

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

Qian Xie (Cornell ORIE)

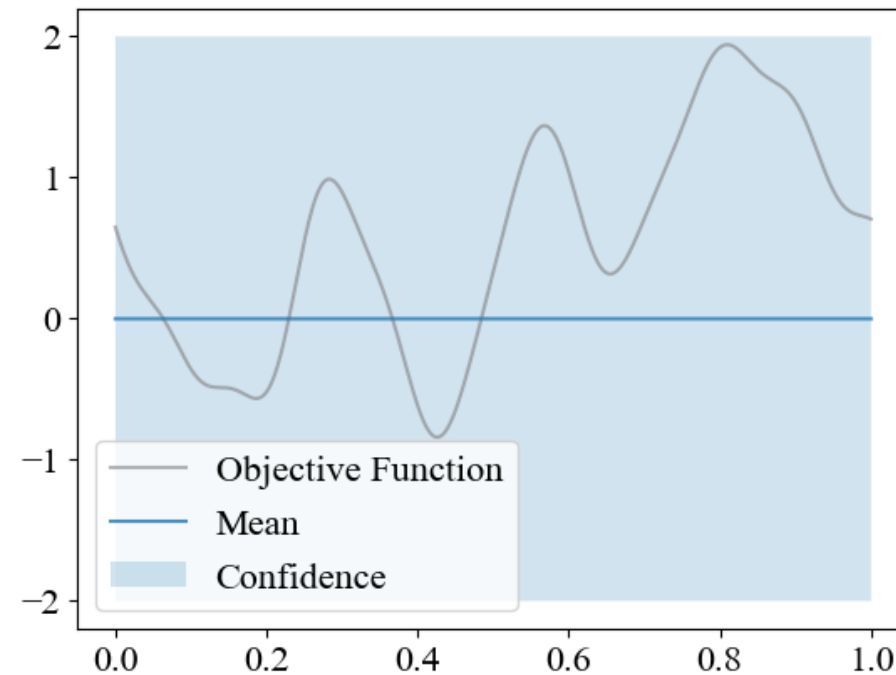
Joint work with Raul Astudillo, Peter Frazier, Ziv Scully, and Alexander Terenin

ECGI'24

# Bayesian Optimization

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

∈ decision-making under uncertainty



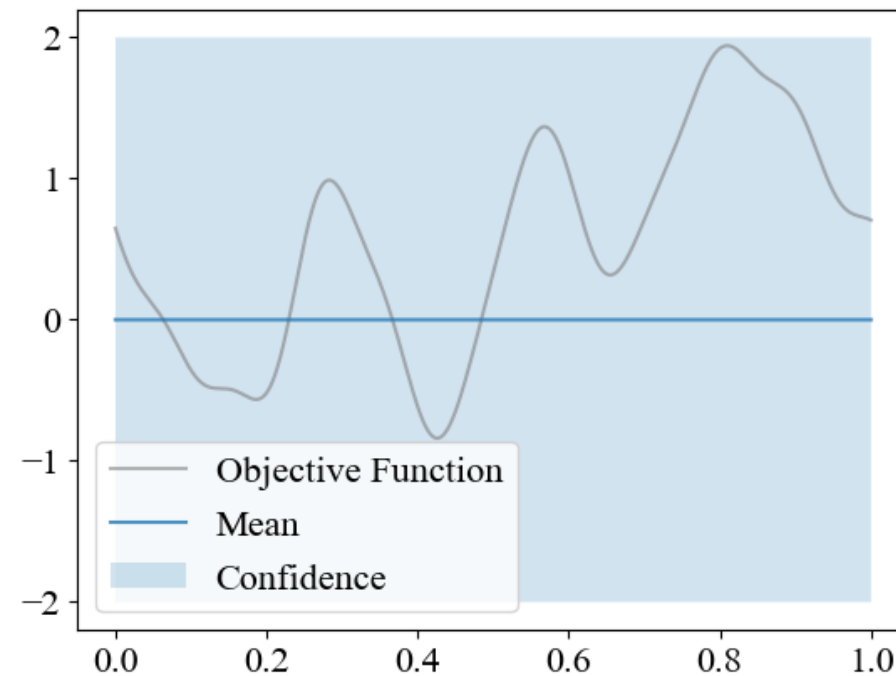
**Applications:**

Hyperparameter tuning  
Drug/material discovery  
Experiment design

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# Bayesian Optimization

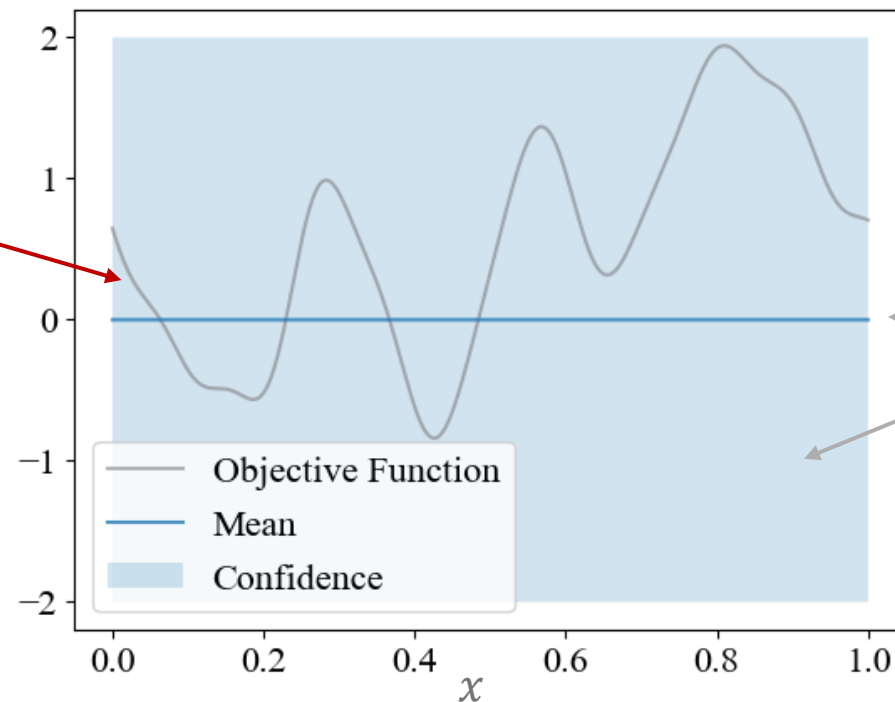
**Goal:** optimize expensive-to-evaluate **black-box** function

An **unknown random** function  $f: \mathcal{X} \rightarrow \mathbb{R}$  drawn from a Gaussian process prior

Gaussian process: infinite-dimensional generalization of multivariate normal distributions



∈ decision-making under uncertainty



**Applications:**

Hyperparameter tuning  
Drug/material discovery  
Experiment design

$x$ : hyperparameter/configuration

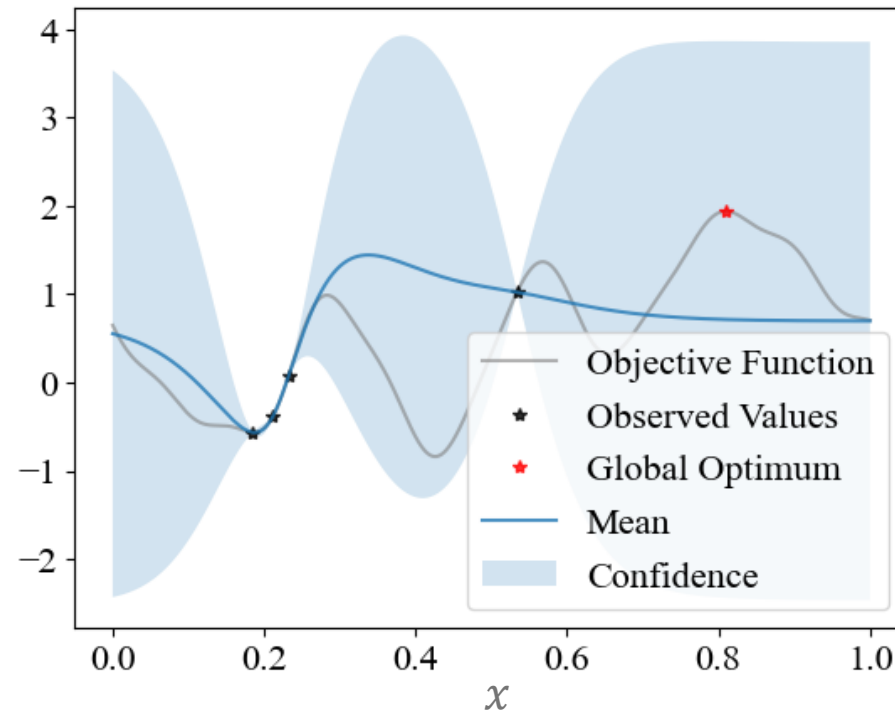
mean: prediction

variance: confidence/uncertainty

# Bayesian Optimization

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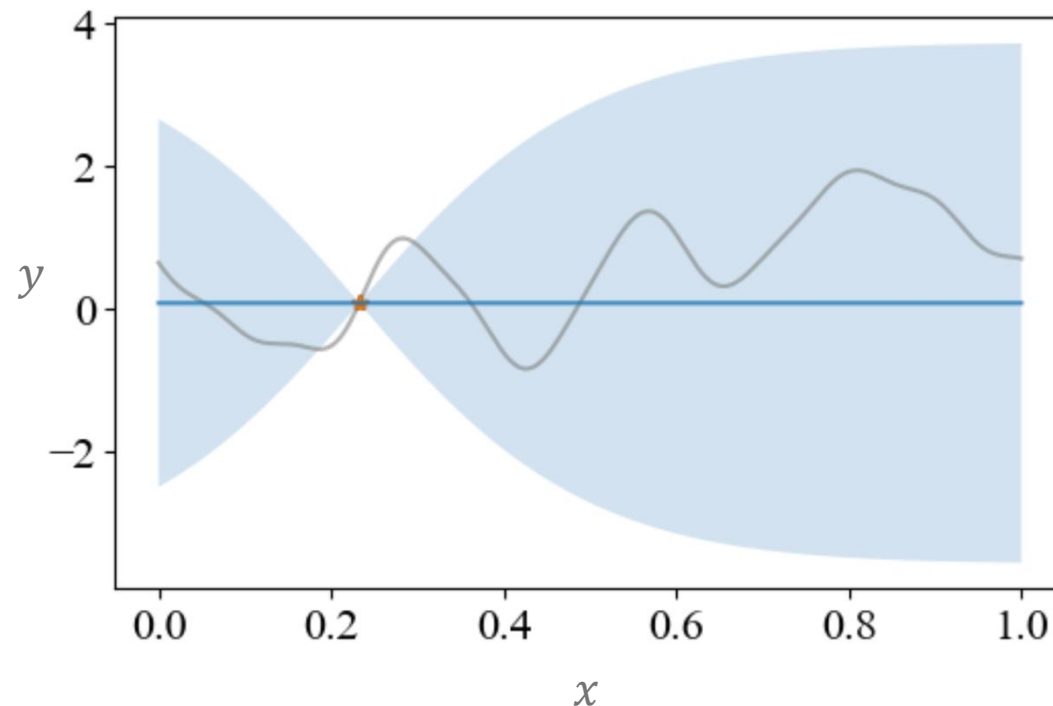
**Objective:** find global optimum  $x^* = \operatorname{argmax}_{x \in \mathcal{X}} f(x)$

**Decision:** evaluate a set of points

# Bayesian Optimization

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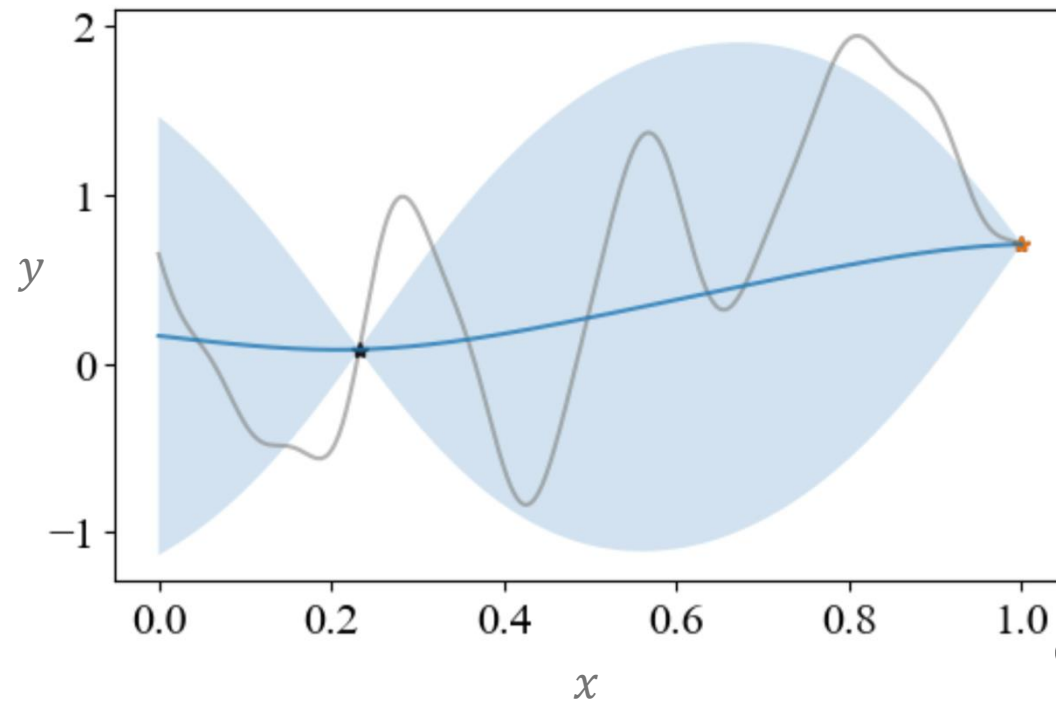
**adaptively**

