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

Qian Xie (Cornell ORIE)

Joint work with Raul Astudillo, Peter Frazier, Ziv Scully, and Alexander Terenin

ECGI'24

**Goal:** optimize expensive-to-evaluate black-box function

∈ decision-making under uncertainty

#### **Applications:**

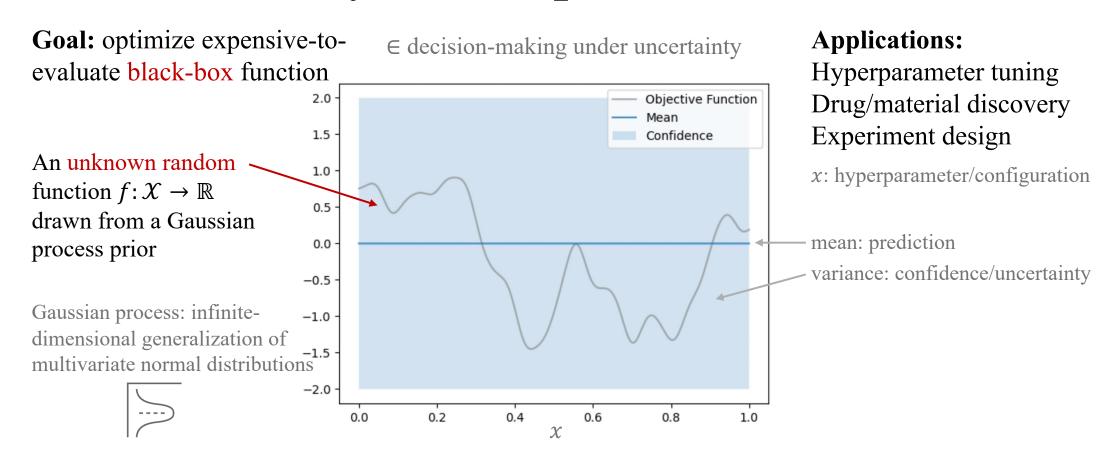
Hyperparameter tuning
Drug/material discovery
Experiment design

**Goal:** optimize expensive-to-evaluate black-box function

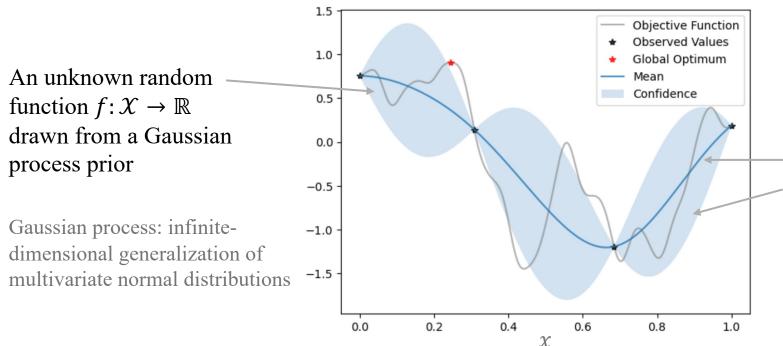
∈ decision-making under uncertainty

#### **Applications:**

Hyperparameter tuning
Drug/material discovery
Experiment design



**Goal:** optimize expensive-to-evaluate black-box function



#### **Applications:**

Hyperparameter tuning Drug/material discovery Experiment design

x: hyperparameter/configuration

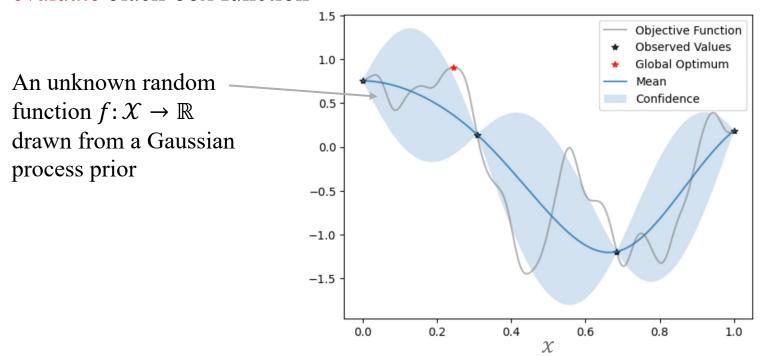
mean: prediction

variance: confidence/uncertainty

**Objective:** find global optimum  $x^* = \operatorname{argmax}_{x \in \mathcal{X}} f(x)$ 

**Decision:** evaluate a set of points

Goal: optimize expensive-toevaluate black-box function



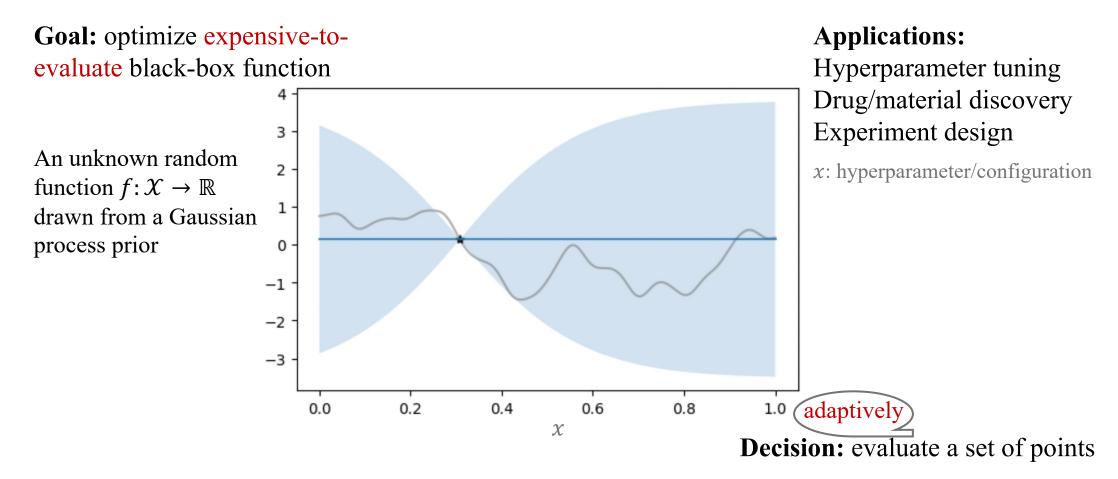
#### **Applications:**

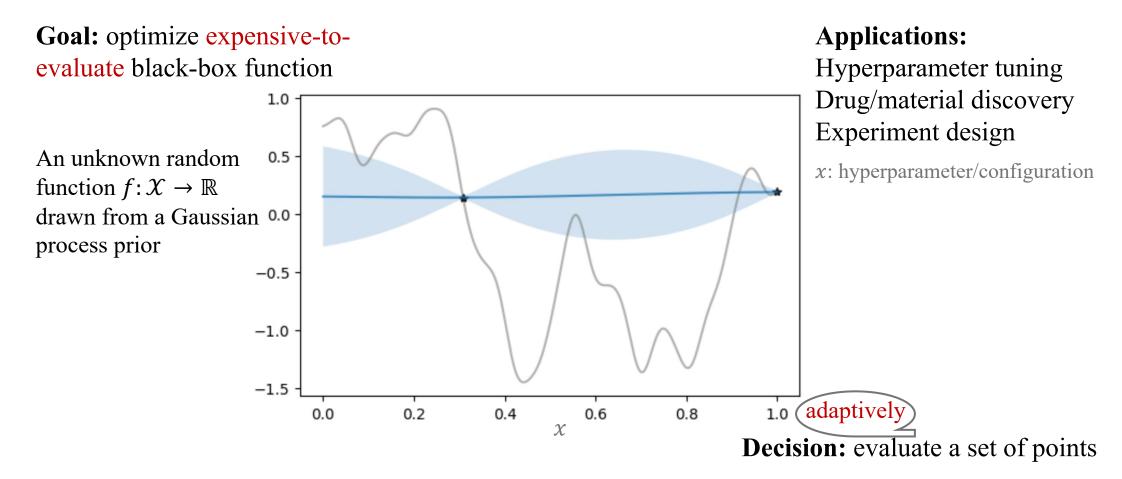
Hyperparameter tuning Drug/material discovery Experiment design

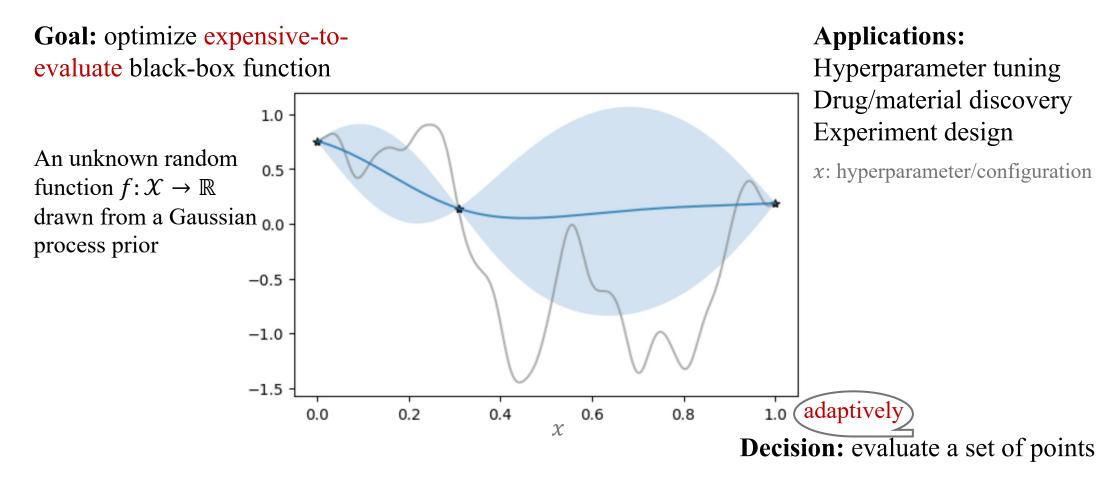
*x*: hyperparameter/configuration

**Objective:** find global optimum  $x^* = \operatorname{argmax}_{x \in \mathcal{X}} f(x)$ 

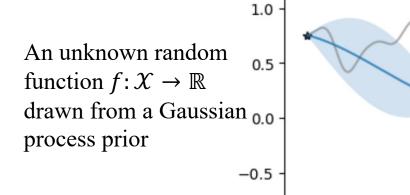
**Decision:** evaluate a set of points







Goal: optimize expensive-toevaluate black-box function



-1.0

-1.5

0.0

0.2

0.4

0.6

0.8



Hyperparameter tuning Drug/material discovery Experiment design

*x*: hyperparameter/configuration

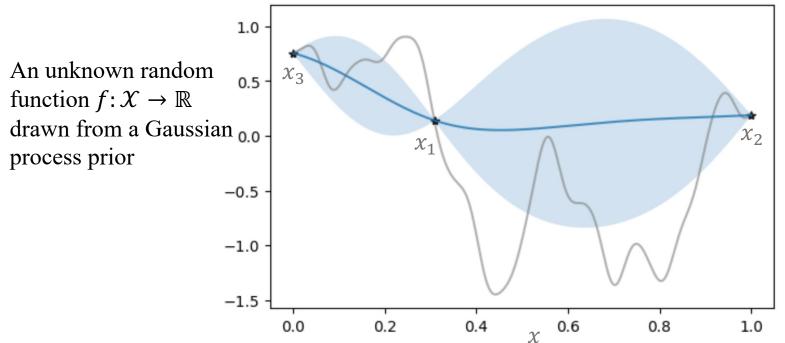
**Decision:** adaptively evaluate a set of points

