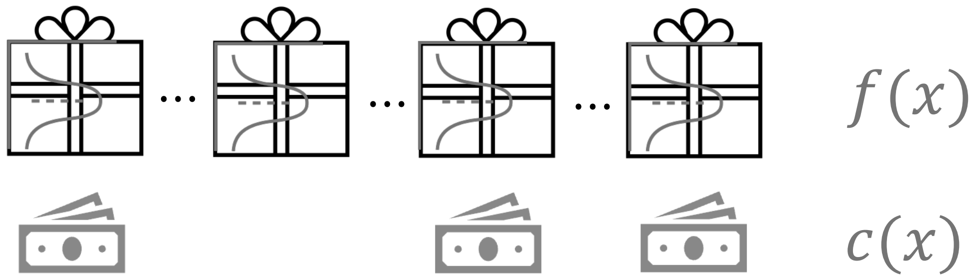


Continuous

Correlated

Expected-budget-constrained

Pandora's Box



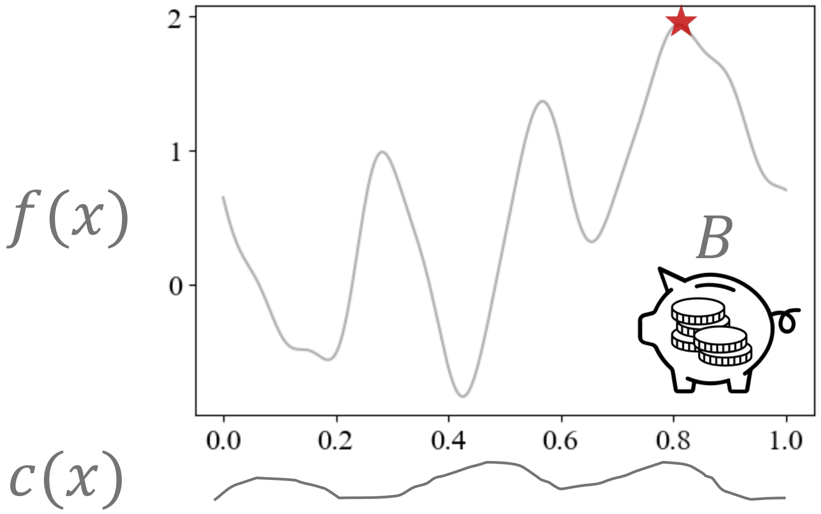
Discrete

Independent

Cost-per-sample

Is Gittins index good? $\xLeftarrow[\text{scale costs}]{\text{incorporate posterior}}$ Gittins index is optimal

Cost-aware Bayesian Optimization



Continuous

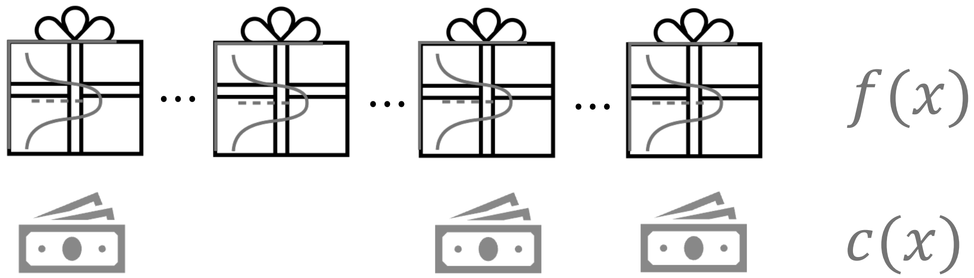
Correlated

Expected-budget-constrained

Is Gittins index empirically good?

this work

Pandora's Box



Discrete

Independent

Cost-per-sample

Gittins index is optimal

Experiment Setup: Objective Functions

Samples from prior

Synthetic

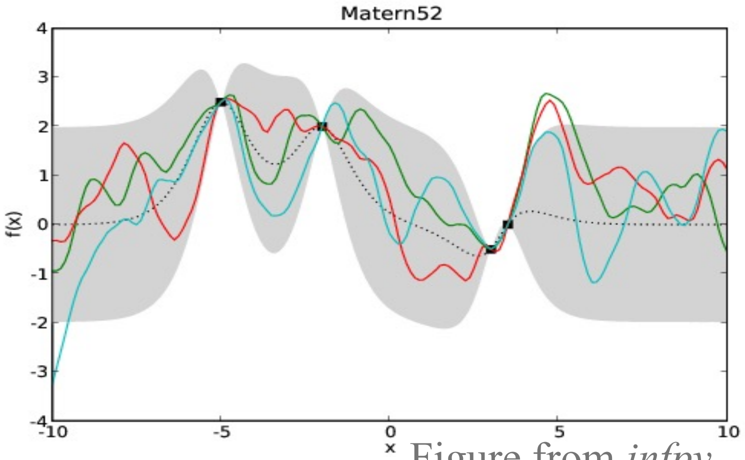


Figure from *infpy*

Ackley function

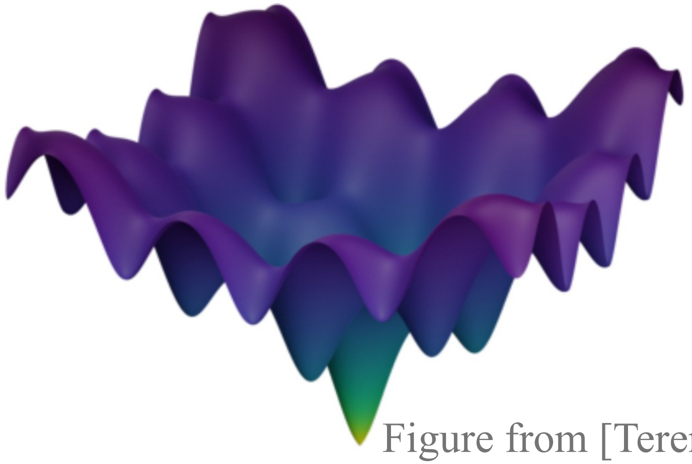


Figure from [Terenin'22]