**Decision:** evaluate a set of points

# Bayesian Optimization

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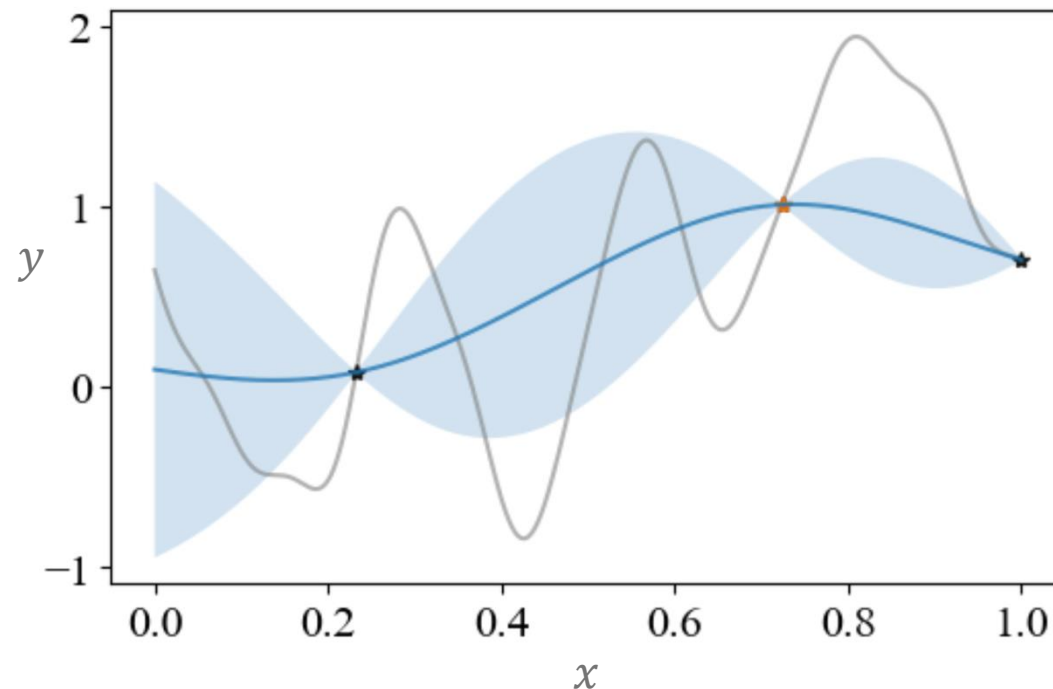
**adaptively**

**Decision:** evaluate a set of points

# Bayesian Optimization

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**Applications:**

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Experiment design

$x$ : hyperparameter/configuration

**adaptively**

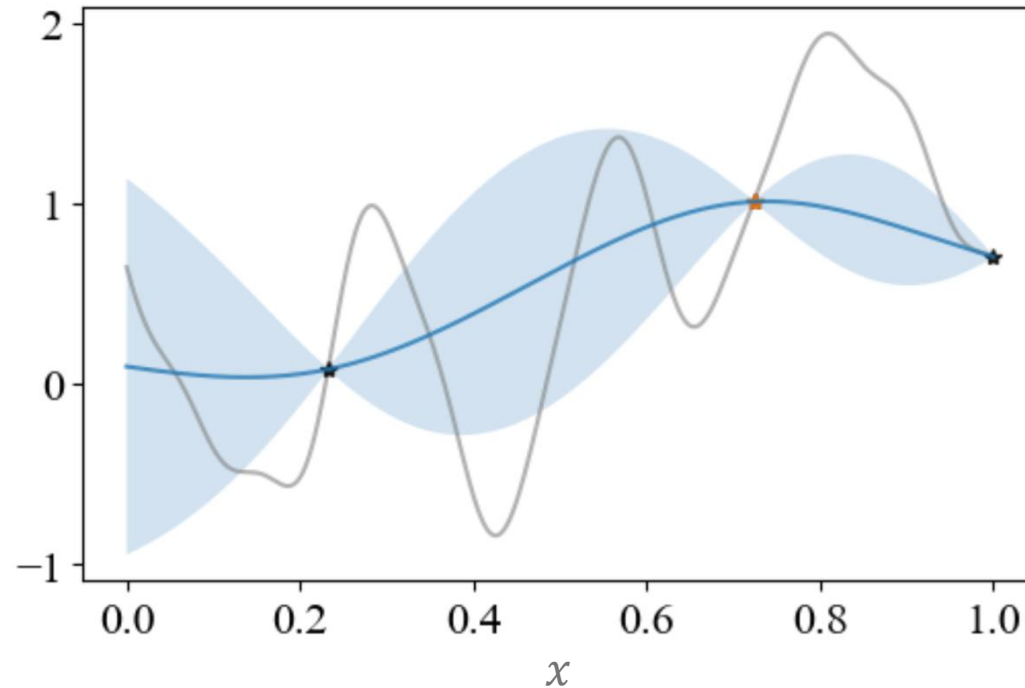
**Decision:** evaluate a set of points



# Bayesian Optimization

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

An unknown random function  $f: \mathcal{X} \rightarrow \mathbb{R}$  drawn from a Gaussian process prior



**Applications:**

Hyperparameter tuning  
Drug/material discovery  
Experiment design

$x$ : hyperparameter/configuration

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

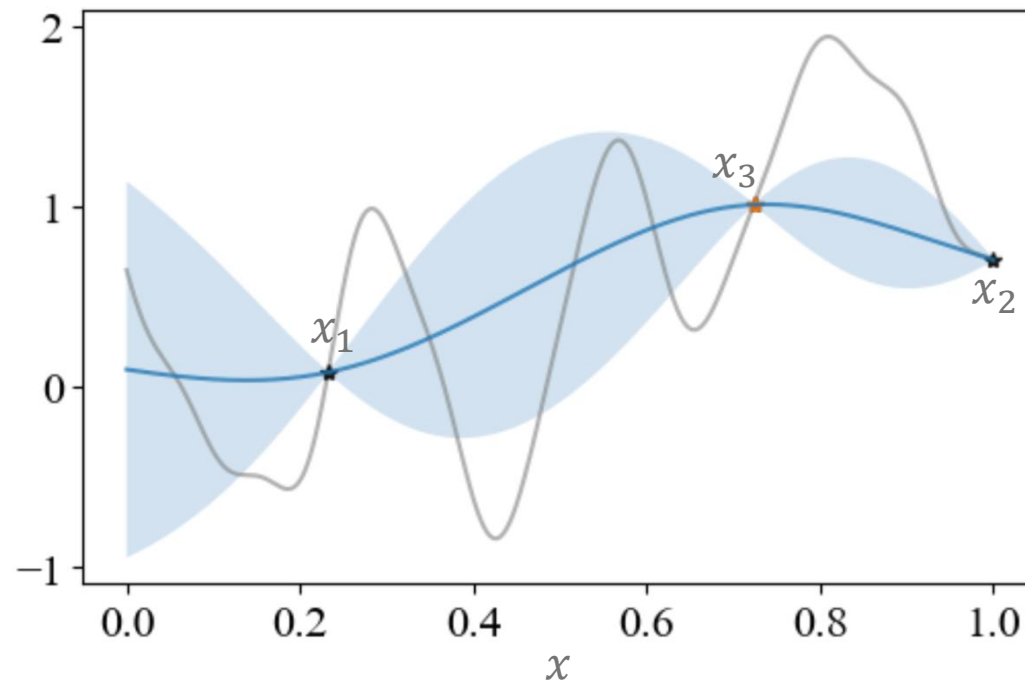
$x_1, x_2, \dots, x_T \in \mathcal{X}$

**$T$ : time budget**

# Bayesian Optimization

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

An unknown random function  $f: \mathcal{X} \rightarrow \mathbb{R}$  drawn from a Gaussian process prior



**Applications:**

Hyperparameter tuning  
Drug/material discovery  
Experiment design

$x$ : hyperparameter/configuration

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

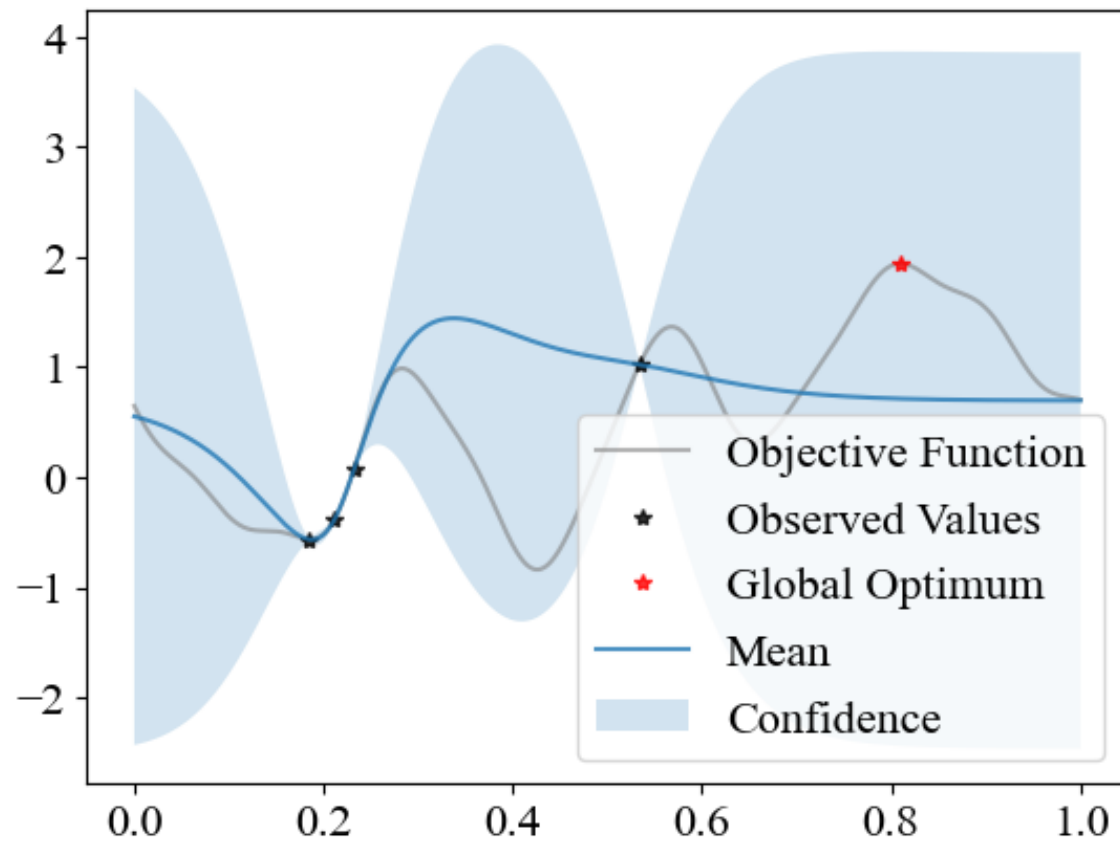
$$\sup_{\text{policy}} \mathbb{E} \max_{t=1,2,\dots,T} f(x_t)$$

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

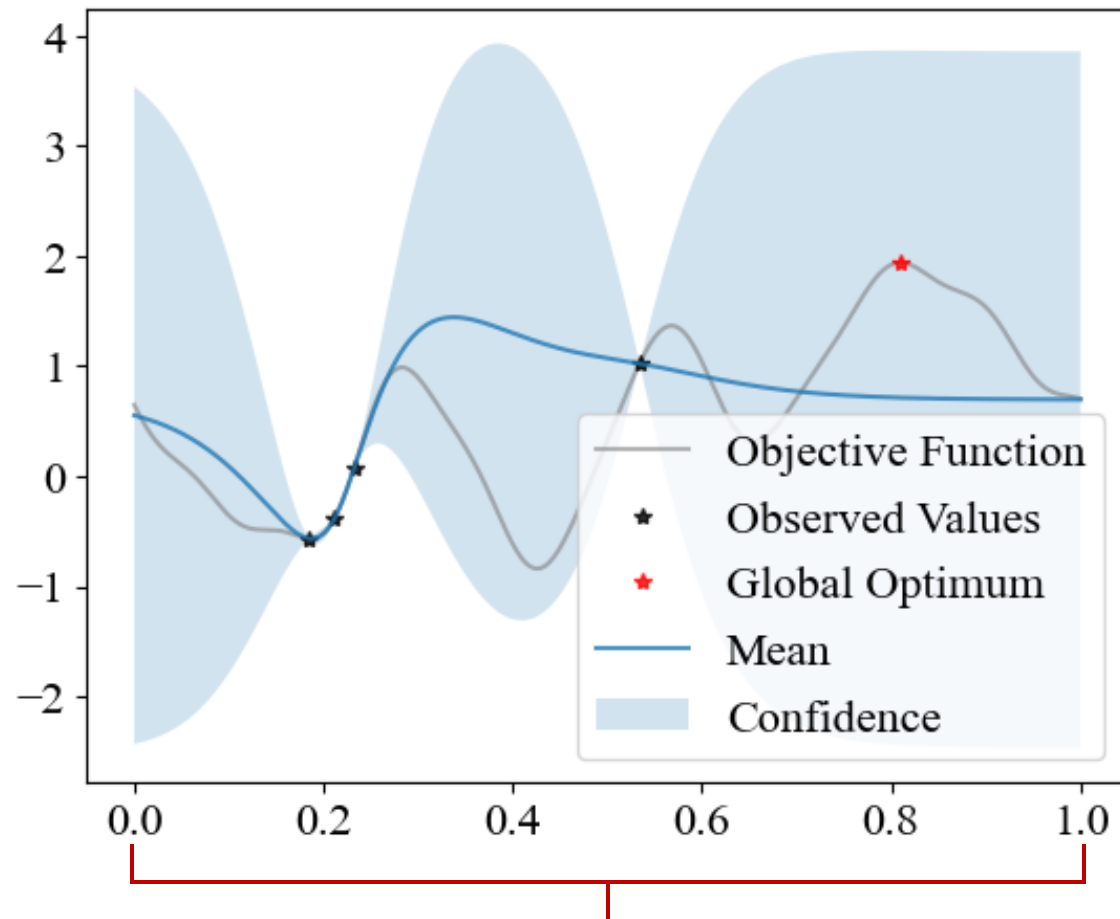
$$x_1, x_2, \dots, x_T \in \mathcal{X}$$