1.0

$$x_1, x_2, \dots, x_T \in \mathcal{X}$$

*T*: time budget

Goal: optimize expensive-toevaluate black-box function



#### **Applications:**

Hyperparameter tuning Drug/material discovery Experiment design

*x*: hyperparameter/configuration

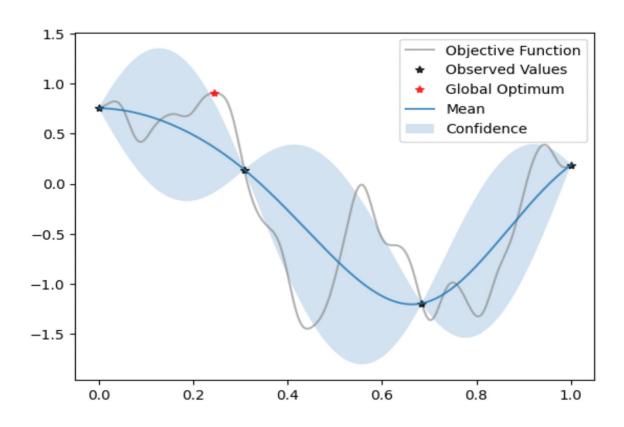
**Objective:** optimize best observed value at time *T* 

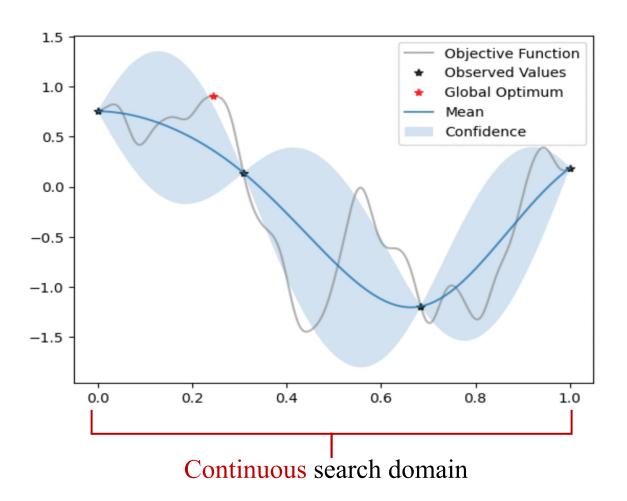
$$\sup_{\text{policy}} \mathbb{E} \max_{t=1,2,\dots,T} f(x_t)$$

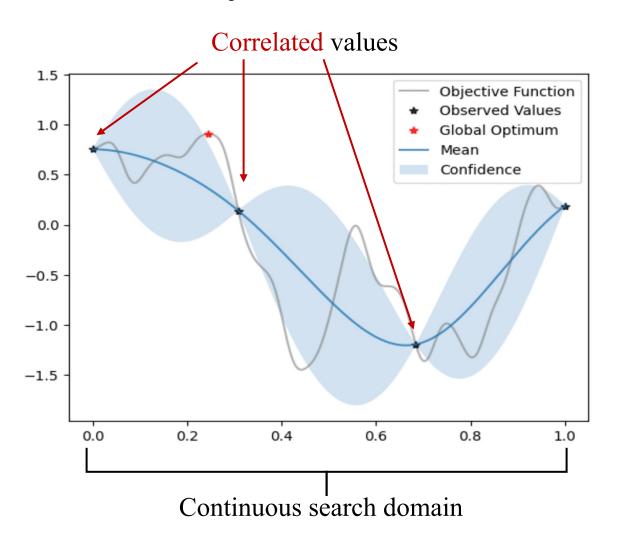
**Decision:** adaptively evaluate a set of points

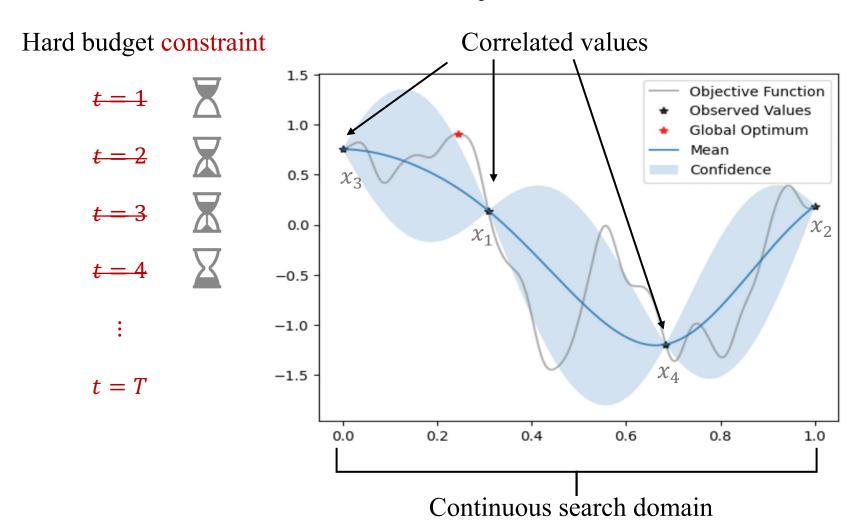
$$x_1, x_2, \dots, x_T \in \mathcal{X}$$

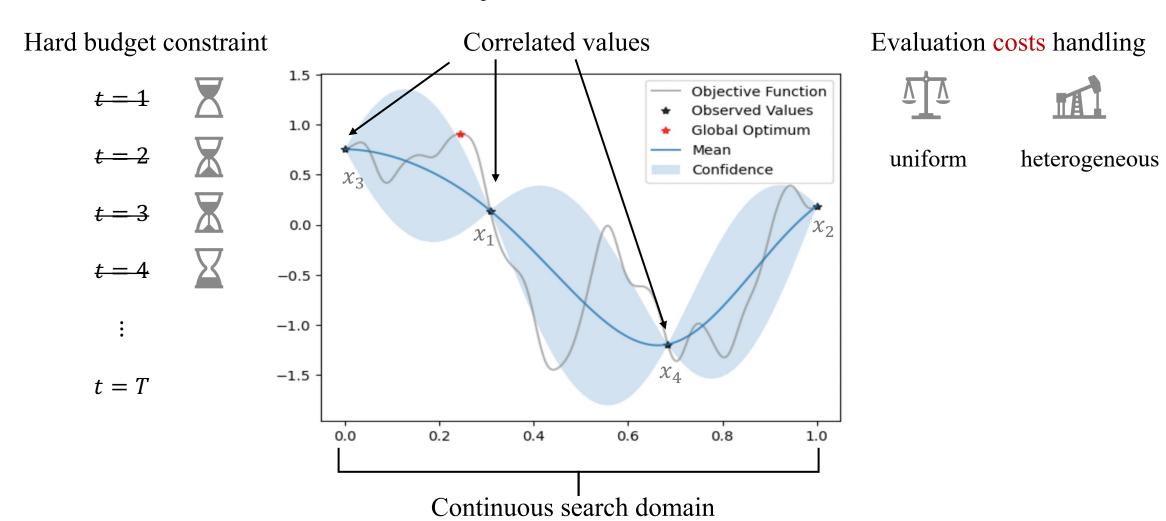
*T*: time budget

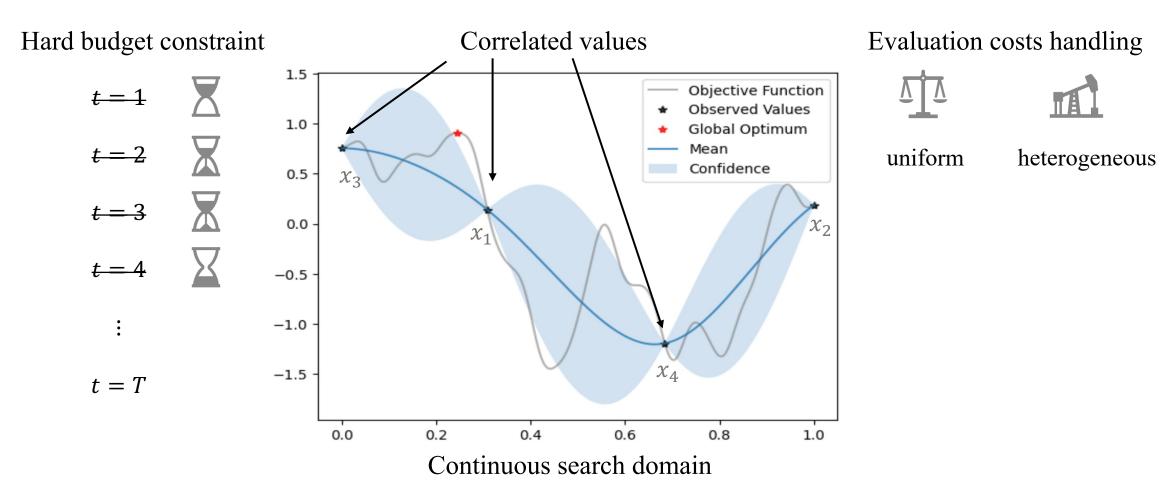




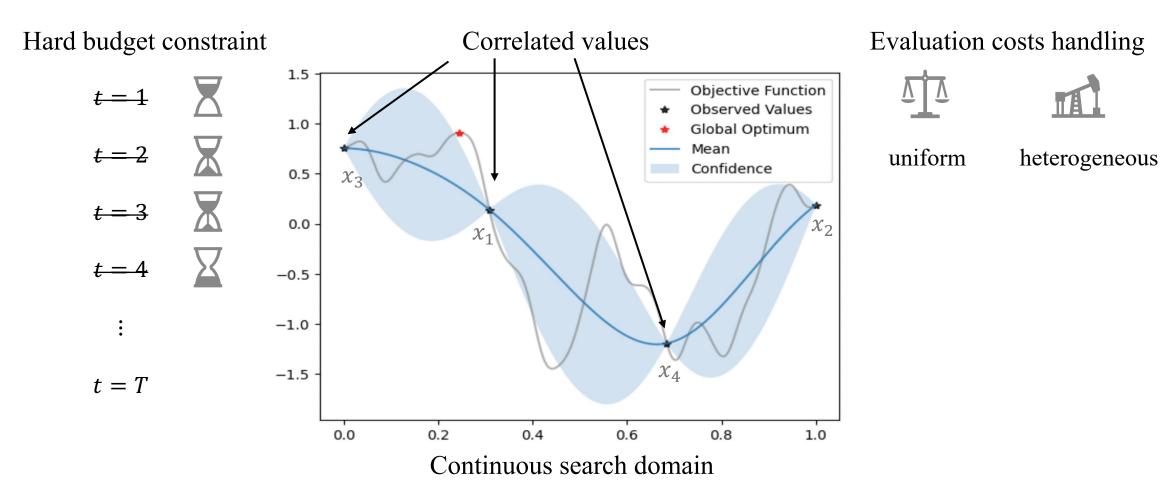




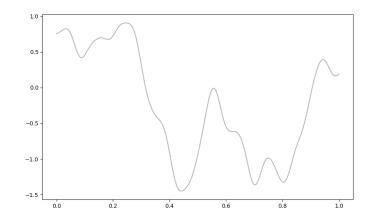




⇒ Optimal policy unknown!