Pest Control

Empirical

Figure from ChatGPT

Lunar Lander

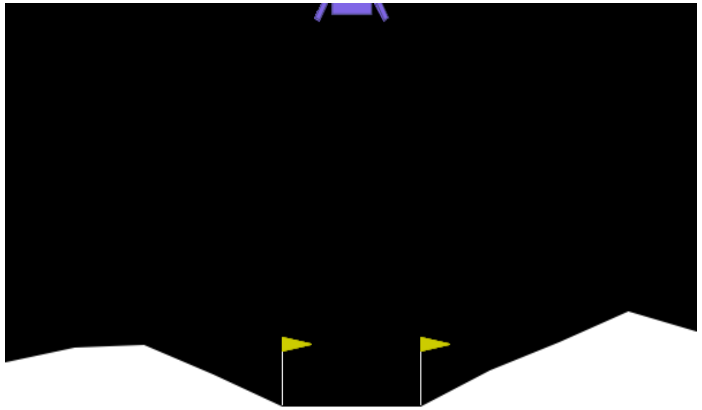
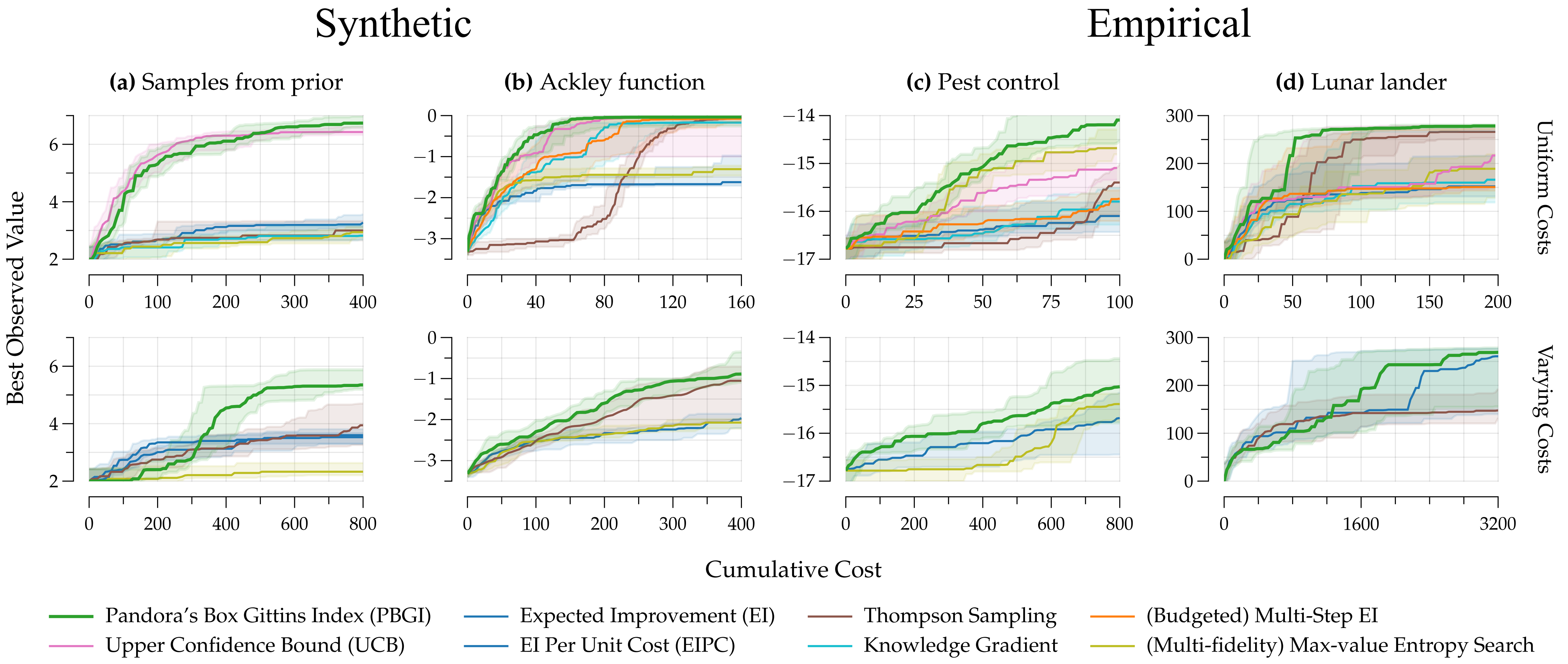
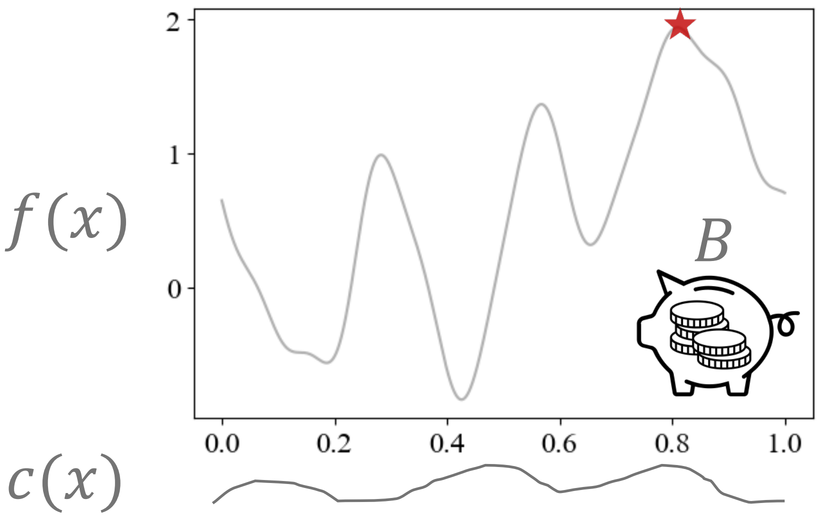