**$T$ : time budget**

# Why is it hard?

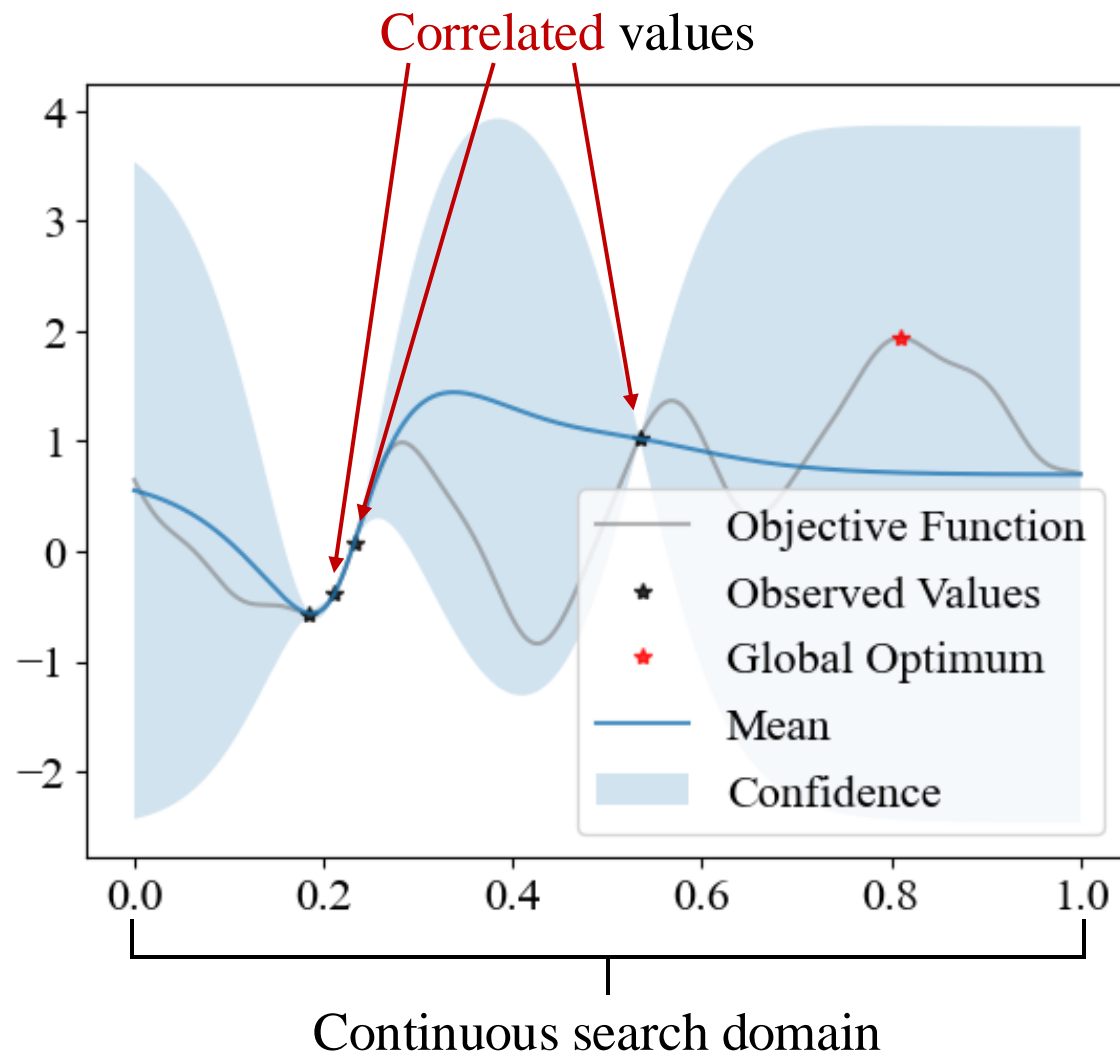


# Why is it hard?



Continuous search domain

# Why is it hard?



# Why is it hard?

Hard budget constraint

$t=1$



$t=2$



$t=3$

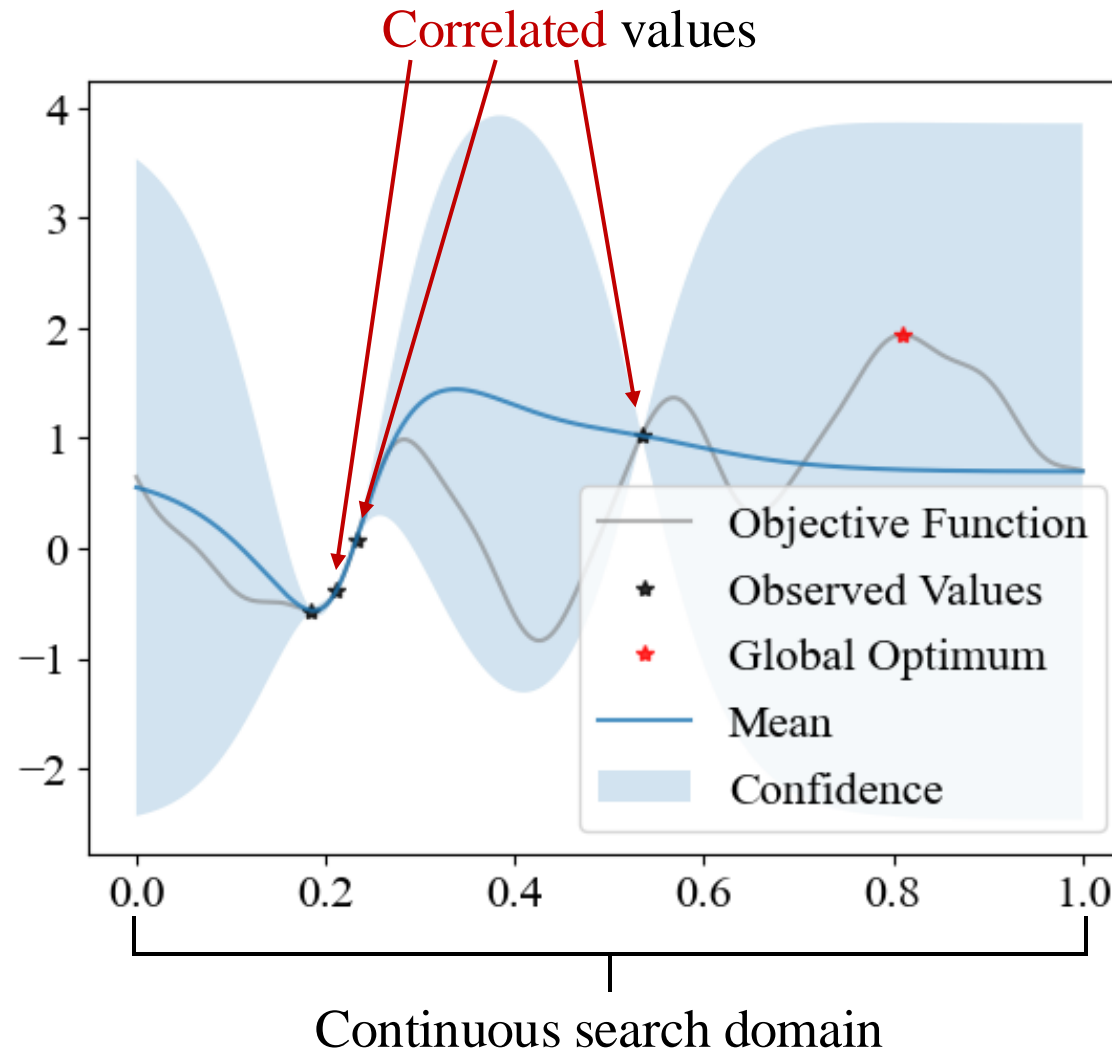


$t=4$







$\vdots$

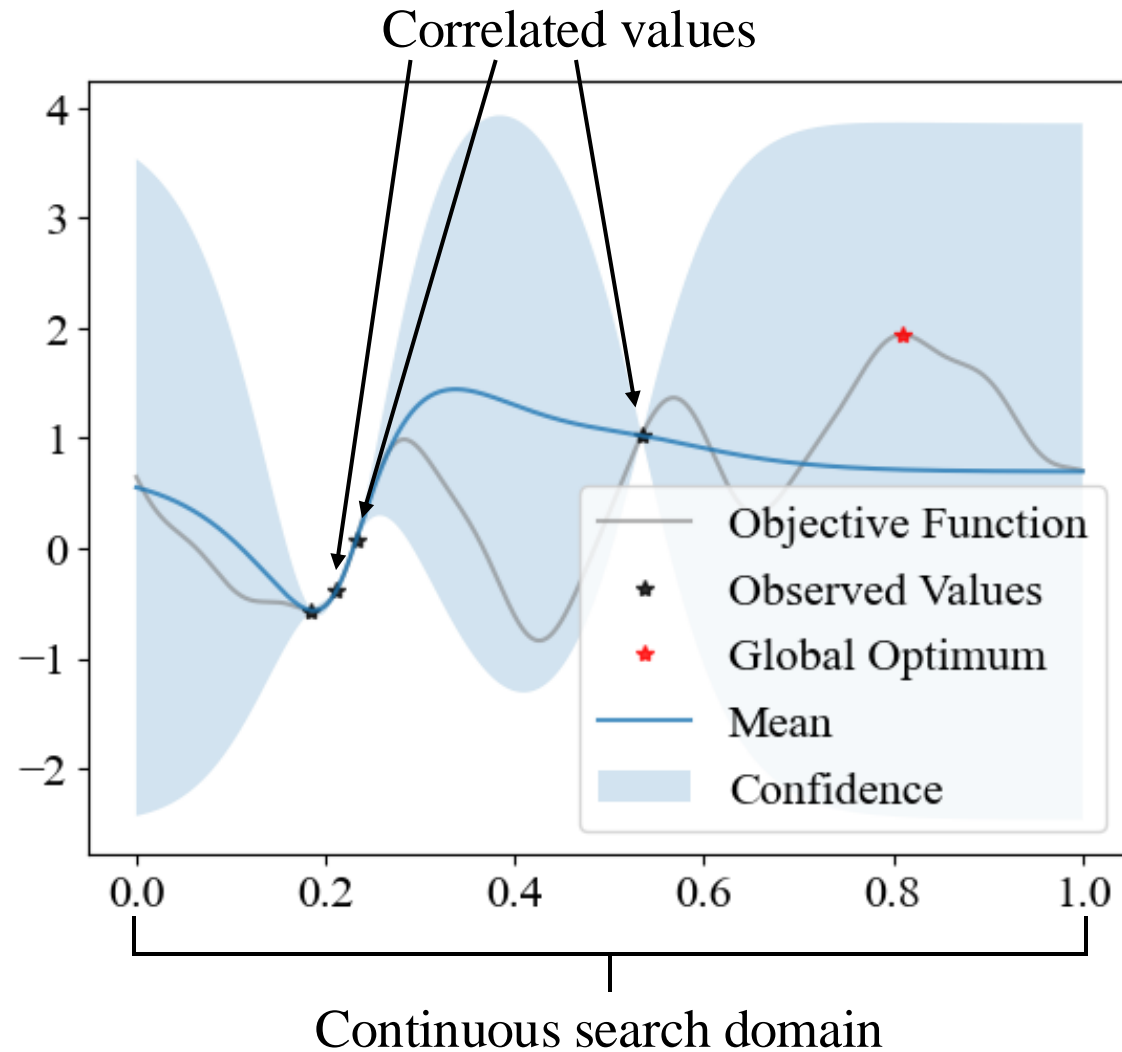
$t=T$



# Why is it hard?

Hard budget constraint

$t=1$    
 $t=2$    
 $t=3$    
 $t=4$    
 $\vdots$   
 $t=T$



Evaluation **costs** handling







uniform

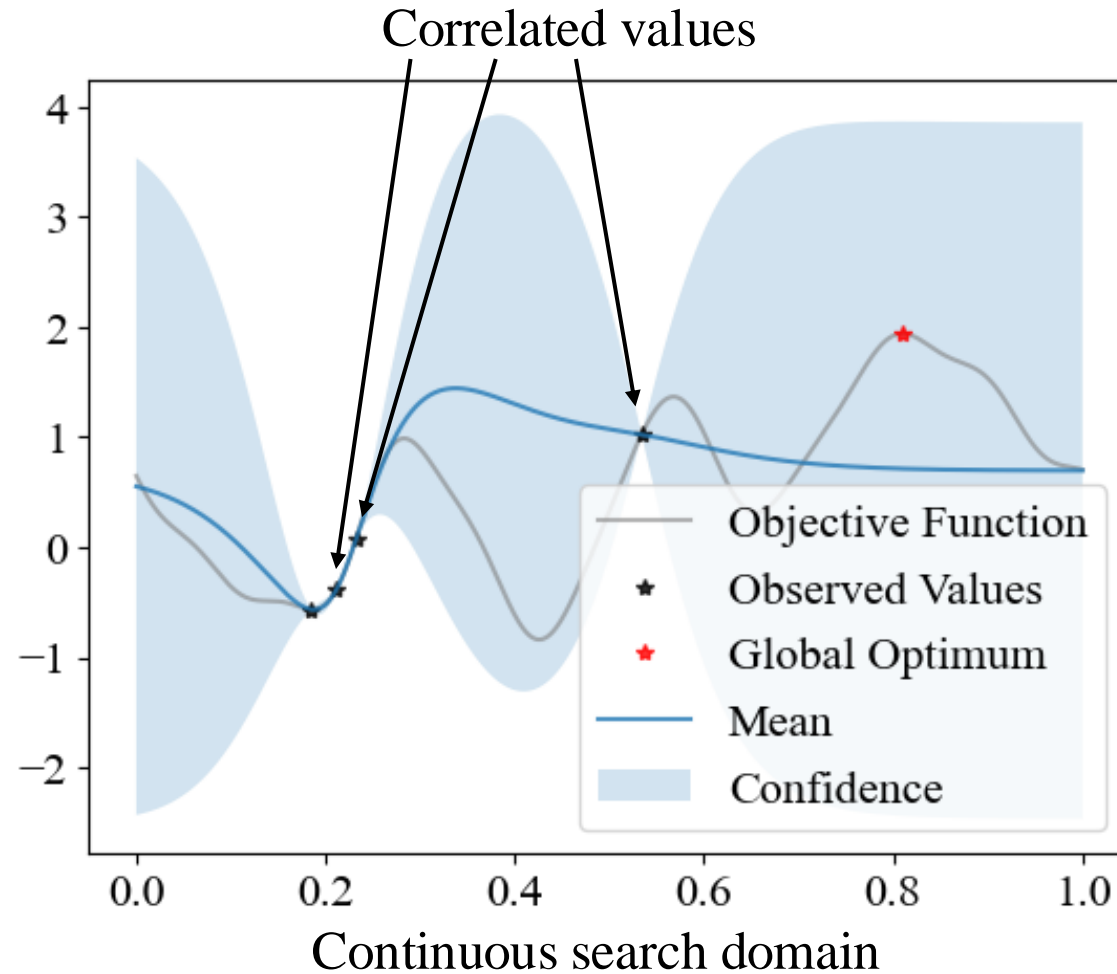


heterogeneous

# Why is it hard?

Hard budget constraint

$t=1$    
 $t=2$    
 $t=3$    
 $t=4$    
 $\vdots$   
 $t=T$



Evaluation costs handling



uniform







heterogeneous

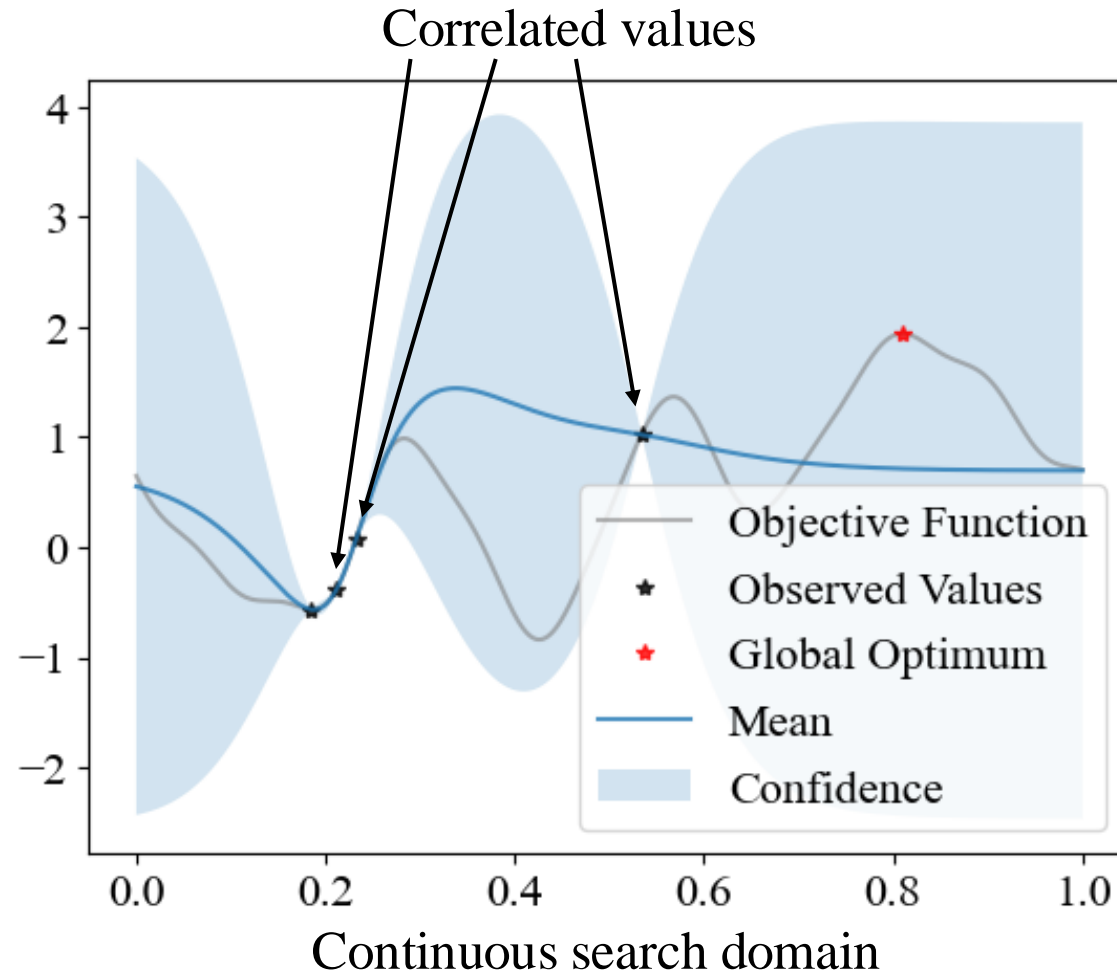
⇒ Optimal policy unknown!



# Why is it hard?

Hard budget constraint

$t=1$    
 $t=2$    
 $t=3$    
 $t=4$    
 $\vdots$   
 $t=T$



Evaluation costs handling



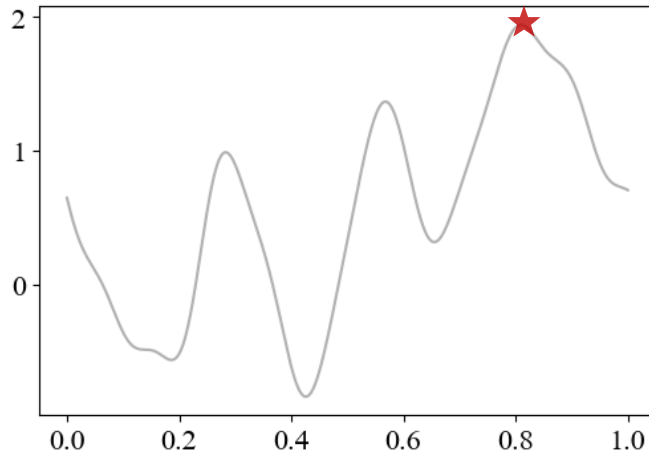
uniform



heterogeneous

Can we convert it to a solvable problem?

# Bayesian Optimization

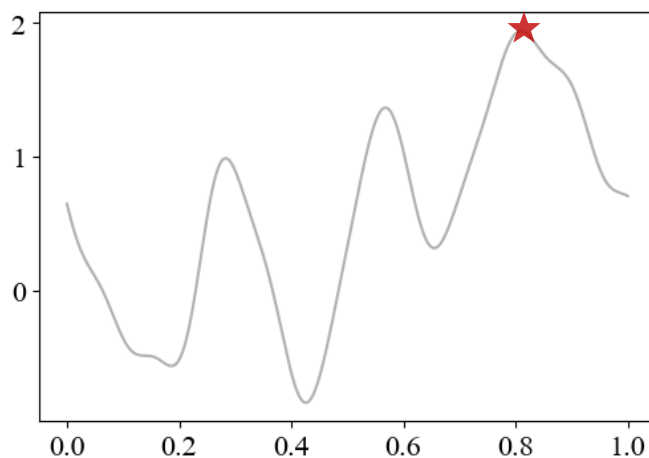


Continuous

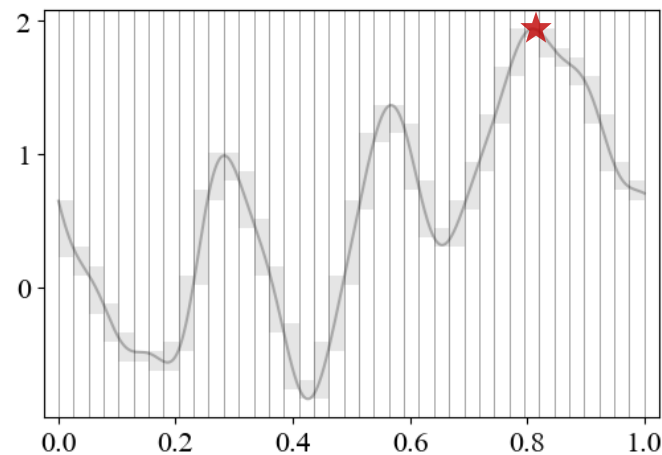
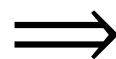
Correlated