Can we convert it to a solvable problem?

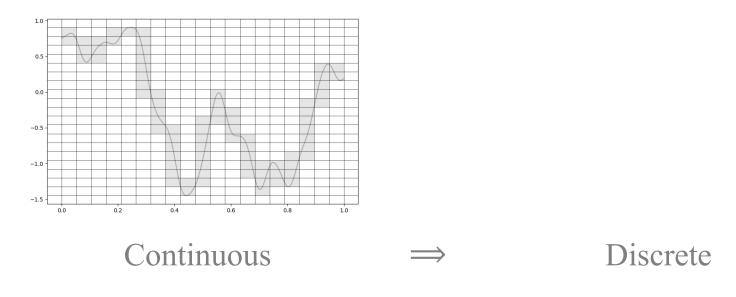


Continuous

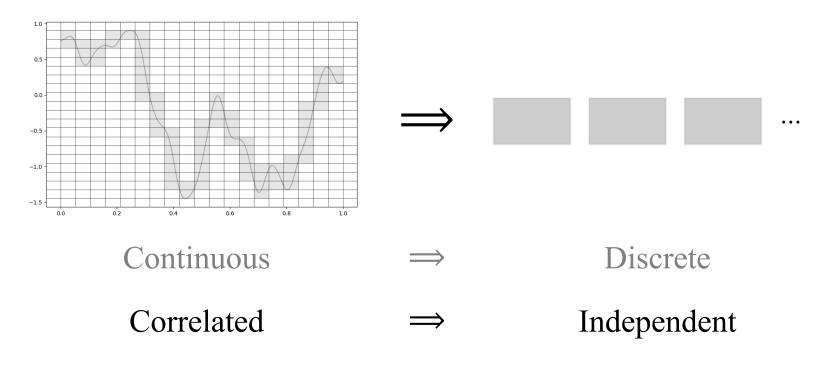
Correlated



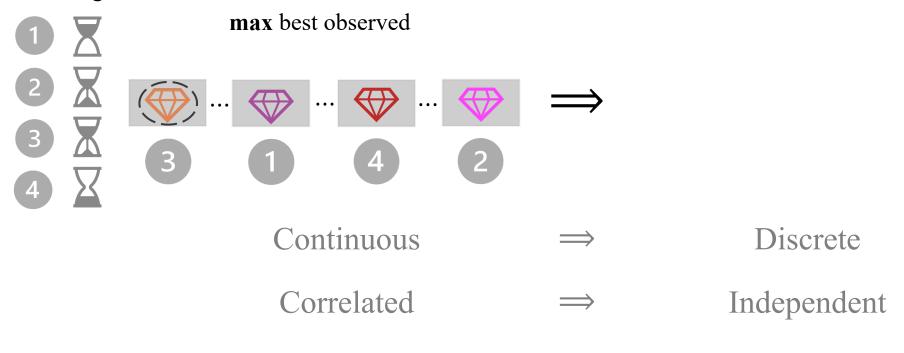
Correlated

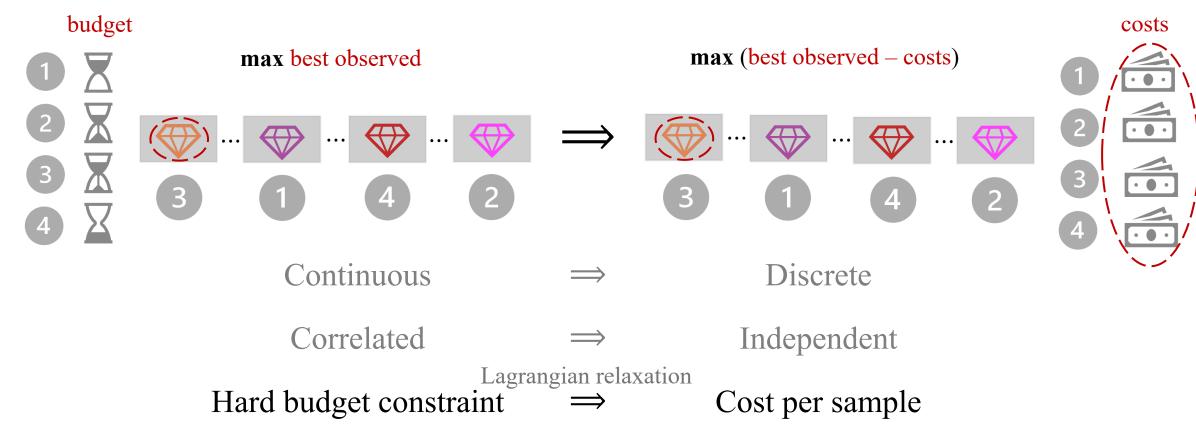


Correlated



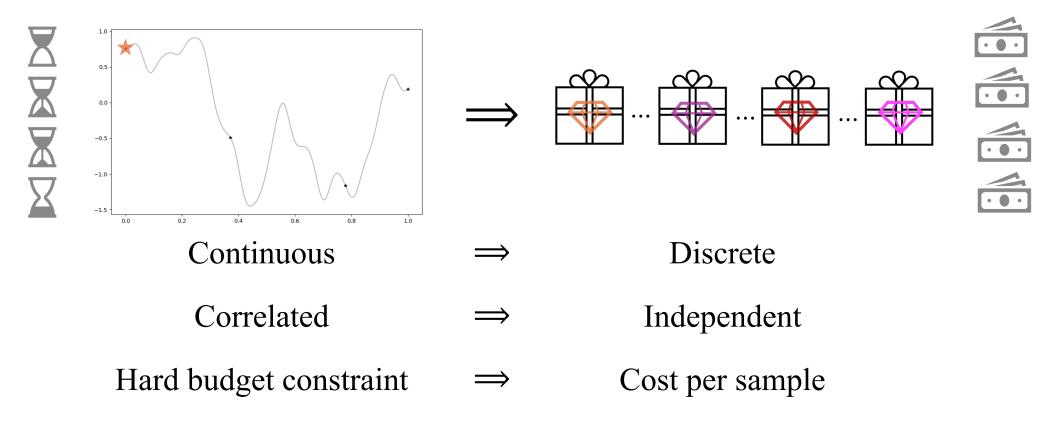
budget



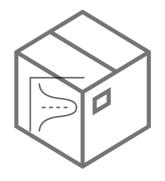


#### Bayesian Optimization ⇒ Pandora's Box

[Weitzman'79]

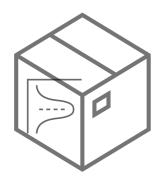


t = 0





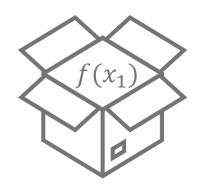




**Objective:** maximize net utility

t = 1







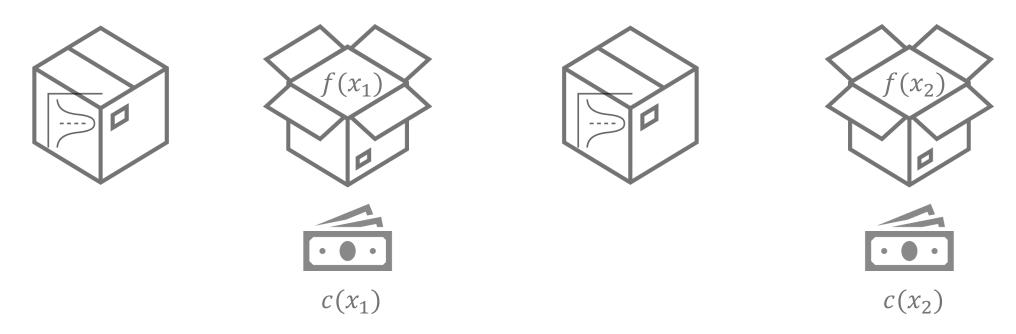




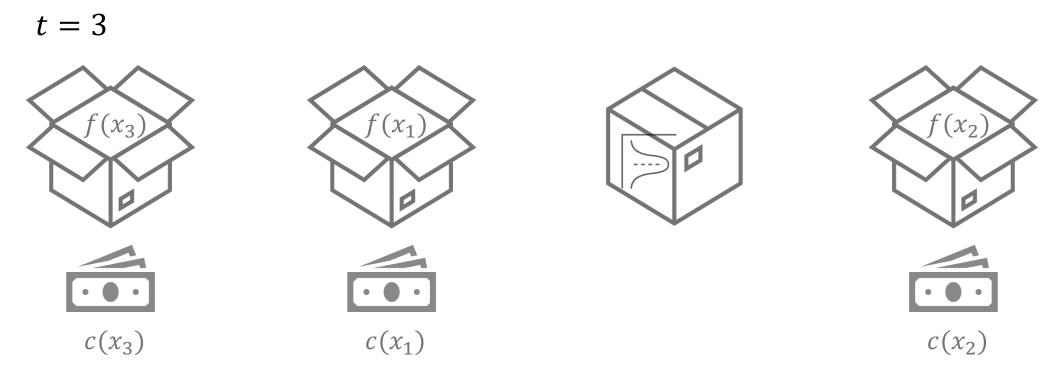
 $c(x_1)$ 

**Objective:** maximize net utility

t = 2

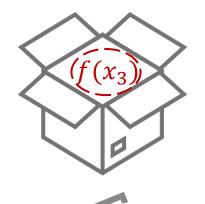


**Objective:** maximize net utility



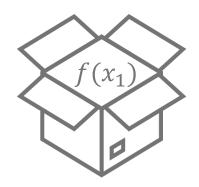
**Objective:** maximize net utility

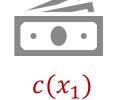




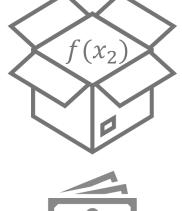














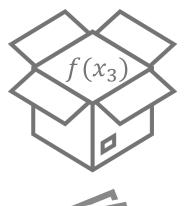
 $c(x_2)$ 

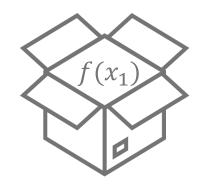
**Objective:** maximize net utility

**Decision:** adaptively evaluate a random number of boxes

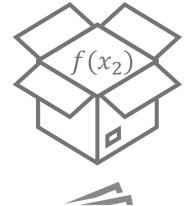
max (best observed value – total costs)