Figure from OpenAI Gym

Experiment Results: PBGI vs Baselines



Cost-aware Bayesian Optimization



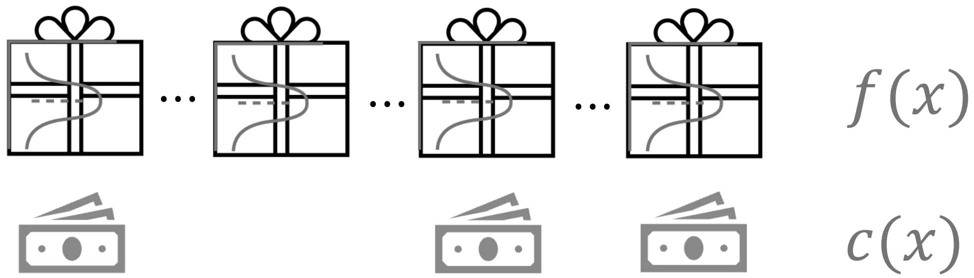
Continuous

Correlated

Expected-budget-constrained

Is Gittins index theoretically good?

Pandora's Box



Discrete

Independent

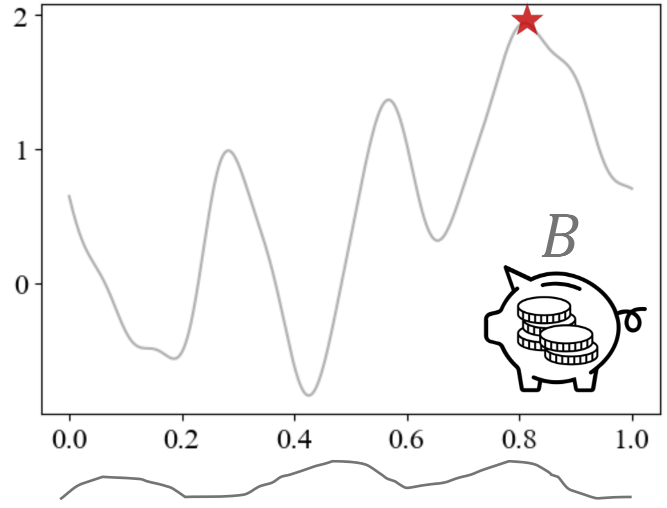
Cost-per-sample

Gittins index is optimal

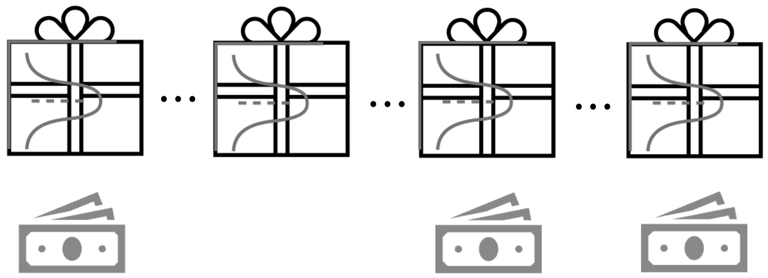
Cost-aware Bayesian Optimization

Pandora's Box

$f(x)$



$c(x)$



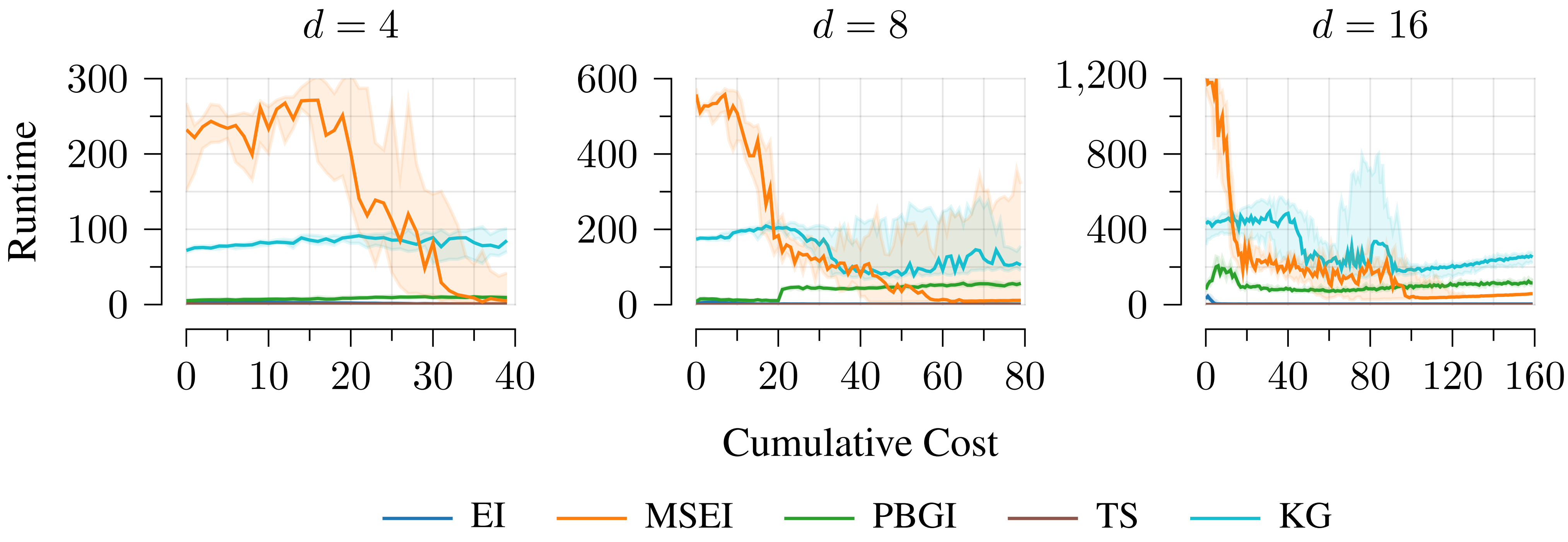
$f(x)$

$c(x)$

Cost-aware Bayesian Optimization	Pandora's Box
Continuous	Discrete
Correlated	Independent
Expected-budget-constrained	Cost-per-sample
Is Gittins index theoretically good?	Gittins index is optimal