Hard budget constraint

# Bayesian Optimization



Continuous



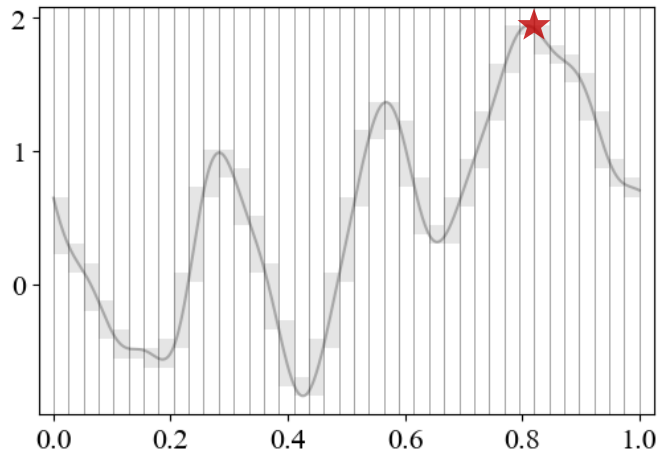
Discrete



Correlated

Hard budget constraint

# Bayesian Optimization



Continuous

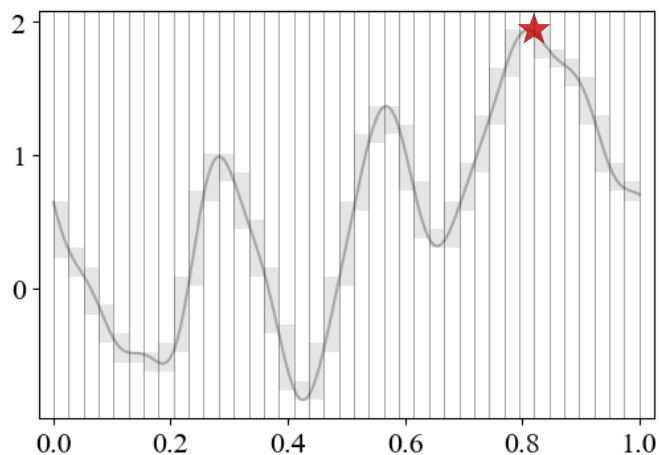
$\Rightarrow$

Discrete

Correlated

Hard budget constraint

# Bayesian Optimization



Continuous



Discrete

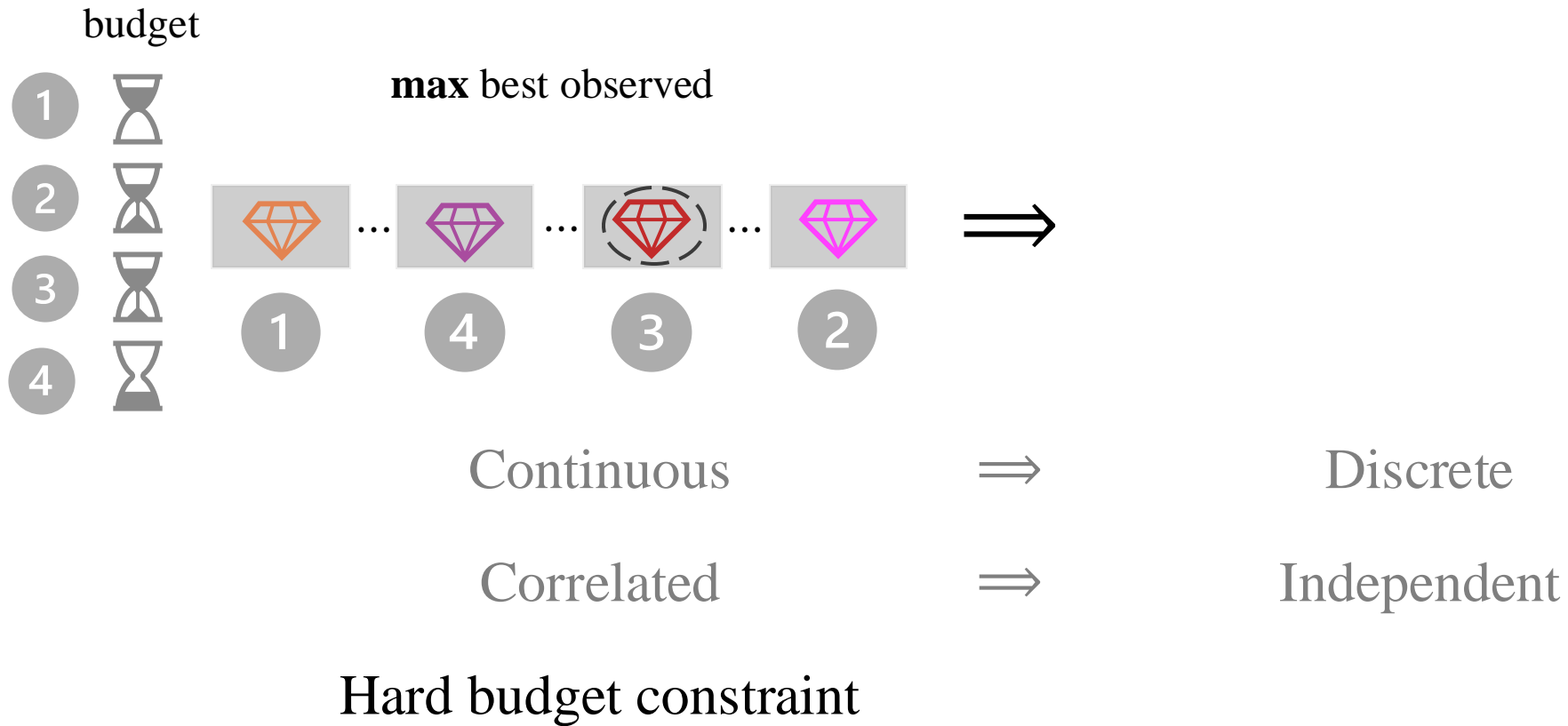
Correlated



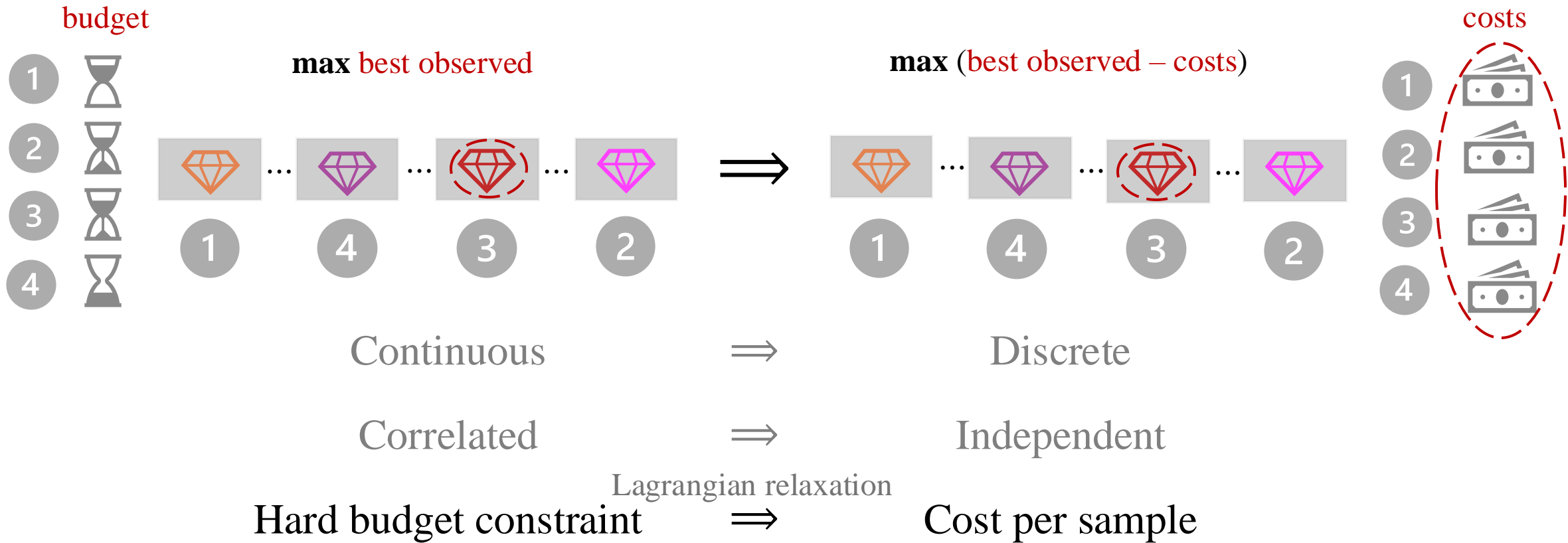
Independent

Hard budget constraint

# Bayesian Optimization

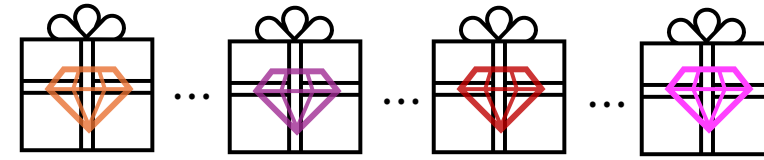
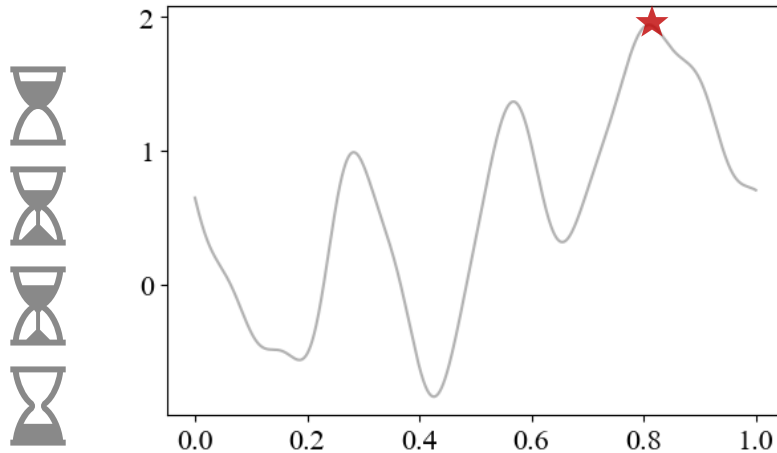


# Bayesian Optimization



# Bayesian Optimization $\Rightarrow$ Pandora's Box

[Weitzman'79]



Continuous



Discrete

Correlated



Independent

Hard budget constraint

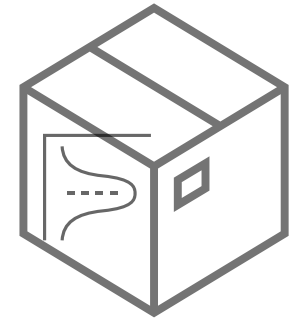
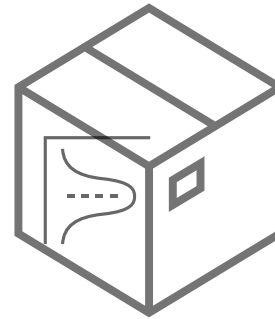
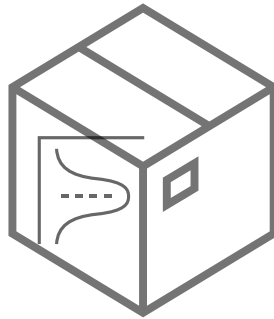
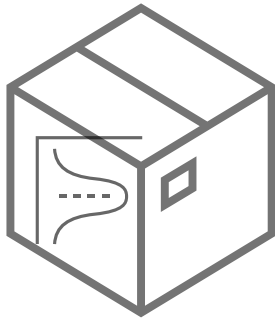


Cost per sample



# Pandora's Box

$t = 0$

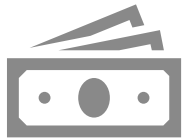
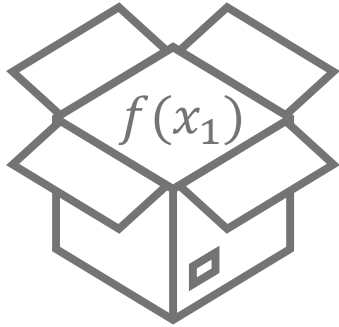


**Objective:** maximize net utility

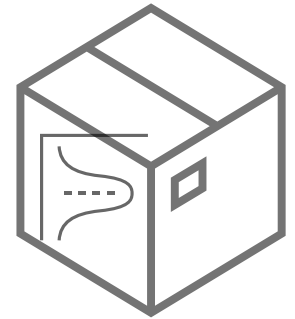
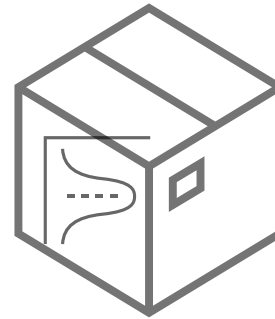
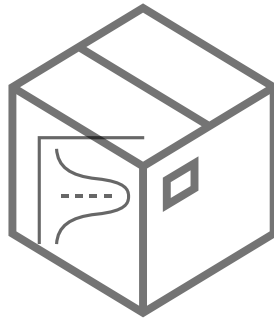
**Decision:** adaptively evaluate a random number of boxes

# Pandora's Box

$t = 1$



$c(x_1)$

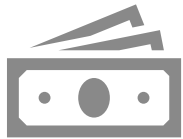
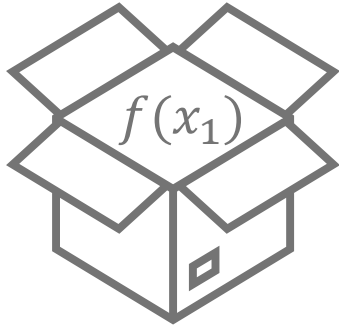