$$t = 3$$









$$c(x_3)$$
  $c(x_1)$ 



$$c(x_2)$$

**Objective:** maximize net utility

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

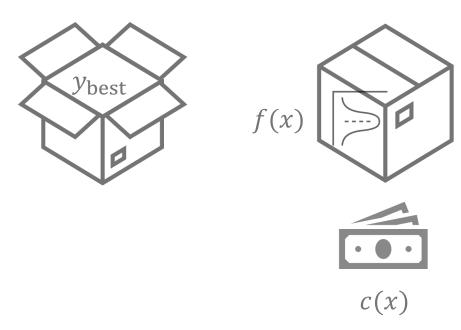
**Decision:** adaptively evaluate a random number of boxes

$$x_1, x_2, \dots, x_T \in \mathcal{X}$$

 $\mathcal{X}$ : discrete

*T*: random stopping time

Naïve Greedy policy



**Inspection rule:**  $\operatorname{argmax}_{x} (\operatorname{EI}_{f}(x; y_{\operatorname{best}}) - c(x))$ 

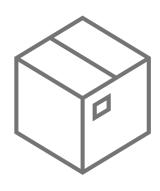
**Stopping rule:**  $\text{EI}_f(x; y_{\text{best}}) \le c(x), \forall x \in \mathcal{X}$ 

expected improvement - cost

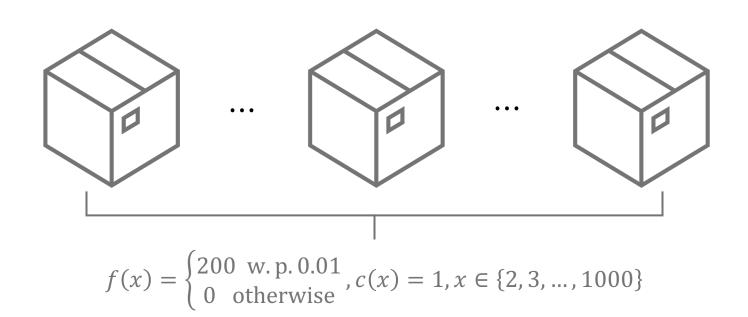
expected improvement  $\leq$  cost

 $y_{\text{best}}$ : current best observed value

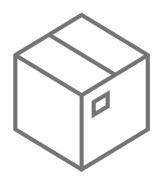
$$EI_f(x; y) = \mathbb{E}[(f(x) - y)^+]$$



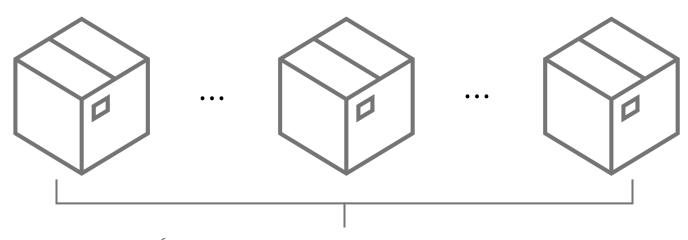
$$f(1) = 200 \text{ w. p. } 1$$
  
 $c(1) = 198$ 



t = 0  $y_{\text{best}} = 0$ 



$$f(1) = 200 \text{ w. p. } 1$$
  
 $c(1) = 198$   
 $EI_f(1; 0) - c(1)$   
 $= 200 - 198 = 2$ 



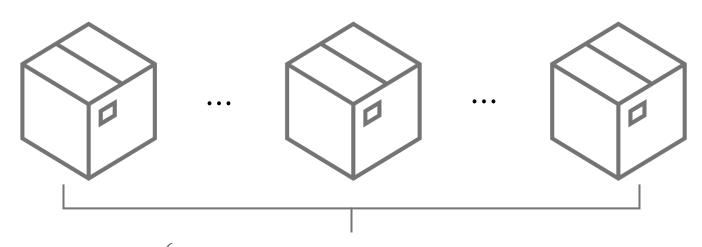
$$f(x) = \begin{cases} 200 \text{ w. p. } 0.01 \\ 0 \text{ otherwise} \end{cases}, c(x) = 1, x \in \{2, 3, ..., 1000\}$$
$$\text{EI}_f(x; 0) - c(x)$$
$$= 2 - 1 = 1$$

**Inspection rule:**  $\operatorname{argmax}_{x} \left( \operatorname{El}_{f}(x; y_{\operatorname{best}}) - c(x) \right)$  **Stopping rule:**  $\operatorname{El}_{f}(x; y_{\operatorname{best}}) \leq c(x), \forall x \in \mathcal{X}$   $\operatorname{El}_{f}(x; y) = \mathbb{E}[(f(x) - y)^{+}]$ 

 $t = 1 y_{\text{best}} = 200$ 



$$f(1) = 200 \text{ w. p. } 1$$
  
 $c(1) = 198$ 



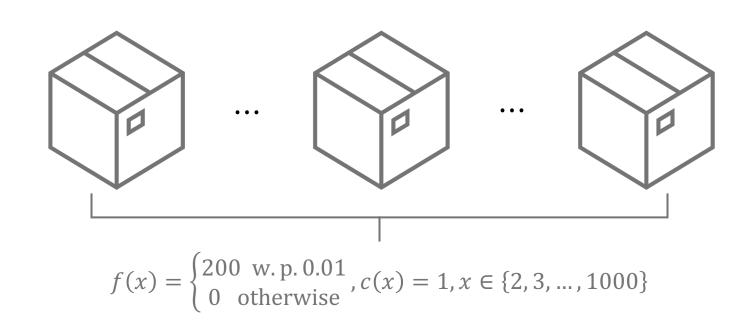
$$f(x) = \begin{cases} 200 \text{ w. p. } 0.01 \\ 0 \text{ otherwise} \end{cases}, c(x) = 1, x \in \{2, 3, ..., 1000\}$$
$$\text{EI}_f(x; 200) - c(x)$$
$$= 0 - 1 = -1 < 0$$

**Inspection rule:**  $\operatorname{argmax}_{x} \left( \operatorname{El}_{f}(x; y_{\operatorname{best}}) - c(x) \right)$  **Stopping rule:**  $\operatorname{El}_{f}(x; y_{\operatorname{best}}) \leq c(x), \forall x \in \mathcal{X}$   $\operatorname{El}_{f}(x; y) = \mathbb{E}[(f(x) - y)^{+}]$ 

$$t = 1$$



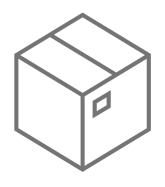
$$f(1) = 200 \text{ w. p. } 1$$
  
 $c(1) = 198$ 



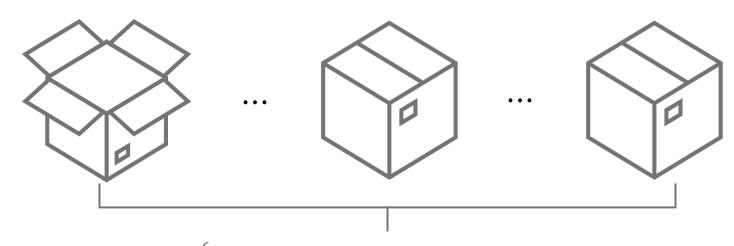
**Inspection rule:**  $\operatorname{argmax}_{x} \left( \operatorname{El}_{f}(x; y_{\operatorname{best}}) - c(x) \right)$  **Stopping rule:**  $\operatorname{El}_{f}(x; y_{\operatorname{best}}) \leq c(x), \forall x \in \mathcal{X}$  Expected utility:  $\mathbb{E}[\operatorname{Greedy}] = 200 - 198 = 2$ 

## Naïve Greedy policy can fail [Singla'18]

 $t \approx 100$   $y_{\text{best}} = 200$ 



$$f(1) = 200 \text{ w. p. } 1$$
  
 $c(1) = 198$ 



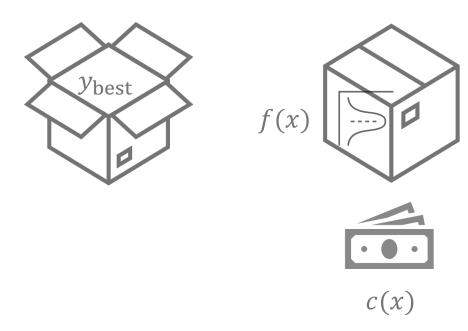
$$f(x) = \begin{cases} 200 \text{ w. p. } 0.01\\ 0 \text{ otherwise} \end{cases}, c(x) = 1, x \in \{2, 3, ..., 1000\}$$

**Inspection rule:**  $x \in \{2, 3, ..., 1000\}$ 

Stopping rule:  $y_{\text{best}} = 200$ 

Expected utility:  $\mathbb{E}[Optimal] = 200 - 100 * 1 = 100$ 

Gittins policy



**Inspection rule:**  $\alpha^*(x)$  s.t.  $\text{EI}_f(x; \alpha^*(x)) = c(x)$  **Stopping rule:**  $\alpha^*(x) \leq y_{\text{best}}, \forall x \in \mathcal{X}$ 

solution to expected improvement = cost

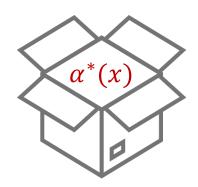
Gittins index  $\leq$  current best

 $y_{\text{best}}$ : current best observed value

$$EI_f(x; y) = \mathbb{E}[(f(x) - y)^+]$$

Gittins policy





**Inspection rule:**  $\alpha^*(x)$  s.t.  $\text{El}_f(x; \alpha^*(x)) = c(x)$  **Stopping rule:**  $\alpha^*(x) \leq y_{\text{best}}, \forall x \in \mathcal{X}$ 