ongoing work

Timing Experiment



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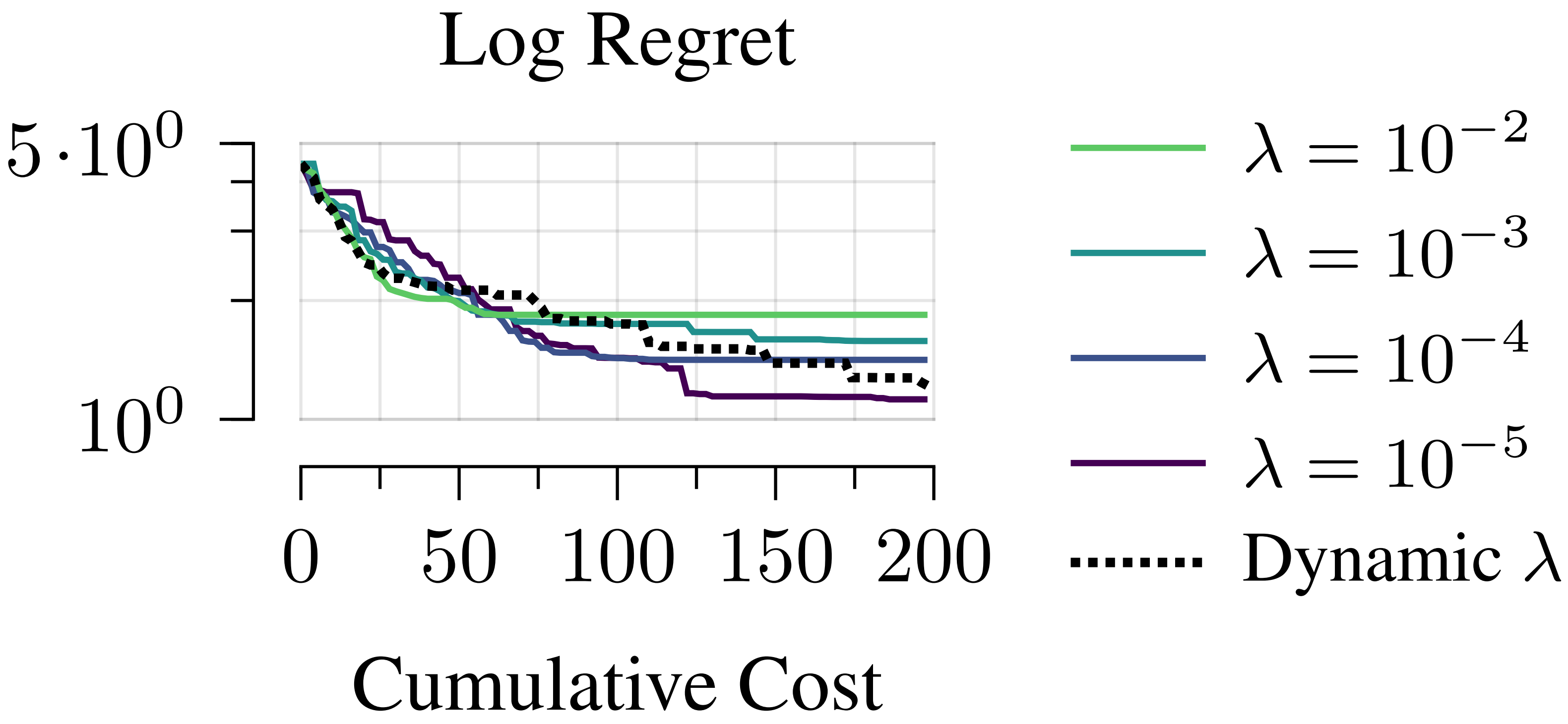
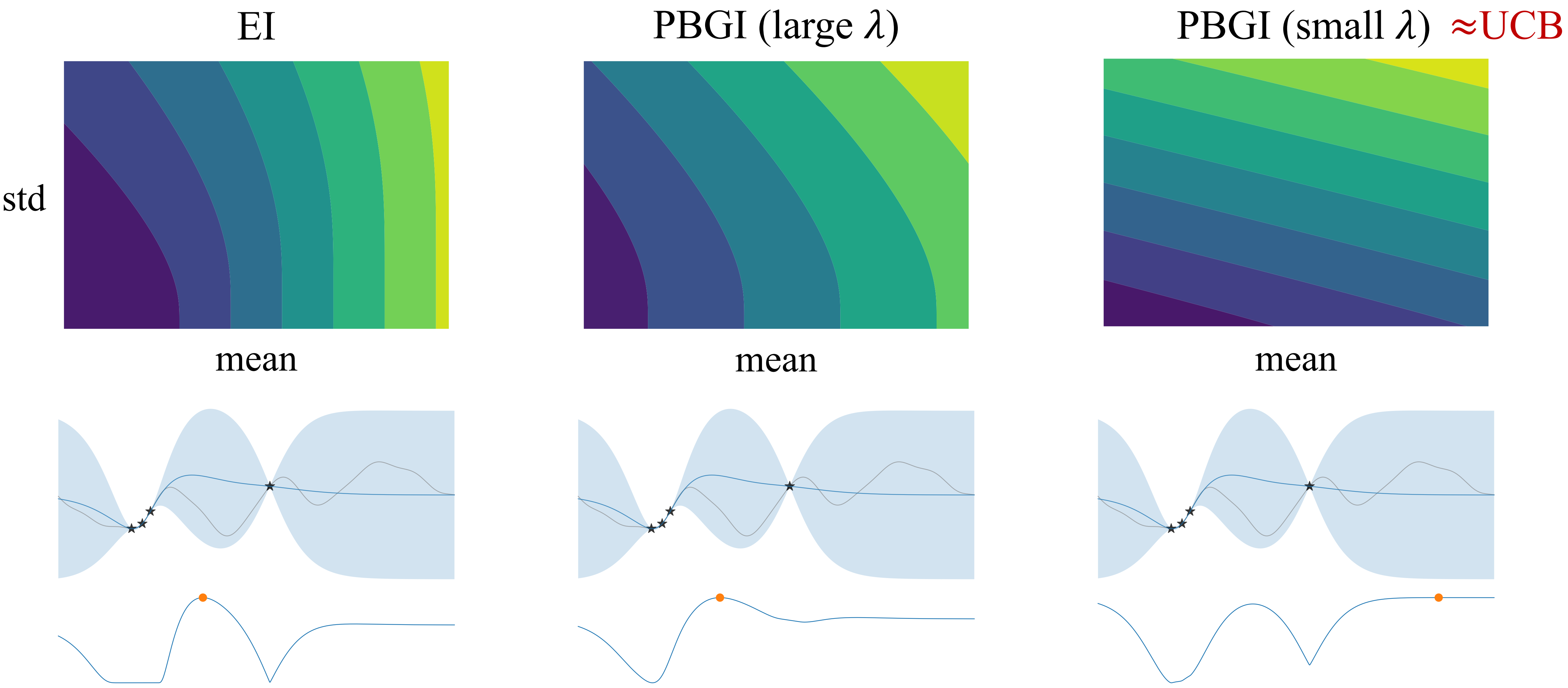
PBGI is easy to compute using EI + bisection search!

Effect of λ



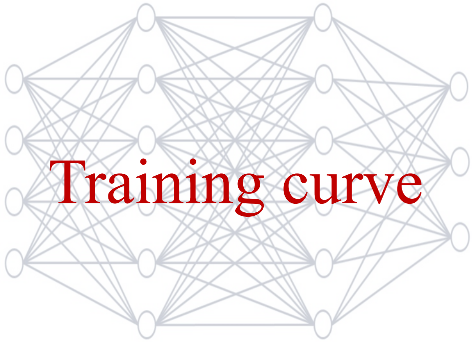
Larger budget, smaller λ, higher exploration

EI vs PBGI


EI
PBGI (large λ)
PBGI (small λ)
≈UCB
std
mean
mean
mean

Part II: Observable Partial Feedback

Hyperparameter tuning:



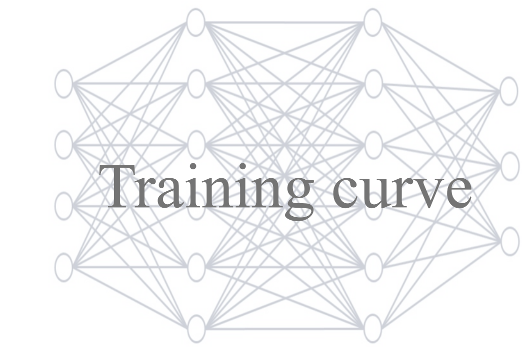
Training parameters → Training curve → Accuracy