**Objective:** maximize net utility

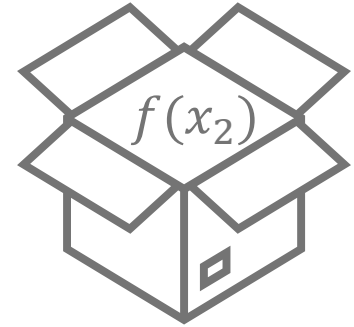
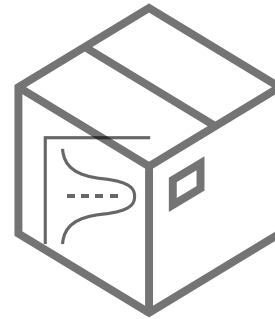
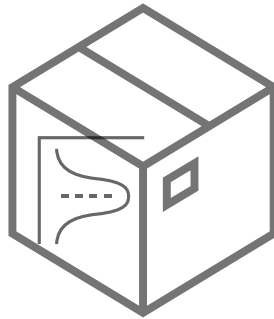
**Decision:** adaptively evaluate a random number of boxes

# Pandora's Box

$t = 2$



$c(x_1)$



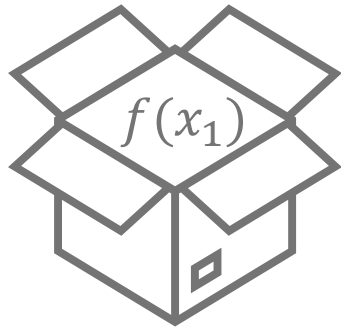
$c(x_2)$

**Objective:** maximize net utility

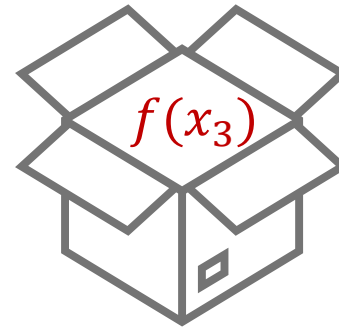
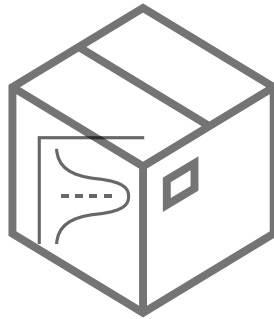
**Decision:** adaptively evaluate a random number of boxes

# Pandora's Box

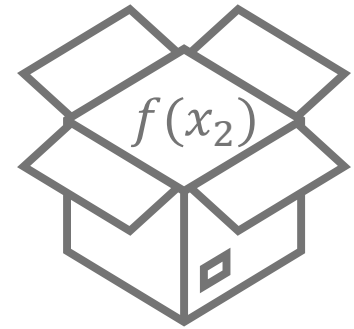
$t = 3$



$c(x_1)$



$c(x_3)$



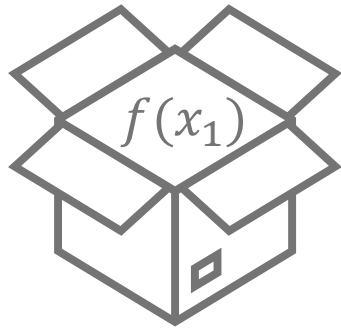
$c(x_2)$

**Objective:** maximize net utility

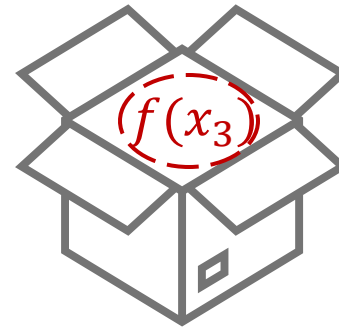
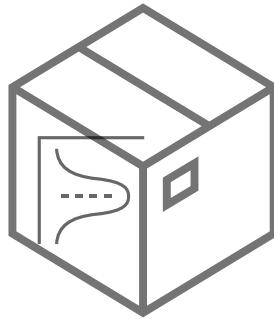
**Decision:** adaptively evaluate a random number of boxes

# Pandora's Box

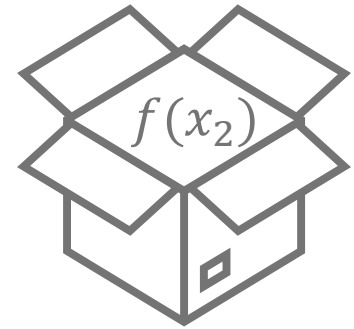
$t = 3$



$c(x_1)$



$c(x_3)$



$c(x_2)$

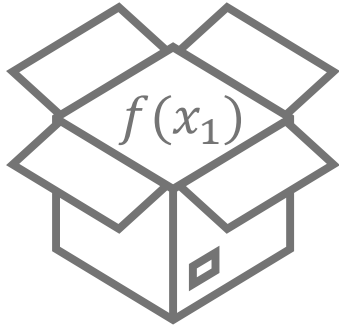
**Objective:** maximize **net utility**

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

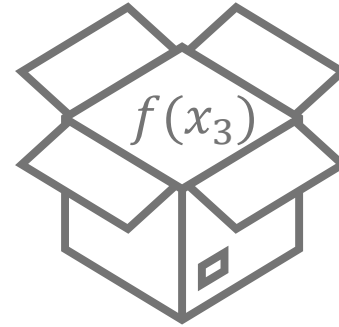
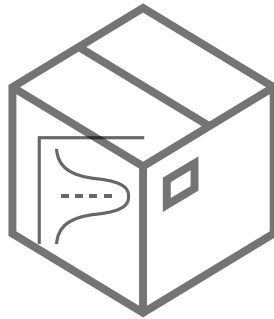
**max** (**best observed value** – **total costs**)

# Pandora's Box

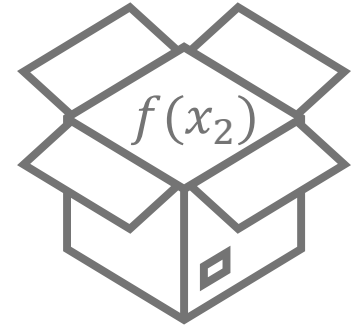
$t = 3$



$c(x_1)$



$c(x_3)$



$c(x_2)$

**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

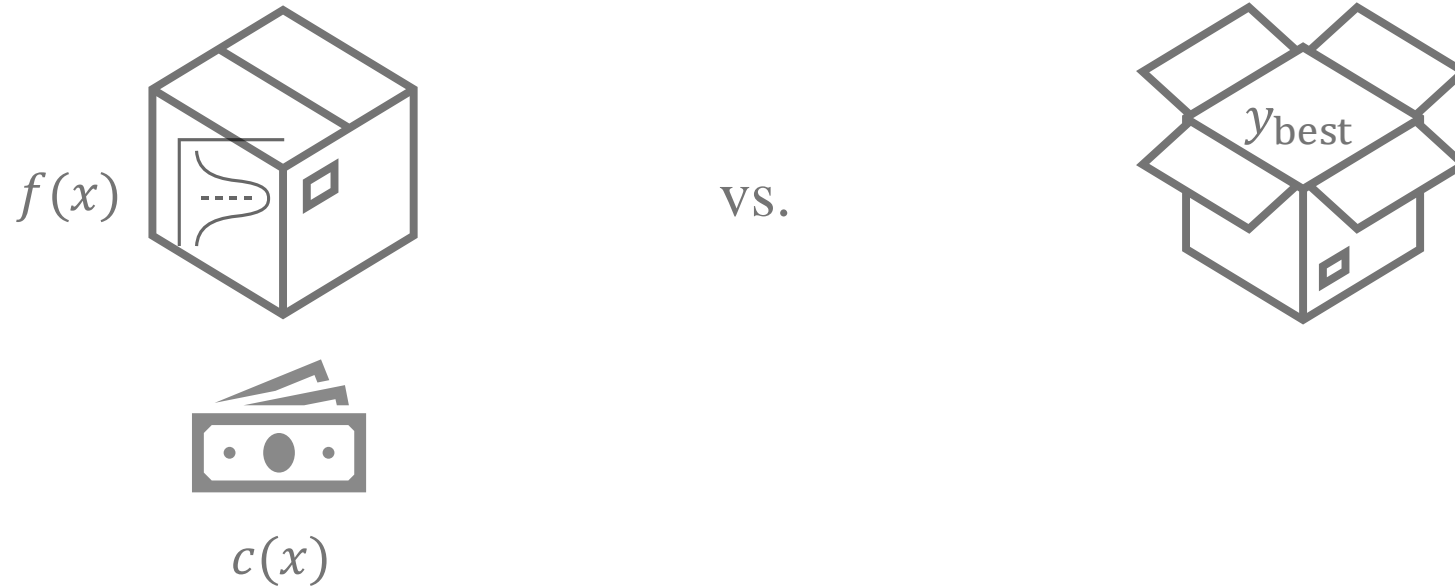
$$x_1, x_2, \dots, x_T \in \mathcal{X}$$