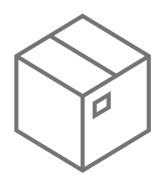
solution to expected improvement = cost

Gittins index  $\leq$  current best

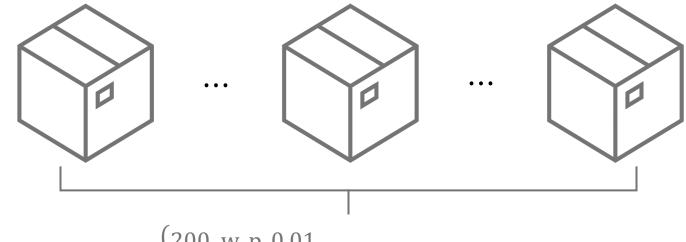
 $y_{\text{best}}$ : current best observed value

$$EI_f(x; y) = \mathbb{E}[(f(x) - y)^+]$$

$$t = 0$$



$$f(1) = 200 \text{ w. p. } 1$$
  
 $c(1) = 198$   
 $200-? = 198$ 

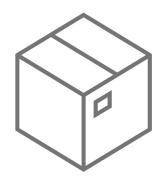


$$f(x) = \begin{cases} 200 \text{ w. p. } 0.01 \\ 0 \text{ otherwise} \end{cases}, c(x) = 1, x \in \{2, 3, ..., 1000\}$$

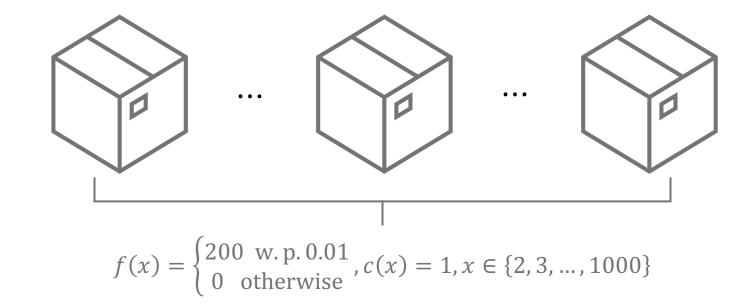
$$(200-?) * 0.01 = 1$$

Inspection rule:  $\alpha^*(x)$  s.t.  $\text{EI}_f(x; \alpha^*(x)) = c(x)$  Stopping rule:  $\alpha^*(x) \leq y_{\text{best}}, \forall x \in \mathcal{X}$   $\text{EI}_f(x; y) = \mathbb{E}[(f(x) - y)^+]$ 

$$t = 0$$



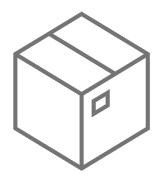
$$f(1) = 200 \text{ w. p. } 1$$
  
 $c(1) = 198$   
 $\alpha^*(1) = 2$ 



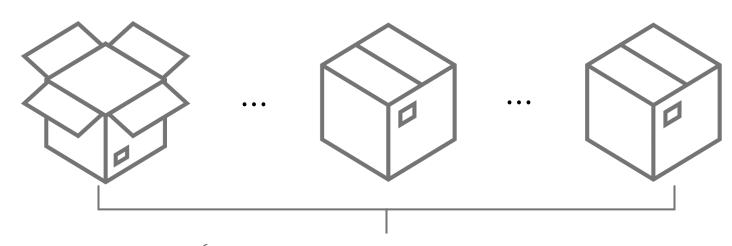
 $\alpha^*(x) = 100$ 

Inspection rule: 
$$\alpha^*(x)$$
 s.t.  $\text{El}_f(x; \alpha^*(x)) = c(x)$  Stopping rule:  $\alpha^*(x) \leq y_{\text{best}}, \forall x \in \mathcal{X}$   $\text{El}_f(x; y) = \mathbb{E}[(f(x) - y)^+]$ 

t = 1  $y_{\text{best}} = 200 \text{ or } 0$ 



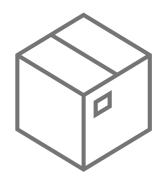
$$f(1) = 200 \text{ w. p. } 1$$
  
 $c(1) = 198$   
 $\alpha^*(1) = 2$ 



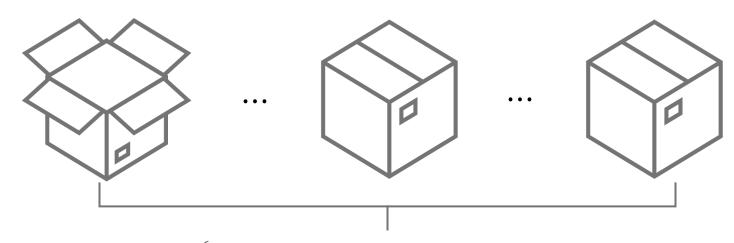
$$f(x) = \begin{cases} 200 \text{ w. p. } 0.01 \\ 0 \text{ otherwise} \end{cases}, c(x) = 1, x \in \{2, 3, ..., 1000\}$$
$$\alpha^*(x) = 100$$

Inspection rule:  $\alpha^*(x)$  s.t.  $\text{EI}_f(x; \alpha^*(x)) = c(x)$  Stopping rule:  $\alpha^*(x) \leq y_{\text{best}}, \forall x \in \mathcal{X}$   $\text{EI}_f(x; y) = \mathbb{E}[(f(x) - y)^+]$ 

 $t \approx 100$   $y_{\text{best}} = 200$ 

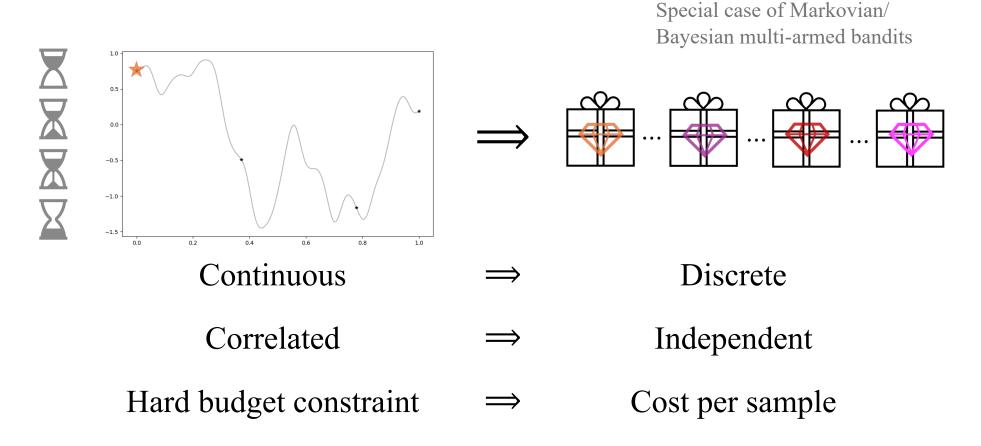


$$f(1) = 200 \text{ w. p. 1}$$
  
 $c(1) = 198$   
 $\alpha^*(1) = 2$ 

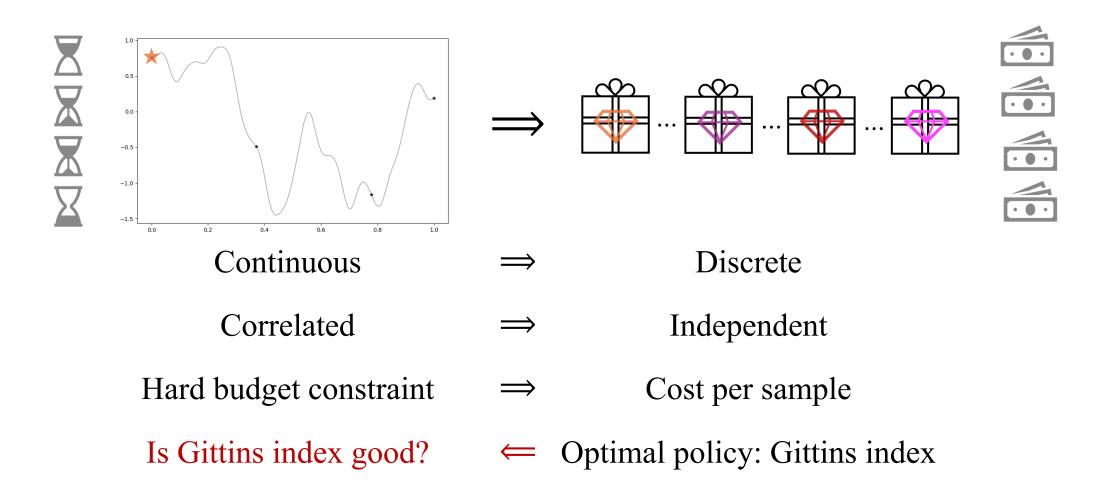


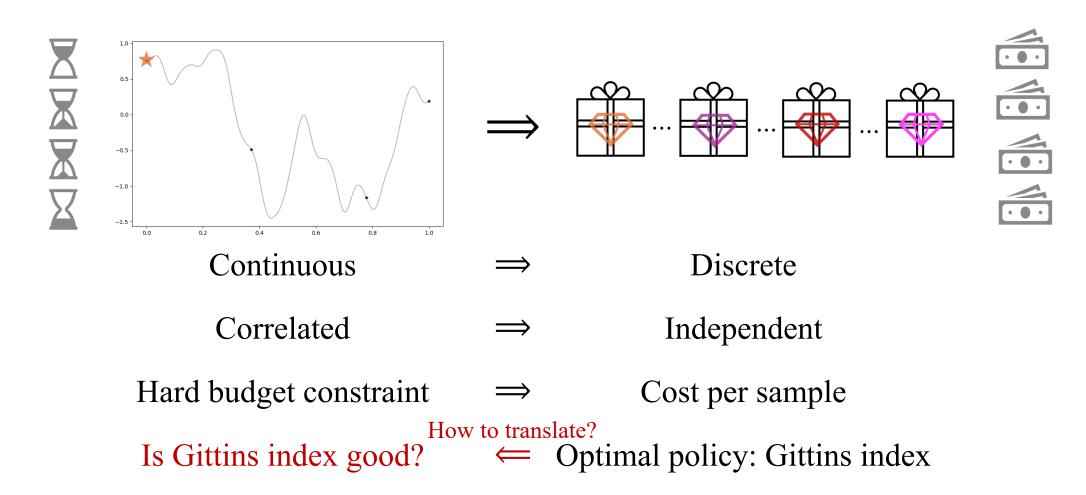
$$f(x) = \begin{cases} 200 \text{ w. p. } 0.01 \\ 0 \text{ otherwise} \end{cases}, c(x) = 1, x \in \{2, 3, ..., 1000\}$$
$$\alpha^*(x) = 100$$