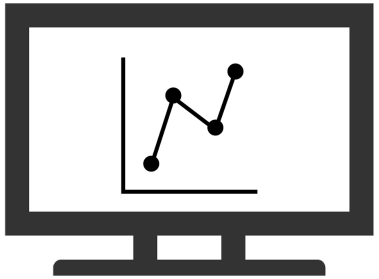
Plasma physics:

Reactor parameters → Convergence curve → Stability

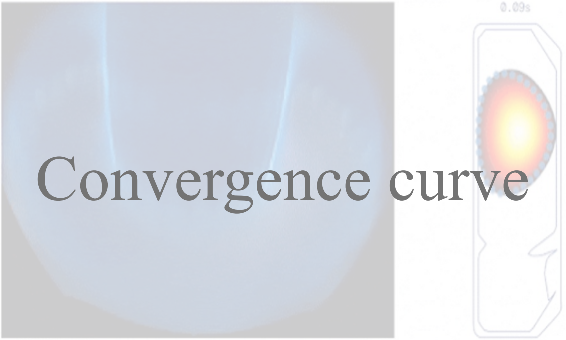
Practical Factor: Observable Partial Feedback

Hyperparameter tuning:

Training parameters ⟶  Training curve ⟶ Accuracy

Input parameters ⟶  ⟶ Performance metric

Plasma physics:

Reactor parameters ⟶  Convergence curve ⟶ Stability

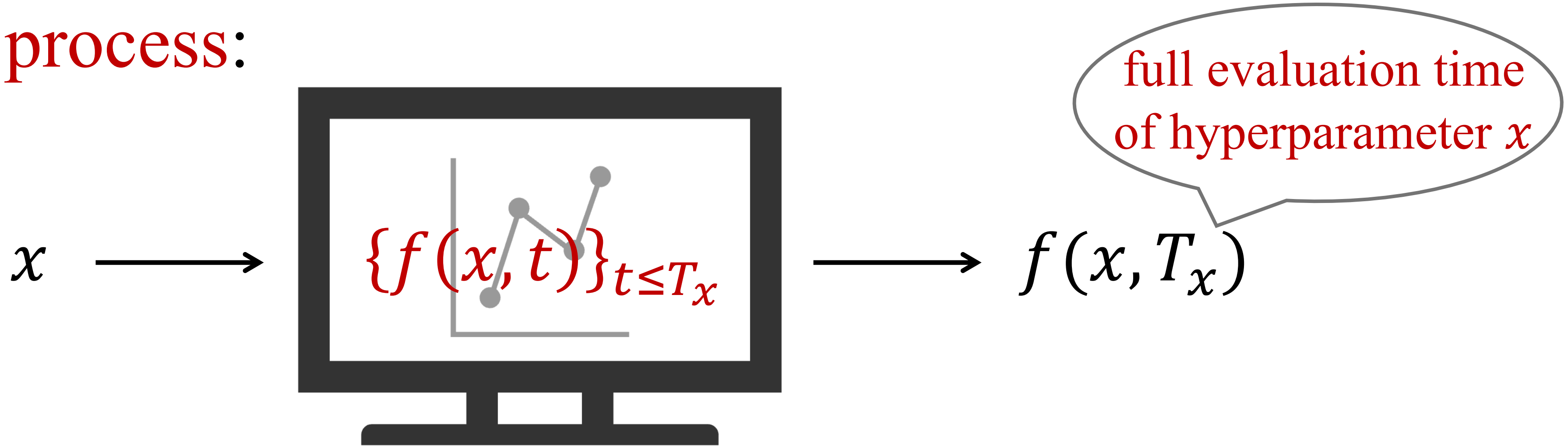
Practical Factor: Observable Partial Feedback

Input parameters → 

→ Performance metric

Practical Factor: Observable Partial Feedback

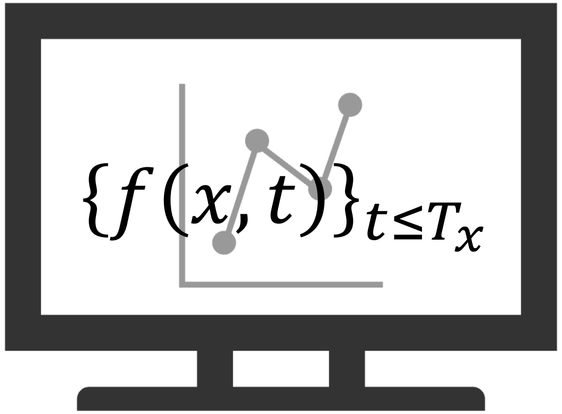
Black-box process:



Optimizing Black-box Processes

Black-box process:

full evaluation time of hyperparameter x



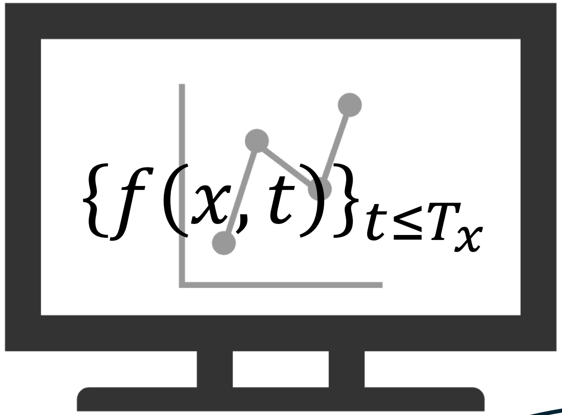
$$x \longrightarrow \{f(x,t)\}_{t \le T_x} \longrightarrow f(x, T_x)$$