$\mathcal{X}$ : discrete

$T$ : random stopping time

# Naïve Greedy policy can fail [Singla'18]

## Naïve Greedy policy



**Inspection rule:**  $\operatorname{argmax}_x (\operatorname{El}_f(x; y_{\text{best}}) - c(x))$

expected improvement - cost

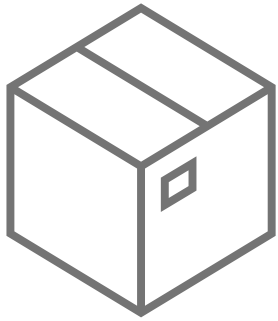
**Stopping rule:**  $\operatorname{El}_f(x; y_{\text{best}}) \leq c(x), \forall x \in \mathcal{X}$

expected improvement  $\leq$  cost

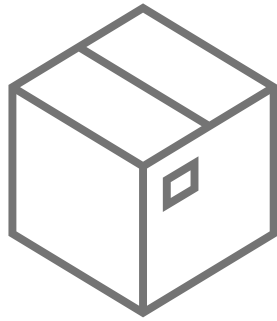
$y_{\text{best}}$ : current best observed value

$\operatorname{El}_f(x; y) := \mathbb{E}[(f(x) - y)^+]$ : expected improvement of  $f(x)$  over  $y$

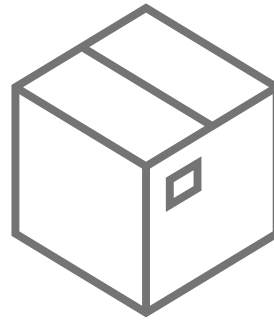
# Naïve Greedy policy can fail [Singla'18]



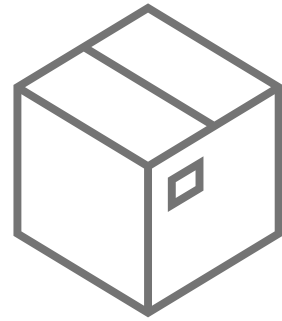
$$\begin{aligned} f(1) &= 200 \text{ w.p. } 1 \\ c(1) &= 198 \end{aligned}$$



...



...



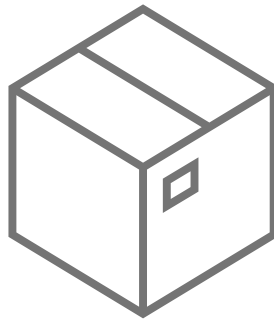
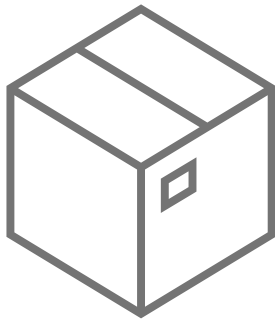
$$f(x) = \begin{cases} 200 & \text{w.p. } 0.01 \\ 0 & \text{otherwise} \end{cases}, c(x) = 1, x \in \{2, 3, \dots, 1000\}$$



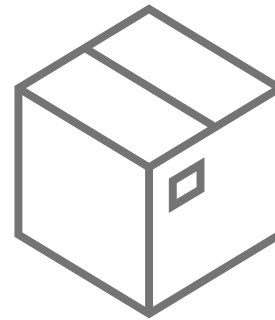
# Naïve Greedy policy can fail [Singla'18]

$t = 0$

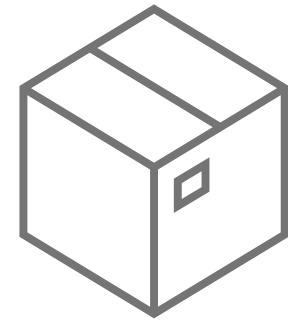
$y_{\text{best}} = 0$



...



...



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

$$\begin{aligned} \text{EI}_f(1; 0) - c(1) \\ &= 200 - 198 = 2 \end{aligned}$$

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

$$\begin{aligned} \text{EI}_f(x; 0) - c(x) \\ &= 2 - 1 = 1 \end{aligned}$$

**Inspection rule:**  $\operatorname{argmax}_x (\text{EI}_f(x; y_{\text{best}}) - c(x))$       **Stopping rule:**  $\text{EI}_f(x; y_{\text{best}}) \leq c(x), \forall x \in \mathcal{X}$

$$\text{EI}_f(x; y) := \mathbb{E}[(f(x) - y)^+]$$

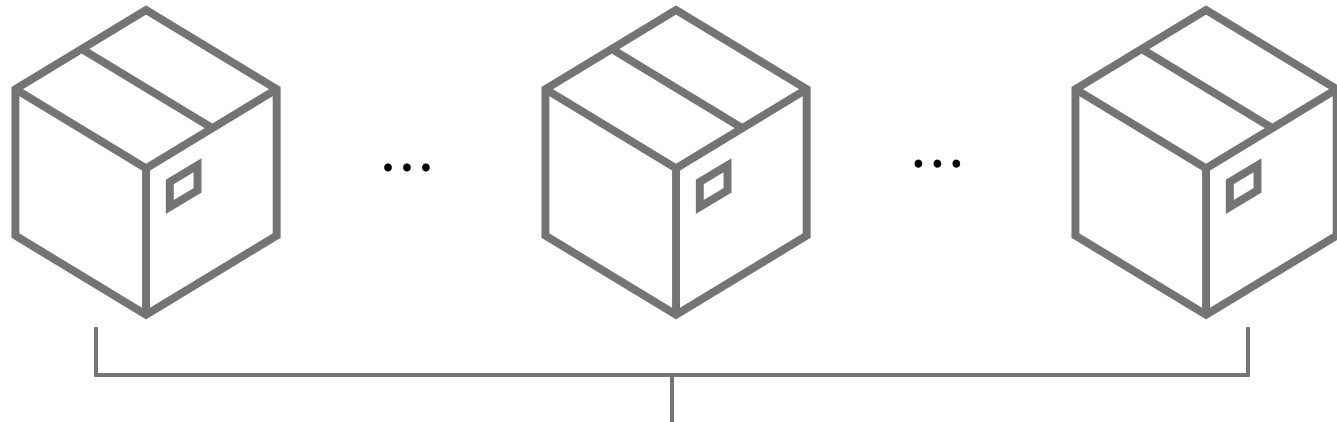
# Naïve Greedy policy can fail [Singla'18]

$t = 1$

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



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



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

$$\begin{aligned} & \text{EI}_f(x; 200) - c(x) \\ &= 0 - 1 = -1 < 0 \end{aligned}$$

**Inspection rule:**  $\operatorname{argmax}_x (\text{EI}_f(x; y_{\text{best}}) - c(x))$       **Stopping rule:**  $\text{EI}_f(x; y_{\text{best}}) \leq c(x), \forall x \in \mathcal{X}$

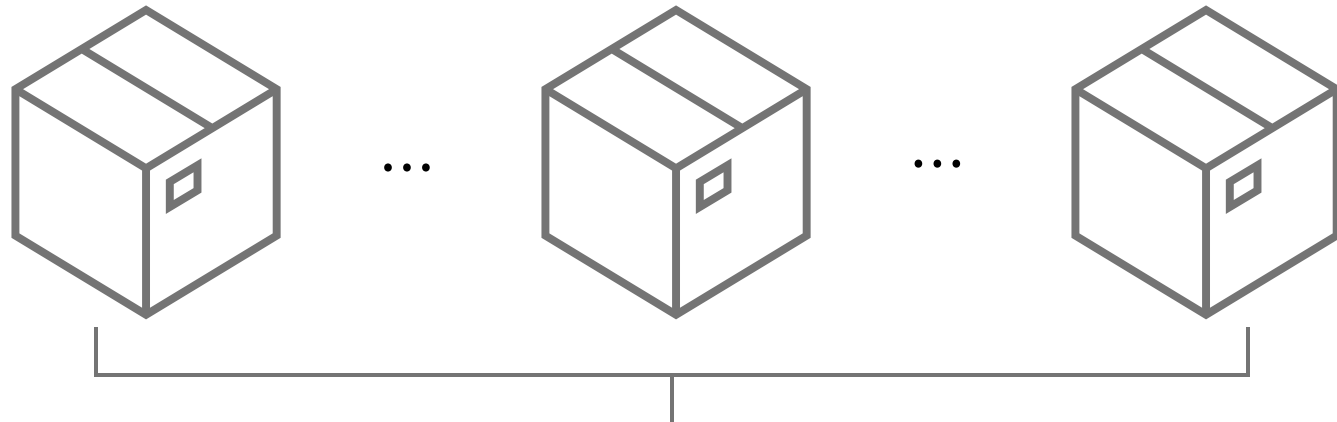
$$\text{EI}_f(x; y) := \mathbb{E}[(f(x) - y)^+]$$

# Naïve Greedy policy can fail [Singla'18]

$t = 1$



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



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

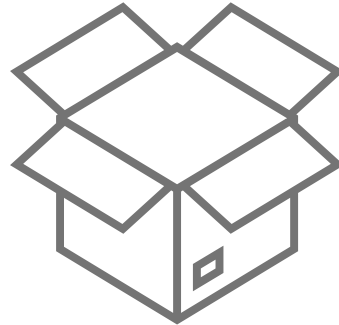
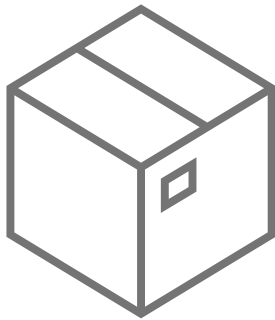
**Inspection rule:**  $\operatorname{argmax}_x (\operatorname{El}_f(x; y_{\text{best}}) - c(x))$       **Stopping rule:**  $\operatorname{El}_f(x; y_{\text{best}}) \leq c(x), \forall x \in \mathcal{X}$

Expected utility:  $\mathbb{E}[\text{Greedy}] = 200 - 198 = 2$

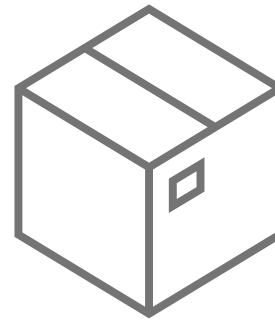
# Naïve Greedy policy can fail [Singla'18]

$t \approx 100$

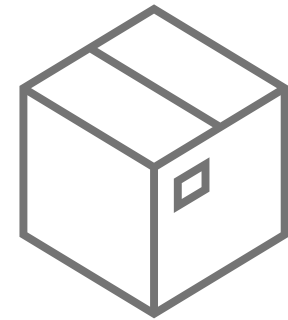
$y_{\text{best}} = 200$



...



...



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

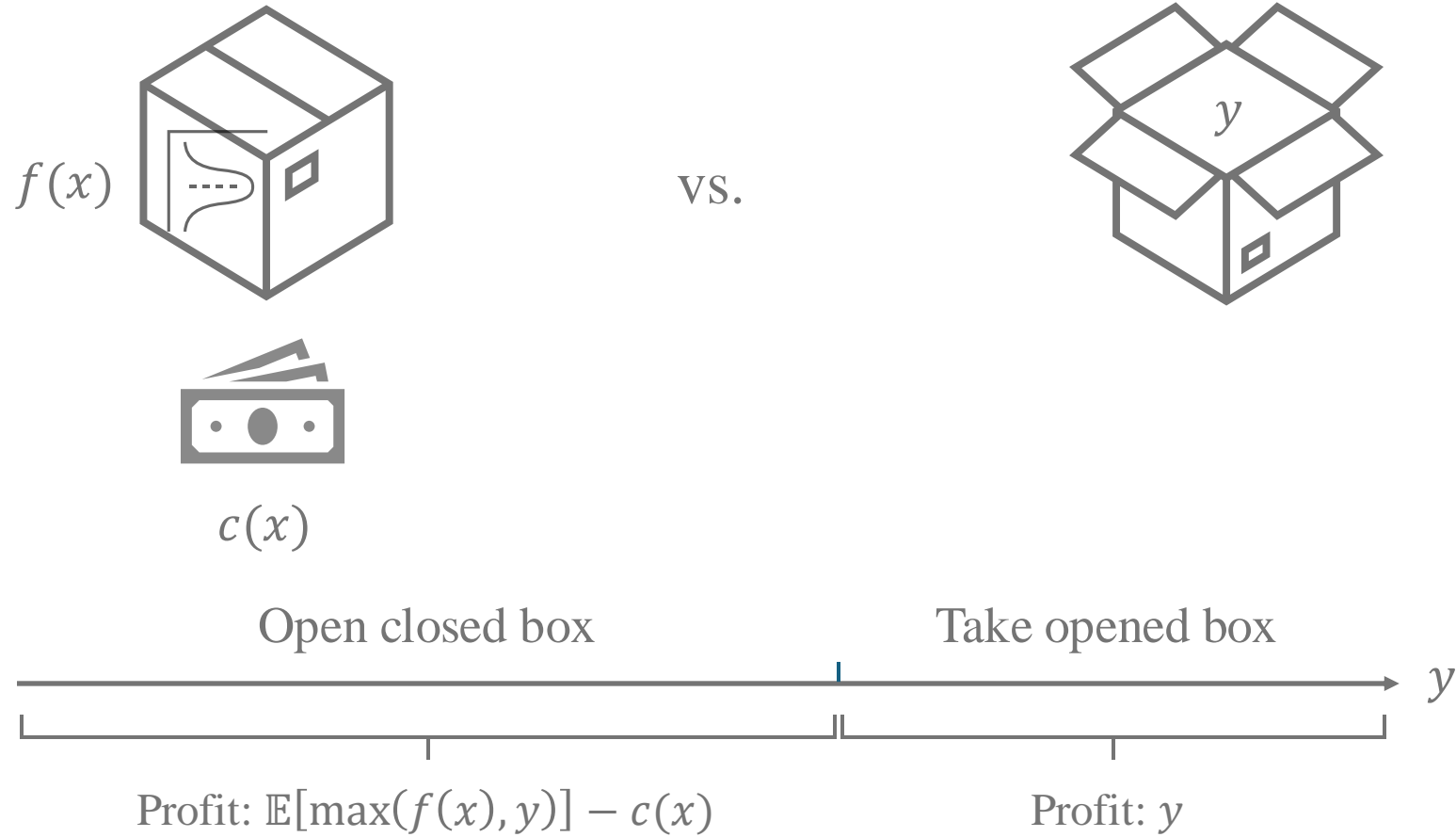
$$f(x) = \begin{cases} 200 & \text{w.p. } 0.01 \\ 0 & \text{otherwise} \end{cases}, c(x) = 1, x \in \{2, 3, \dots, 1000\}$$