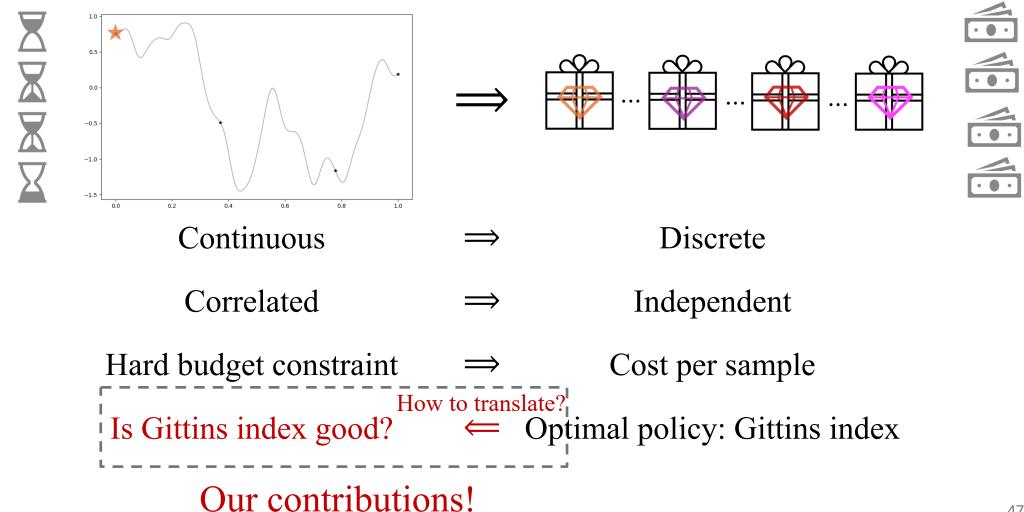
**Inspection rule:** argmax<sub>x</sub>  $\alpha^*(x)$  s.t.  $\text{EI}_f(x; \alpha^*(x)) = c(x)$  **Stopping rule:**  $\alpha^*(x) \leq y_{\text{best}}, \forall x \in \mathcal{X}$  Expected utility:  $\mathbb{E}[\text{Gittins}] = 200 - 100 * 1 = 100$ 

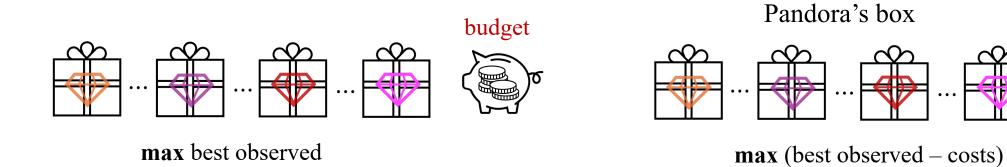


Optimal policy: Gittins index [Weitzman'79]







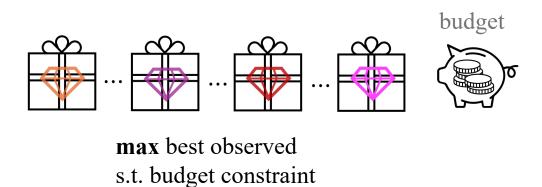


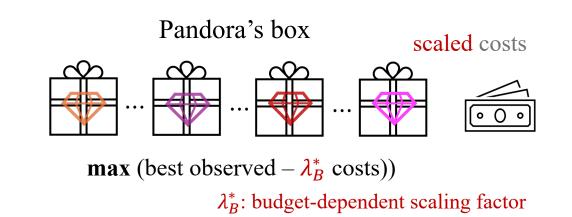
s.t. budget constraint

Expected budget constraint  $\iff$  Cost per sample

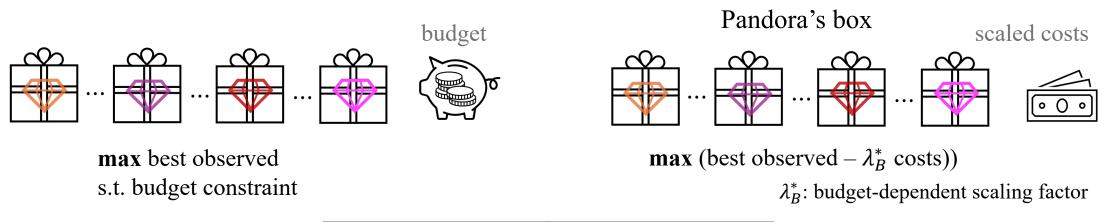
Optimal policy? ← Optimal policy: Gittins index

costs



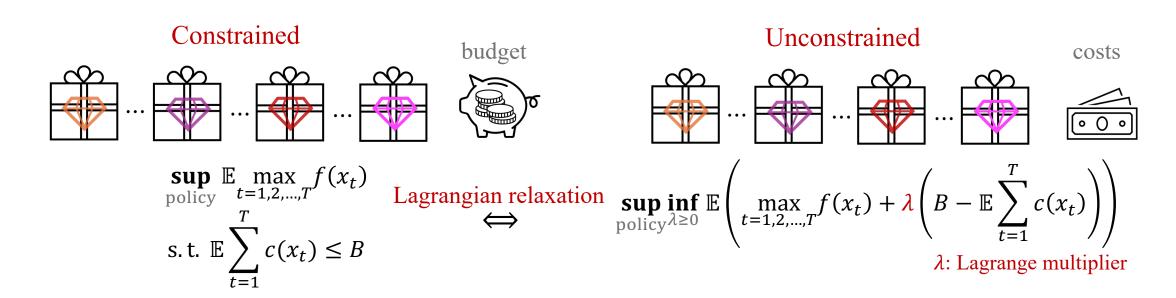


Optimal policy: Gittins solution to  $\leftarrow$  Optimal policy: Gittins index Pandora's box with scaled costs



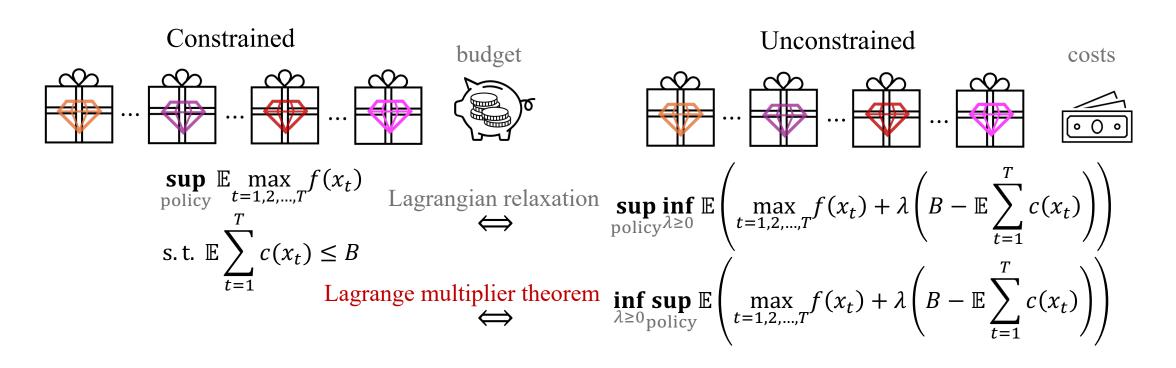
Reward distribution	Reference
finite support	[Aminian et al.'24]
general support	our work

Optimal policy: Gittins solution to  $\leftarrow$  Optimal policy: Gittins index Pandora's box with scaled costs



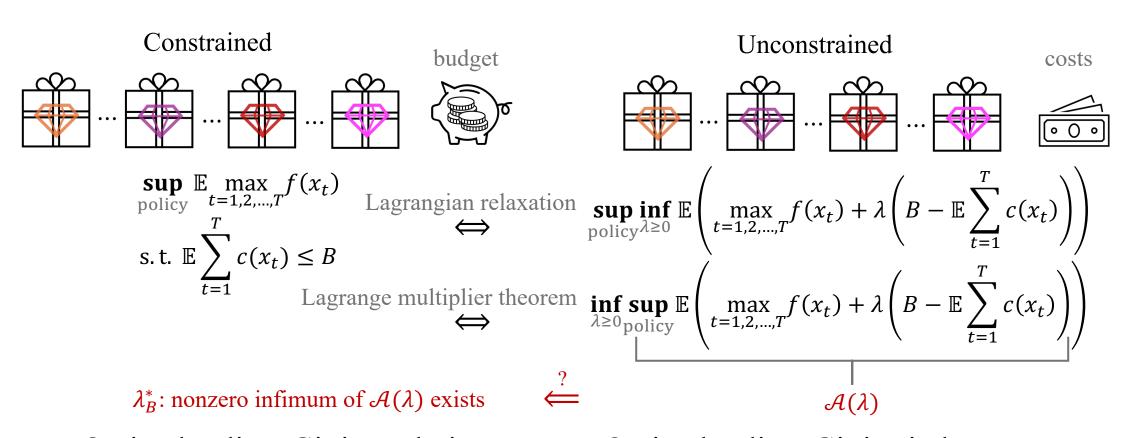
Optimal policy: Gittins solution to ← Optimal policy: Gittins index Pandora's box with scaled costs

Extension to [Aminian et al.'24]



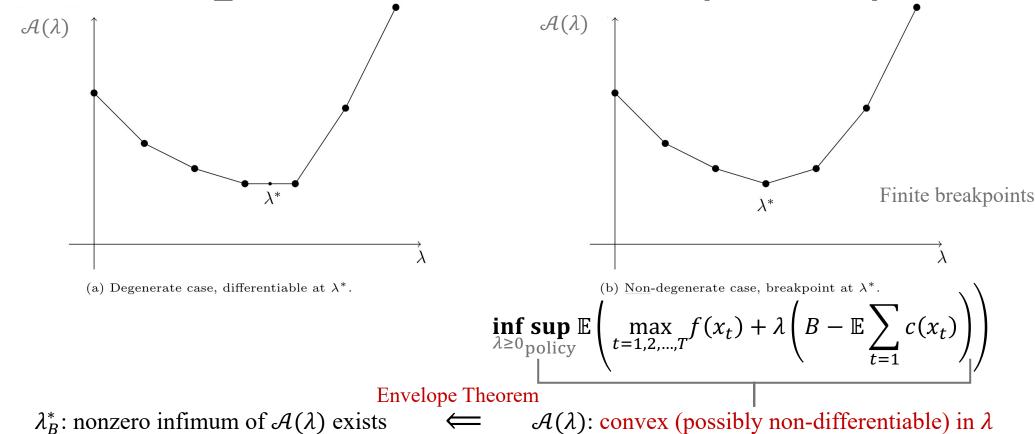
Optimal policy: Gittins solution to ← Optimal policy: Gittins index Pandora's box with scaled costs

Extension to [Aminian et al.'24]



Optimal policy: Gittins solution to  $\leftarrow$  Optimal policy: Gittins index Pandora's box with scaled costs