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

Optimizing Black-box Processes

Black-box process:

full evaluation time of hyperparameter x

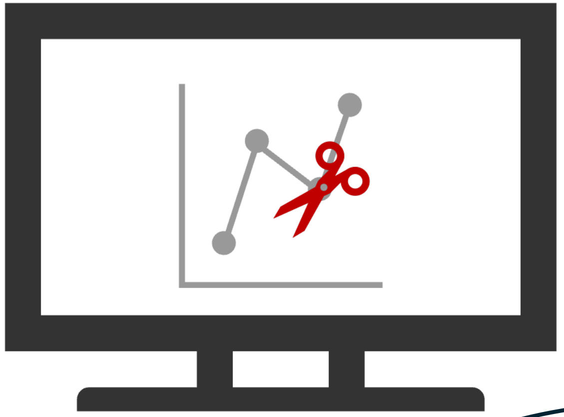
$x \longrightarrow$  $\longrightarrow f(x, T_x)$

expensive-to-evaluate

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

Freeze-thaw Bayesian Optimization

[Swersky, Snoek, Adams'14]

$x \longrightarrow$  $\longrightarrow f(x, T_x)$

full evaluation time of hyperparameter x

expensive-to-evaluate

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

Allow pauses and resumes of hyperparameter tests

Freeze-thaw Bayesian Optimization

[Swersky, Snoek, Adams'14]

full evaluation time
of hyperparameter x

$x \longrightarrow$  $\longrightarrow f(x, T_x)$

Goal: $\mathbf{sup}_{\text{policy}}\ \mathbb{E} \max_{\text{completed } x \in \mathcal{X}} f(x, T_x)$

s.t. total evaluation time within budget

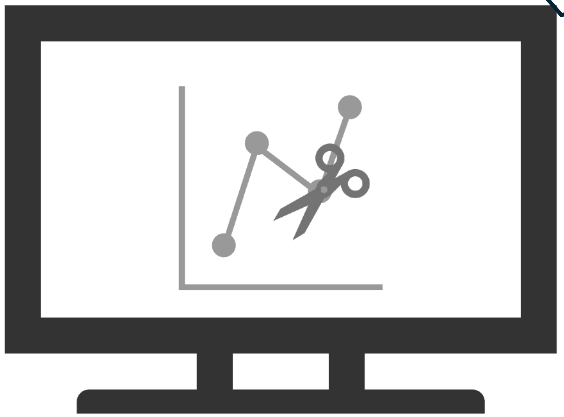
Allow pauses and resumes of hyperparameter tests

Freeze-thaw Bayesian Optimization

[Swersky, Snoek, Adams'14]

~Temporal GP

full evaluation time
of hyperparameter x

$x \longrightarrow$  $\longrightarrow f(x, T_x)$

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Allow pauses and resumes of hyperparameter tests

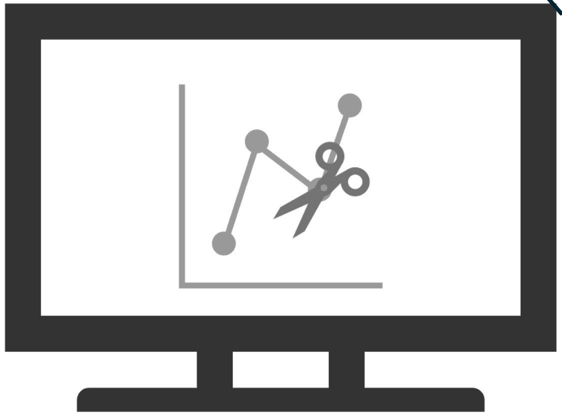
Freeze-thaw Bayesian Optimization

[Swersky, Snoek, Adams'14]