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

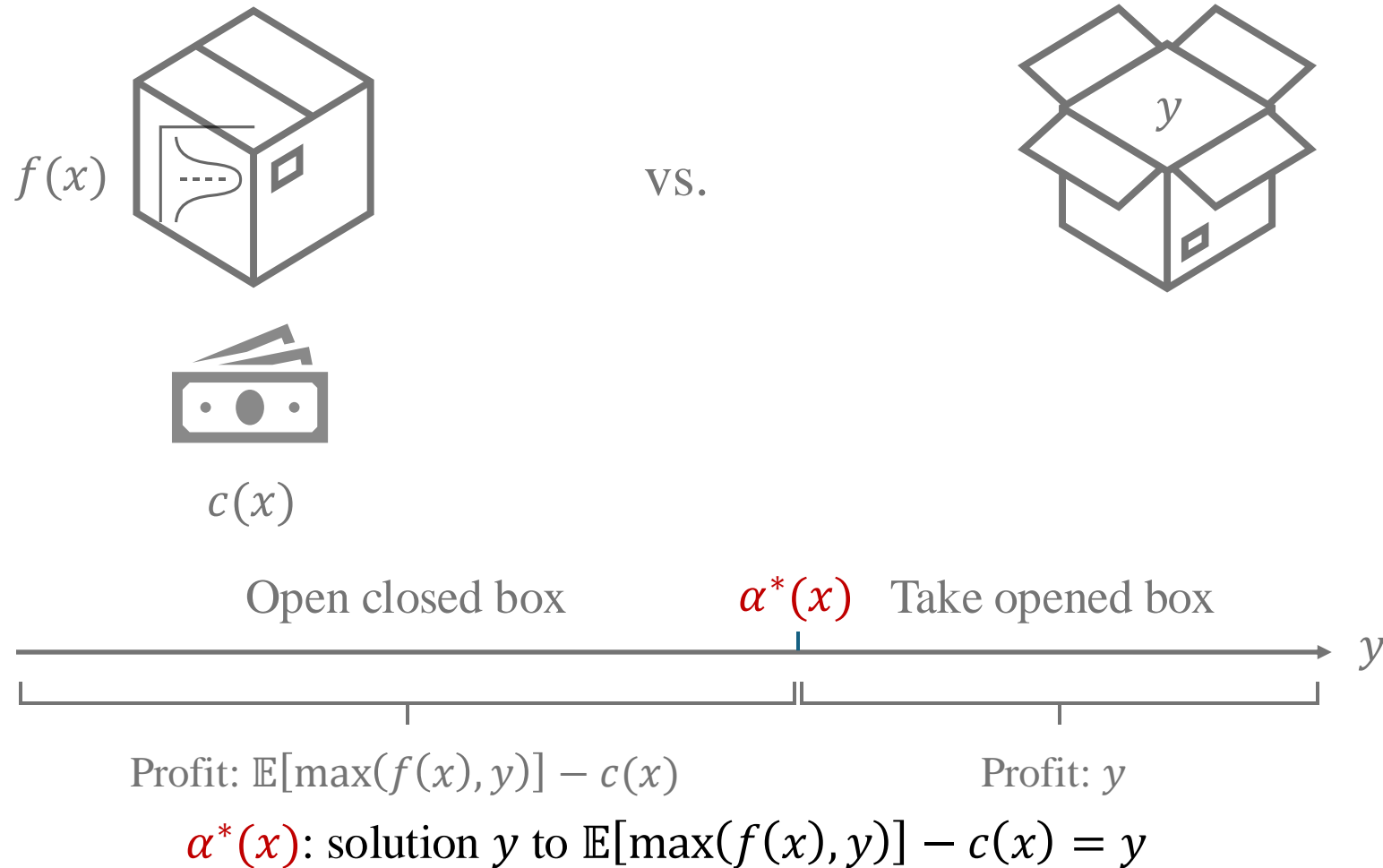
**Stopping rule:**  $y_{\text{best}} = 200$

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

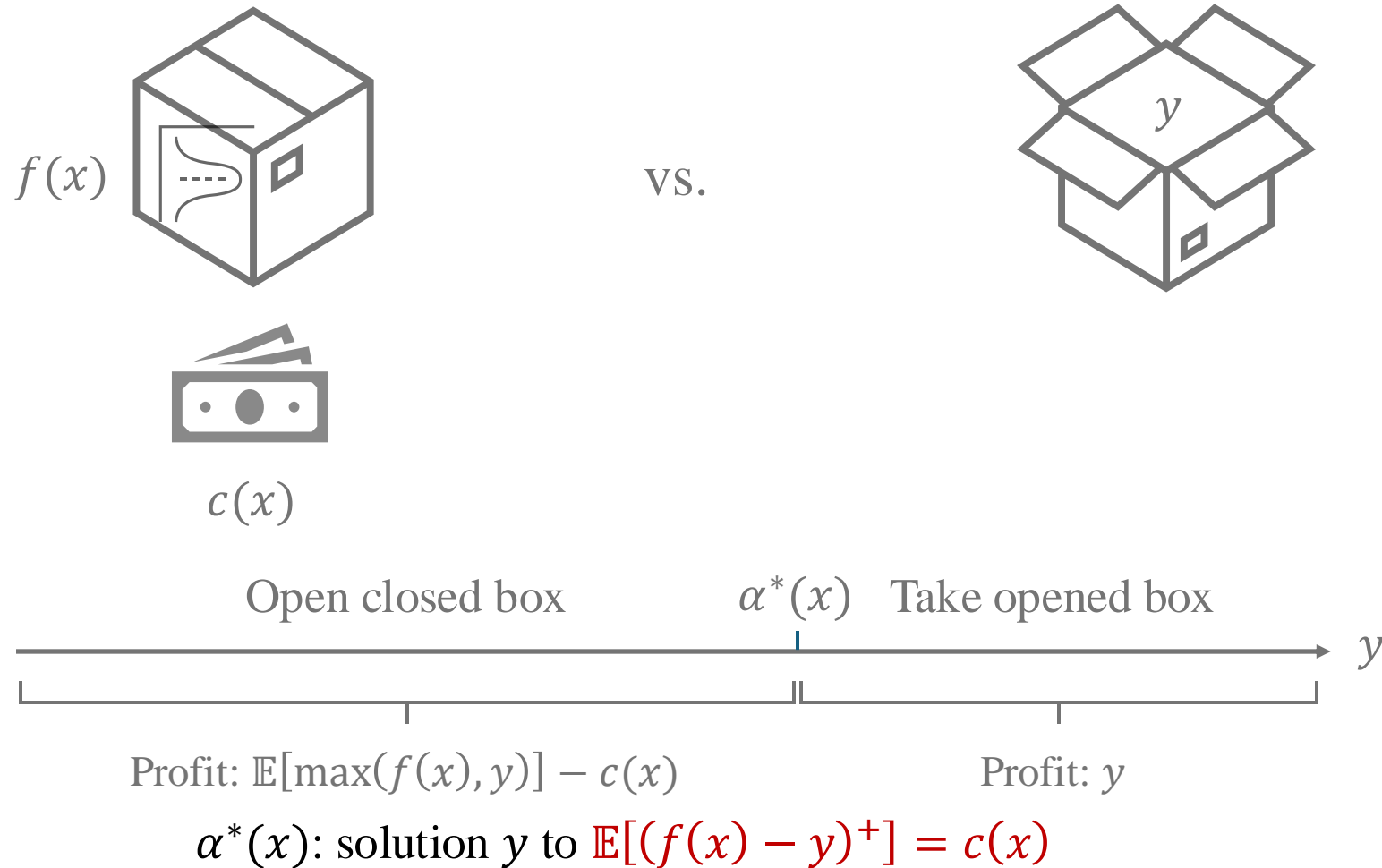
# 1.5-Box Problem



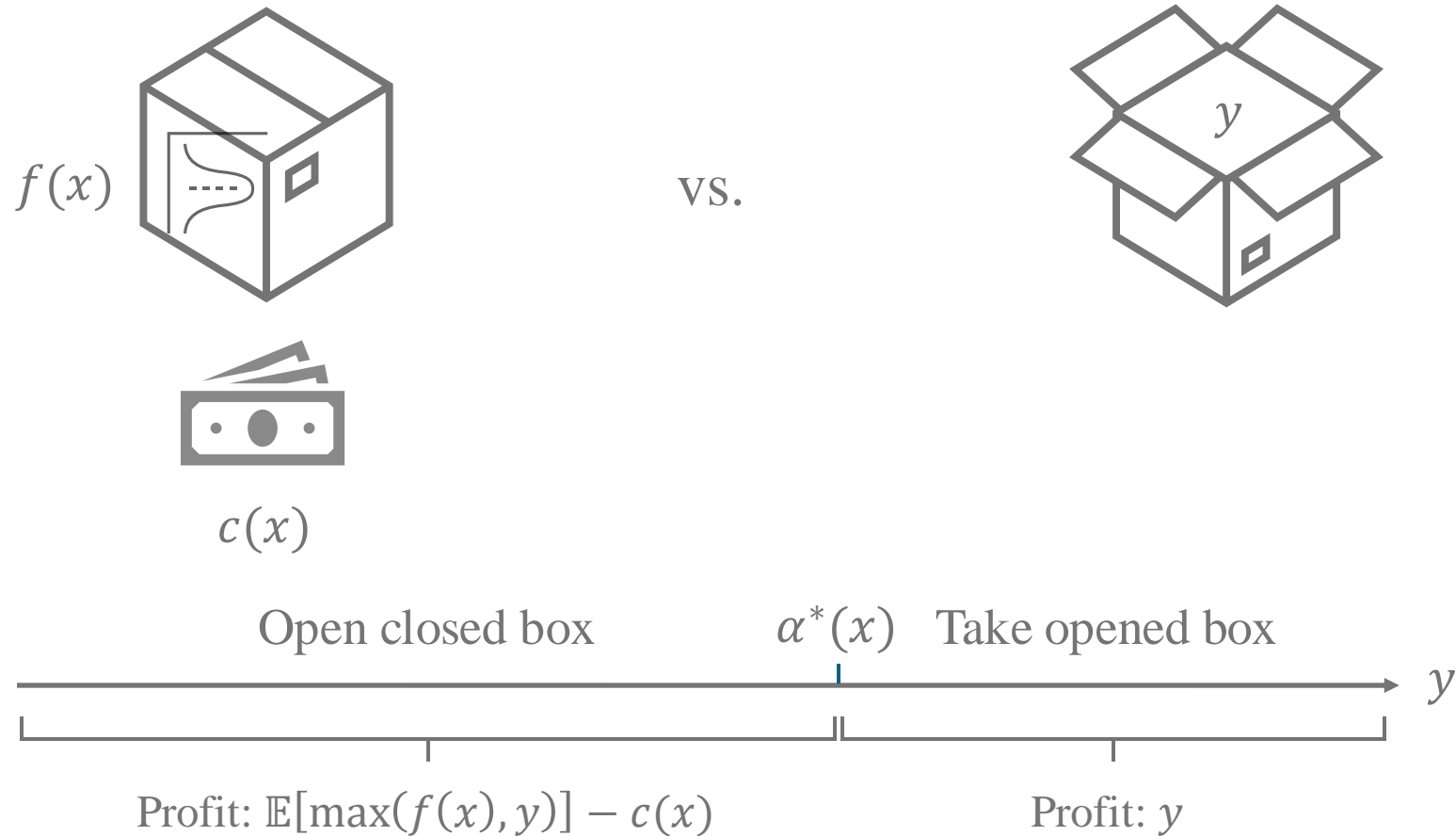
# 1.5-Box Problem



# 1.5-Box Problem



# 1.5-Box Problem



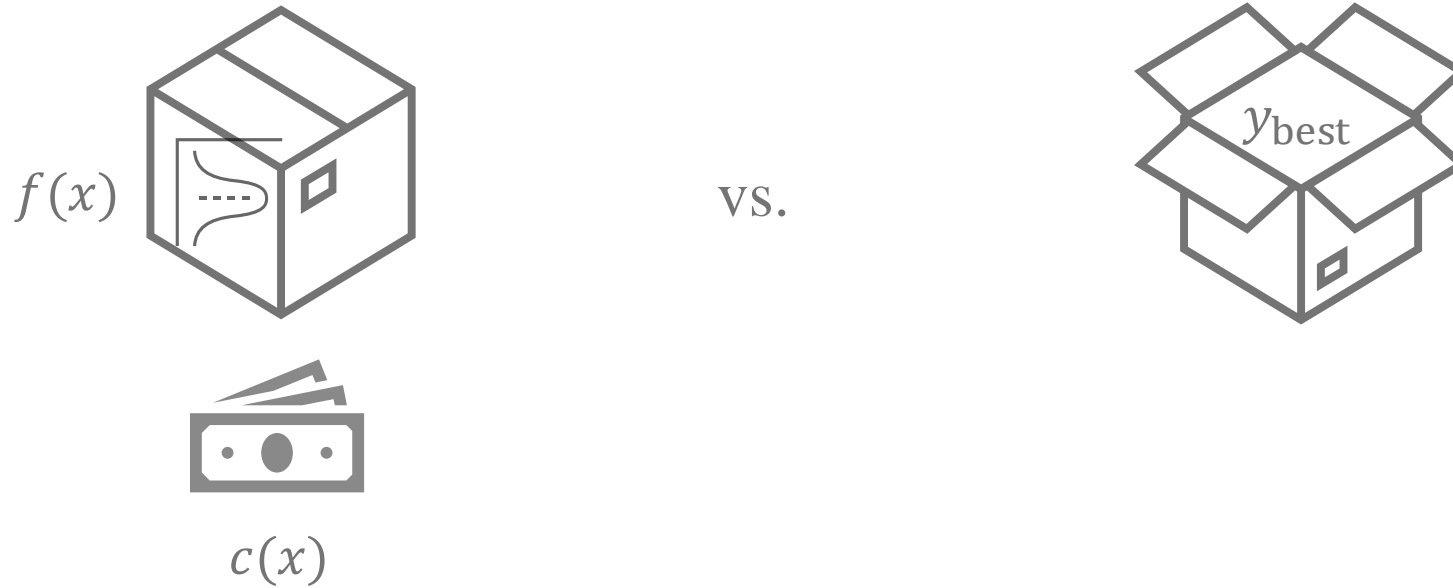
$\alpha^*(x)$ : solution  $y$  to  $\mathbb{E}[(f(x) - y)^+] = c(x)$

$\alpha^*(x)$ : Gittins index!