Extension to [Aminian et al.'24]

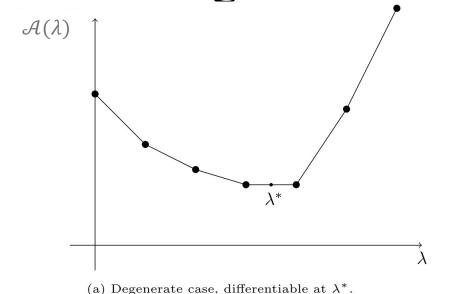


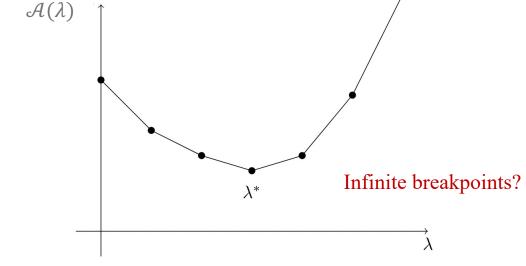
Optimal policy: Gittins solution to  $\leftarrow$  Optimal policy: Gittins index

Pandora's box with scaled costs

Extension to [Aminian et al.'24]

Figure from [Aminian et al.'24]





$$\inf_{\lambda \geq 0} \sup_{\text{policy}} \mathbb{E} \left( \max_{t=1,2,\dots,T} f(x_t) + \lambda \left( B - \mathbb{E} \sum_{t=1}^{\infty} c(x_t) \right) \right)$$

 $\lambda_B^*$ : nonzero infimum of  $\mathcal{A}(\lambda)$  exists

 $\Leftarrow$ 

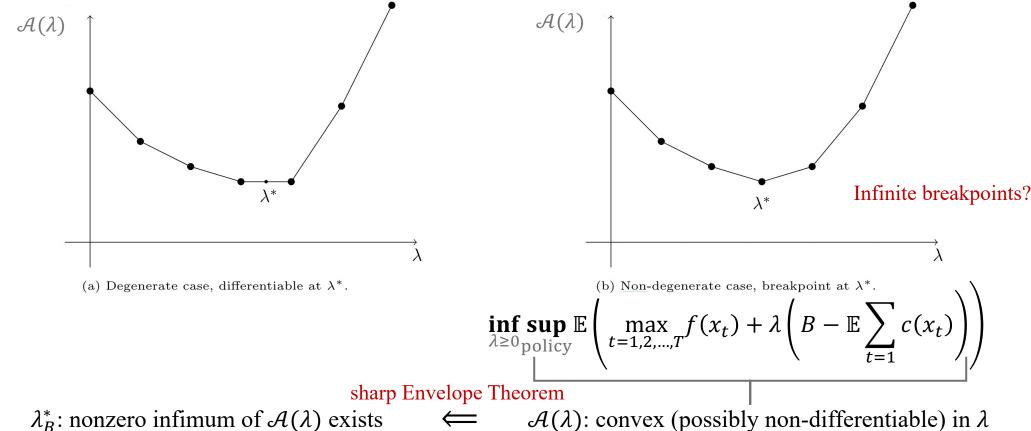
 $\mathcal{A}(\lambda)$ : convex (possibly non-differentiable) in  $\lambda$ 

Optimal policy: Gittins solution to  $\leftarrow$  Optimal policy: Gittins index Pandora's box with scaled costs

Extension to [Aminian et al.'24]

Figure from [Aminian et al.'24]

Expected budget constraint ⇔ Cost per sample



 $\mathcal{A}_B$ . Holizero infilitum of  $\mathcal{A}(\lambda)$  exists  $\longrightarrow \mathcal{A}(\lambda)$ . Convex (possibly non-differentiable

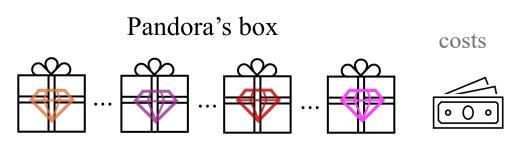
Optimal policy: Gittins solution to  $\leftarrow$  Optimal policy: Gittins index Pandora's box with scaled costs

Extension to [Aminian et al.'24]

Figure from [Aminian et al.'24]



max best observed
s.t. budget constraint



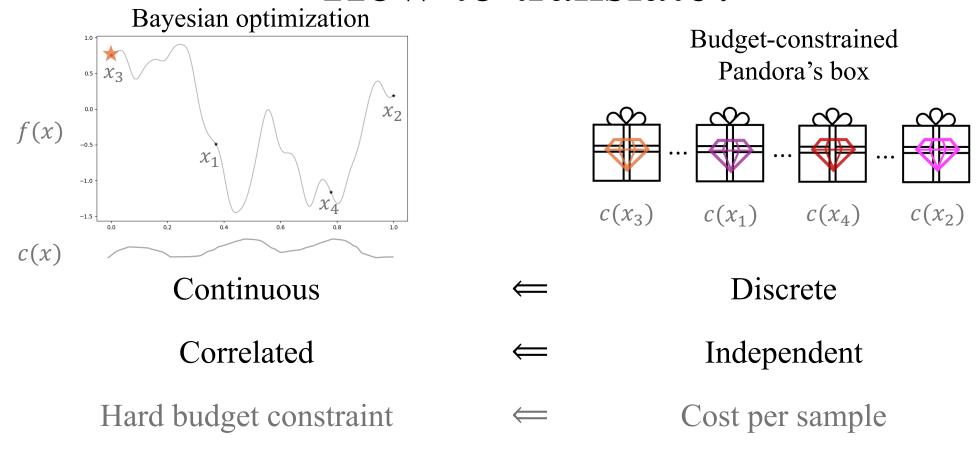
max (best observed – costs)

Hard budget constraint

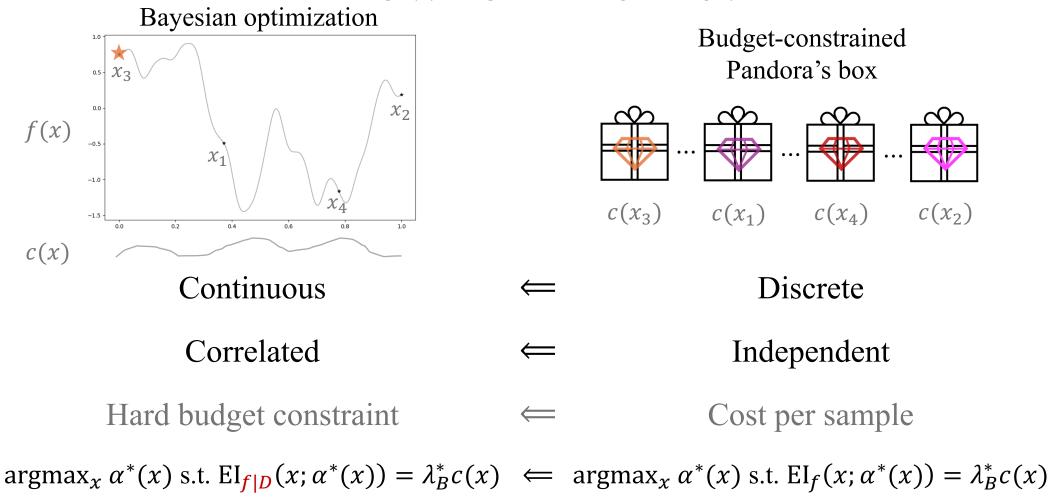
 $\leftarrow$ 

Cost per sample

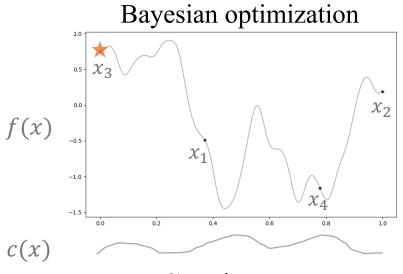
 $\operatorname{argmax}_{x} \alpha^{*}(x) \text{ s.t. } \operatorname{EI}_{f}(x; \alpha^{*}(x)) = \lambda_{B}^{*} c(x) \iff \operatorname{argmax}_{x} \alpha^{*}(x) \text{ s.t. } \operatorname{EI}_{f}(x; \alpha^{*}(x)) = c(x)$ 



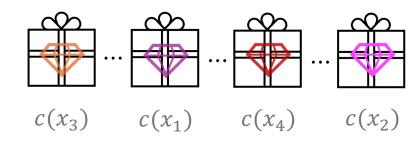
How to incorporate Gaussian process? ← Optimal policy: Gittins solution to Pandora's box with scaled costs



D: observed data



Budget-constrained Pandora's box



Continuous

 $\Leftarrow$ 

Discrete

Correlated

 $\leftarrow$ 

Independent

Hard budget constraint

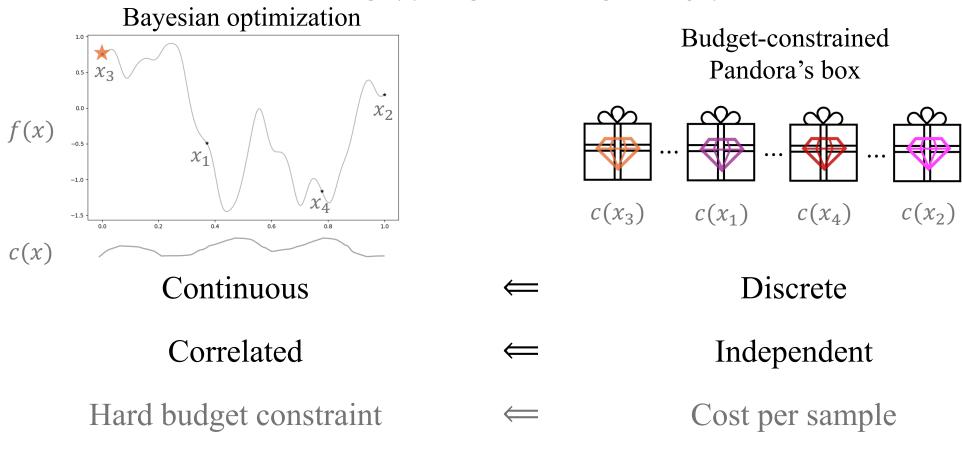
 $\leftarrow$ 

Cost per sample

 $\operatorname{argmax}_{x} \alpha^{*}(x) \text{ s.t. } \operatorname{EI}_{f|D}(x; \alpha^{*}(x)) = \lambda_{B}^{*} c(x) \iff \operatorname{argmax}_{x} \alpha^{*}(x) \text{ s.t. } \operatorname{EI}_{f}(x; \alpha^{*}(x)) = \lambda_{B}^{*} c(x)$ 