entropy-based

~Temporal GP

full evaluation time of hyperparameter x

$x \longrightarrow$  $\longrightarrow f(x, T_x)$

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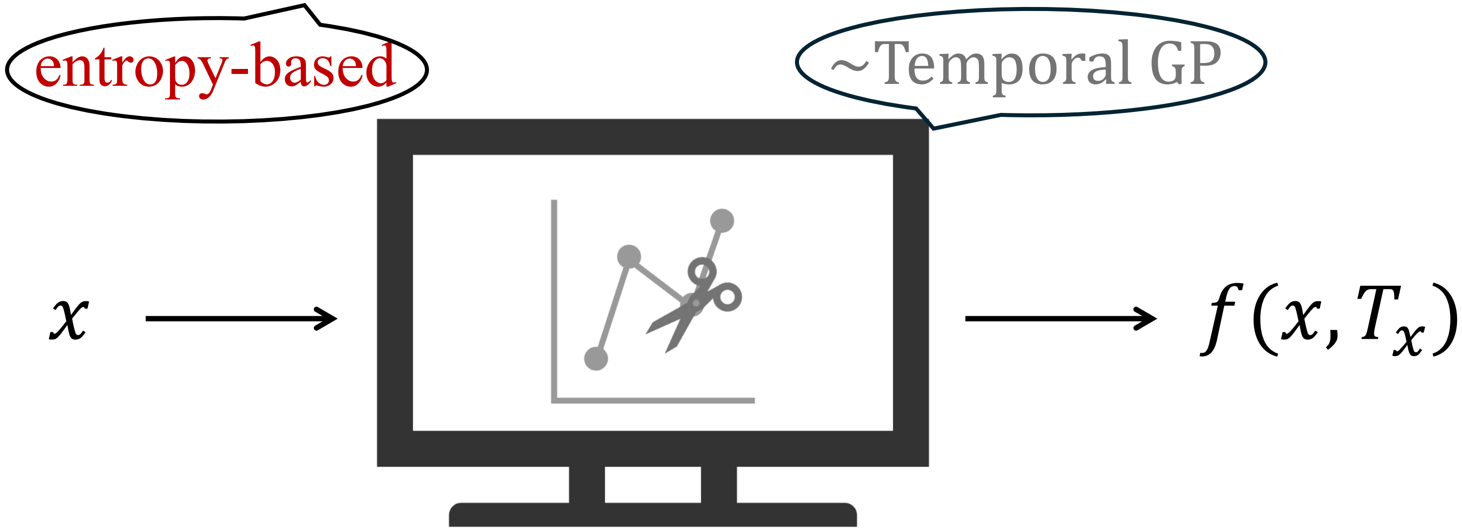
s.t. total evaluation time within budget

Allow pauses and resumes of hyperparameter tests

Freeze-thaw Bayesian Optimization

[Swersky, Snoek, Adams'14]



Our view: lack of a guidance to incorporate partial feedback

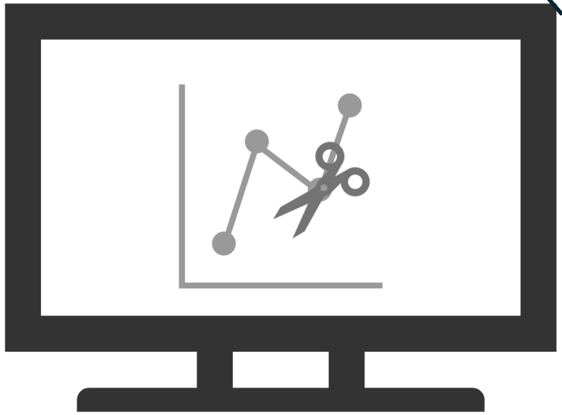
Freeze-thaw Bayesian Optimization

[Swersky, Snoek, Adams’14]

entropy-based

~Temporal GP

$x \longrightarrow$



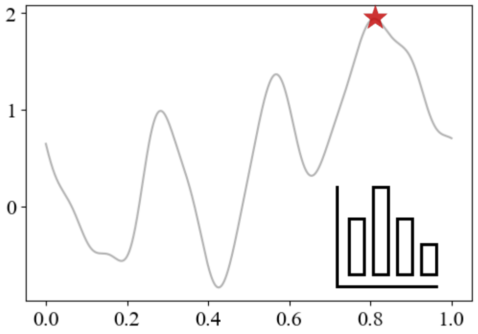
$\longrightarrow f(x, T_x)$

New design principle: Gittins Index

inherently feedback-aware

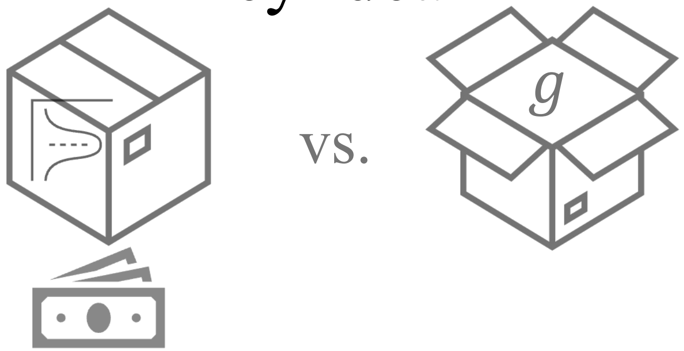
New Design Principle: Gittins Index

Studied Problem



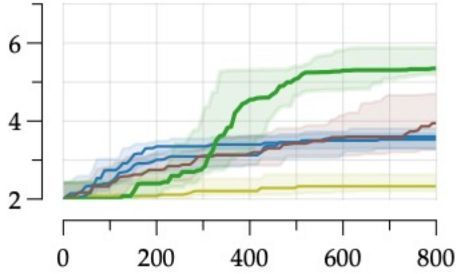
Cost-aware Bayesian optimization for
black-box function with varying costs

Key idea



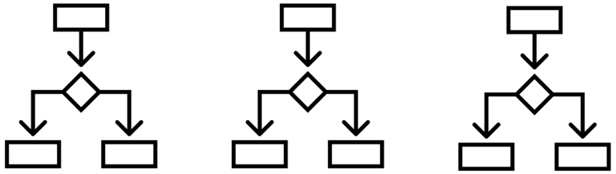
Link to Pandora’s box
and Gittins index theory

Impact



Competitive empirical performance

Ongoing work



Freeze-thaw Bayesian optimization for
black-box process with partial feedback

Find our paper on ArXiv!

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