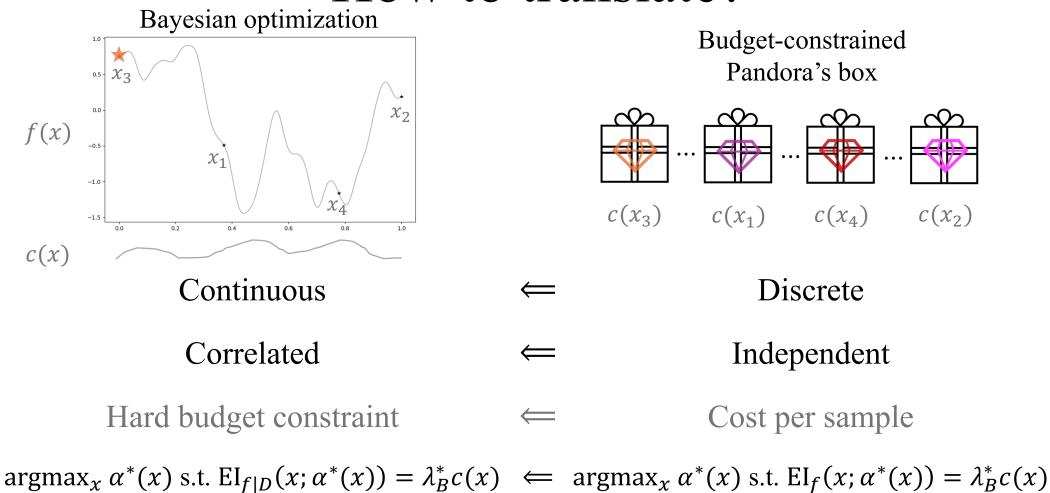
popular one-step

heuristic: EI policy



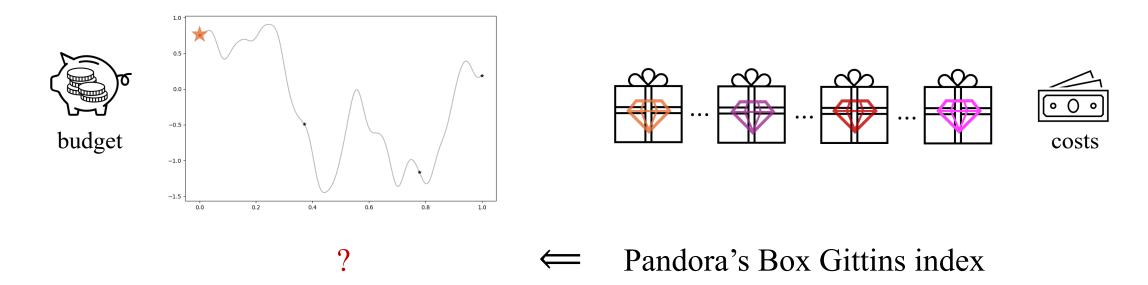
 $\operatorname{argmax}_{x} \alpha^{*}(x) \text{ s.t. } \operatorname{EI}_{f|D}(x; \alpha^{*}(x)) = \lambda_{B}^{*} c(x) \iff \operatorname{argmax}_{x} \alpha^{*}(x) \text{ s.t. } \operatorname{EI}_{f}(x; \alpha^{*}(x)) = \lambda_{B}^{*} c(x)$ 

ratio of EI and cost: EIPC policy



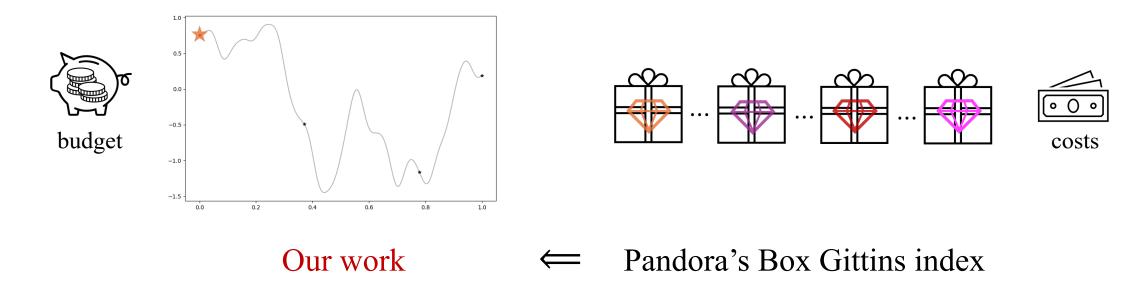
### Our Contributions

- How to translate?
- Is Pandora's Box Gittins index (PBGI) good?



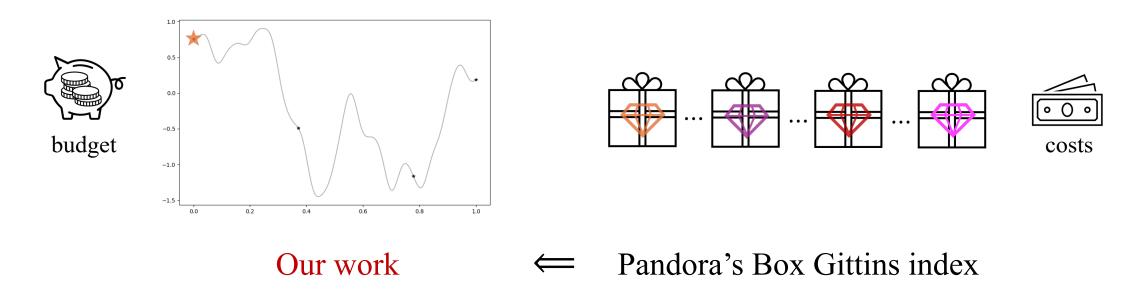
### Our Contributions

- Develop PBGI policy for cost-aware Bayesian optimization
- Is Pandora's Box Gittins index (PBGI) good?

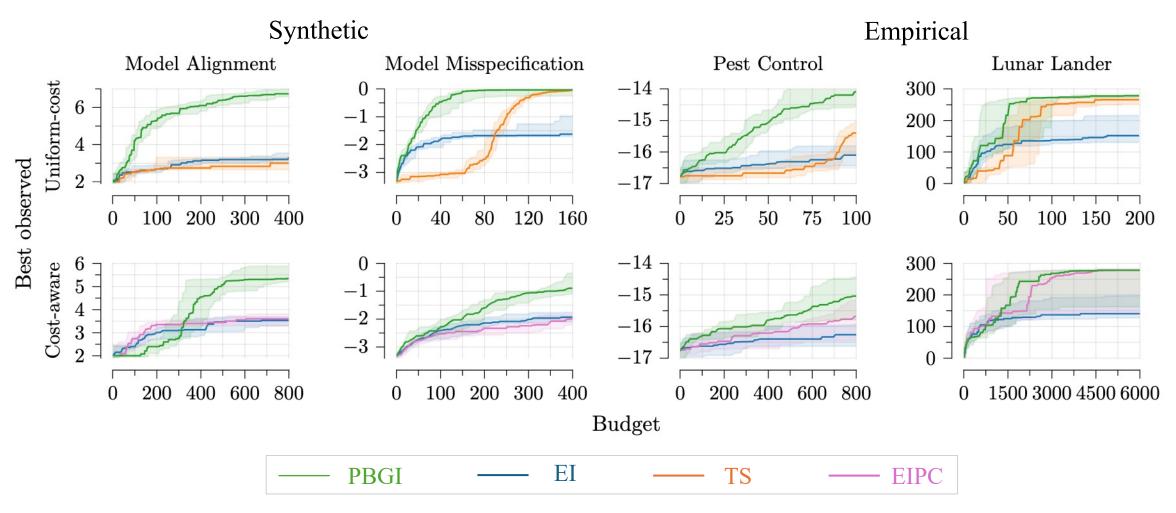


#### Our Contributions

- Develop PBGI policy for Bayesian optimization
- Show performance against baselines on synthetic & empirical experiments

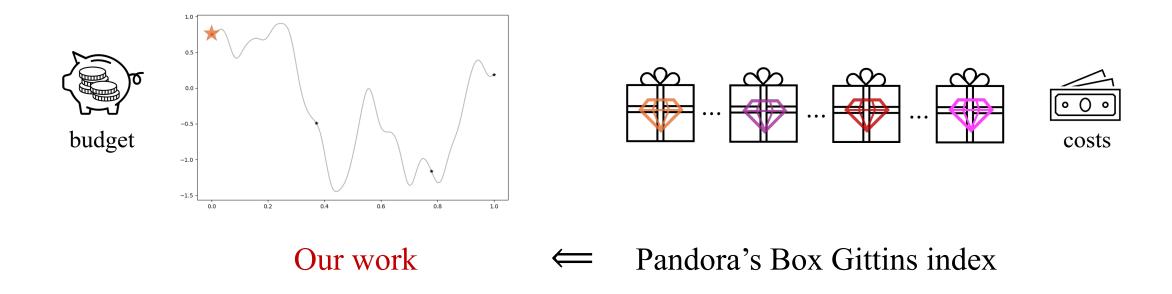


# Experiment Results: PBGI vs Baselines



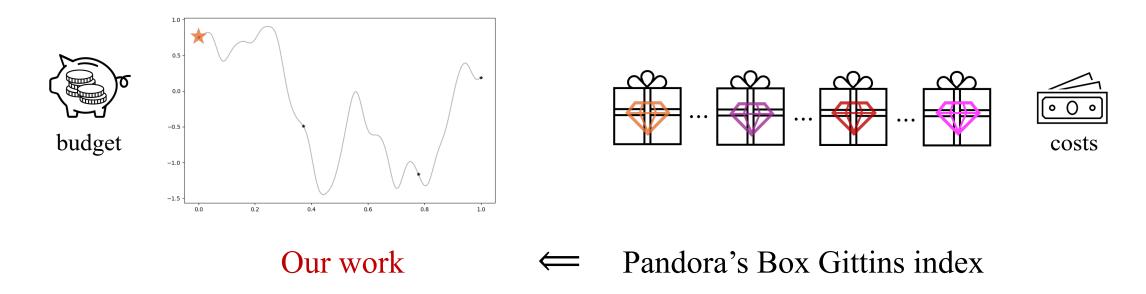
### Conclusions

• Propose easy-to-compute PBGI policy for Bayesian optimization



### Conclusions

- Propose easy-to-compute PBGI policy for Bayesian optimization
- Show the effectiveness of PBGI on synthetic & empirical experiments



### Conclusions

- Propose easy-to-compute PBGI policy for Bayesian optimization
- Show the effectiveness of PBGI on synthetic & empirical experiments
- Open door for more-complex BO (freeze-thaw, multi-fidelity, function network, etc.) via Gittins variants ("golf" Markovian MAB, optional inspection, etc.)