# Optimal policy: Gittins policy

Gittins policy



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

solution to expected improvement = cost

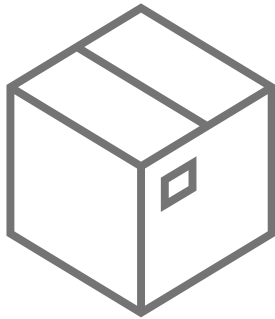
Gittins index  $\leq$  current best

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

$\operatorname{El}_f(x; y) := \mathbb{E}[(f(x) - y)^+]$ : expected improvement of  $f(x)$  over  $y$

# Optimal policy: Gittins policy

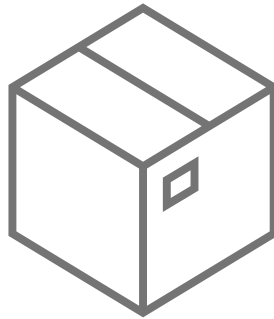
$t = 0$



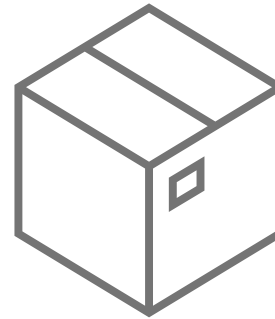
$$f(1) = 200 \text{ w. p. } 1$$

$$c(1) = 198$$

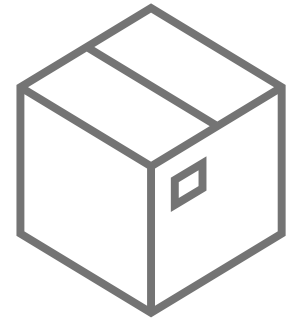
$$200 - ? = 198$$



...



...



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

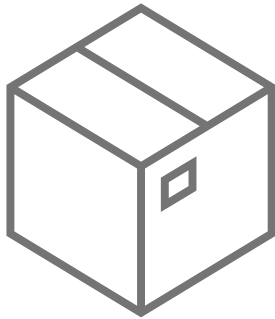
$$(200 - ?) * 0.01 = 1$$

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

$$\operatorname{El}_f(x; y) := \mathbb{E}[(f(x) - y)^+]$$

# Optimal policy: Gittins policy

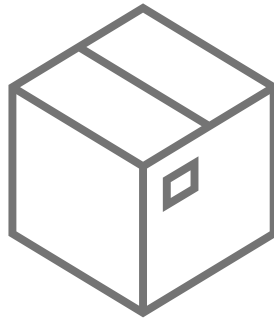
$t = 0$



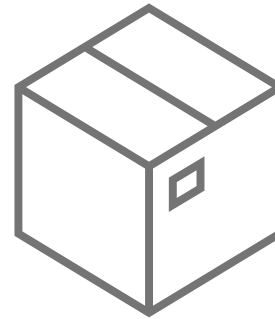
$$f(1) = 200 \text{ w.p. } 1$$

$$c(1) = 198$$

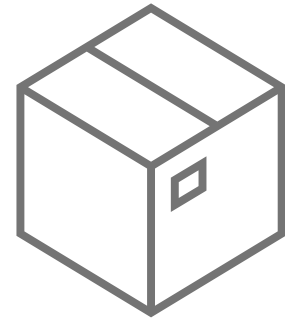
$$\alpha^*(1) = 2$$



...



...



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

$$\alpha^*(x) = 100$$

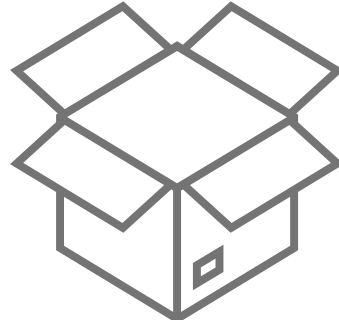
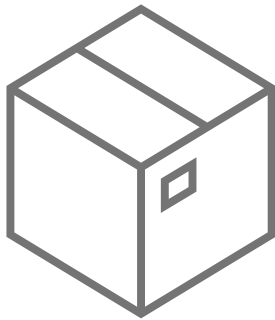
**Inspection rule:**  $\operatorname{argmax}_x \alpha^*(x)$  s.t.  $\operatorname{El}_f(x; \alpha^*(x)) = c(x)$  **Stopping rule:**  $\alpha^*(x) \leq y_{\text{best}}, \forall x \in \mathcal{X}$

$$\operatorname{El}_f(x; y) := \mathbb{E}[(f(x) - y)^+]$$

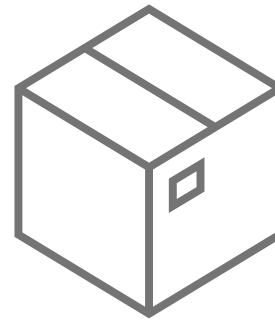
# Optimal policy: Gittins policy

$t = 1$

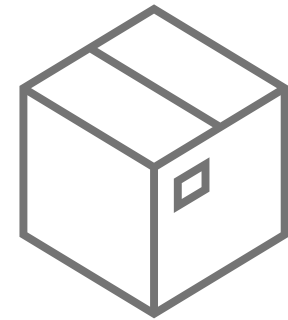
$y_{\text{best}} = 200 \text{ or } 0$



...



...



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

$$\alpha^*(1) = 2$$

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

$$\alpha^*(x) = 100$$

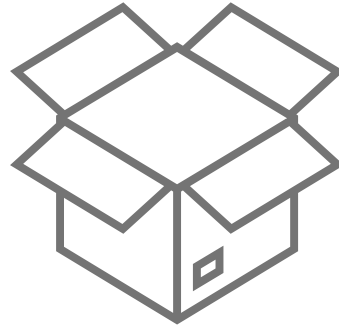
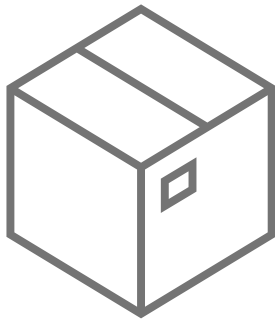
**Inspection rule:**  $\operatorname{argmax}_x \alpha^*(x)$  s.t.  $\operatorname{El}_f(x; \alpha^*(x)) = c(x)$  **Stopping rule:**  $\alpha^*(x) \leq y_{\text{best}}, \forall x \in \mathcal{X}$

$$\operatorname{El}_f(x; y) := \mathbb{E}[(f(x) - y)^+]$$

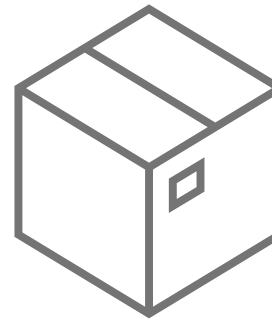
# Optimal policy: Gittins policy

$t \approx 100$

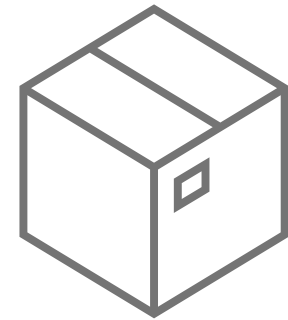
$y_{\text{best}} = 200$



...



...



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

$$\alpha^*(1) = 2$$

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

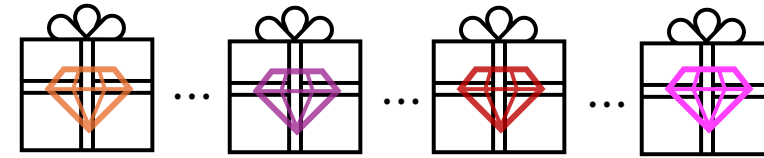
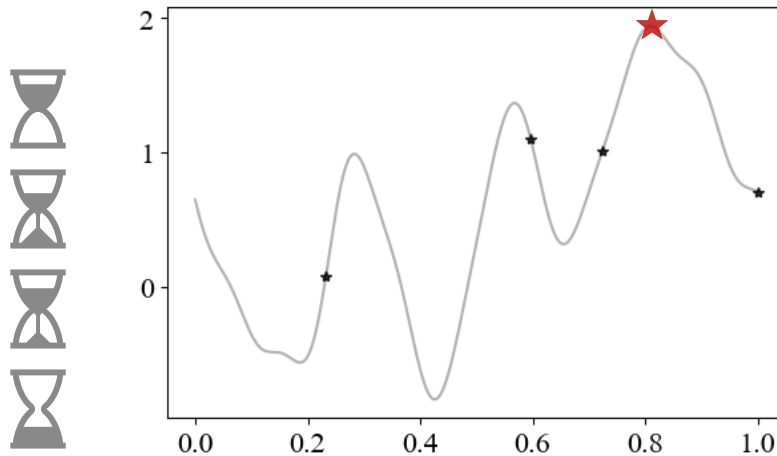
$$\alpha^*(x) = 100$$

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

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

# Bayesian Optimization $\Rightarrow$ Pandora's Box

Special case of Markovian/  
Bayesian multi-armed bandits



Continuous



Discrete

Correlated



Independent

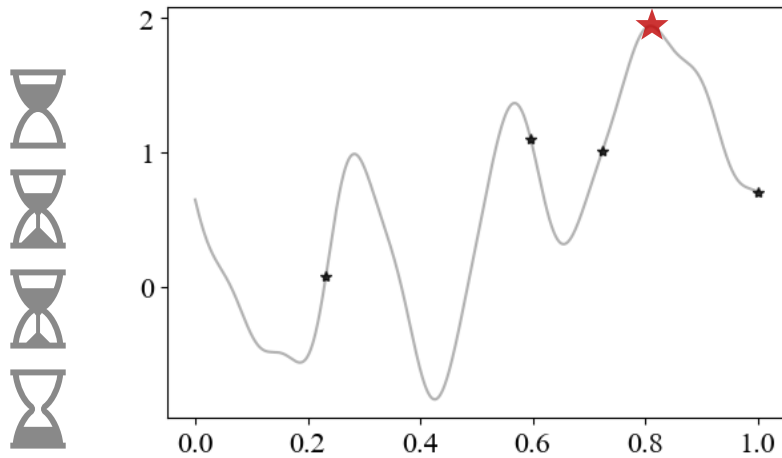
Hard budget constraint



Cost per sample

Optimal policy: Gittins index [Weitzman'79]

# Bayesian Optimization $\Rightarrow$ Pandora's Box

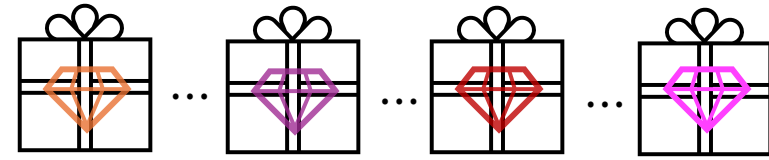


Continuous

Correlated

Hard budget constraint

Is Gittins index good?



Discrete

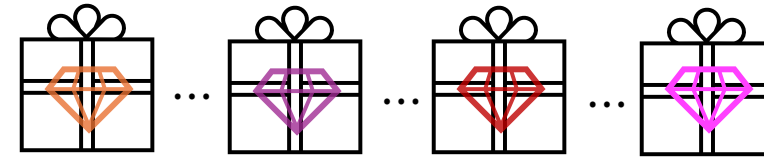
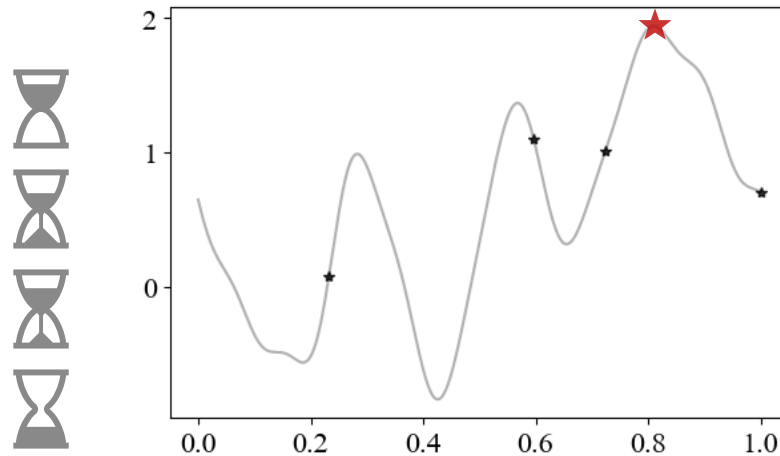
Independent

Cost per sample



Optimal policy: Gittins index

# Bayesian Optimization $\Rightarrow$ Pandora's Box



Continuous



Discrete

Correlated



Independent

Hard budget constraint



Cost per sample

Is Gittins index good?

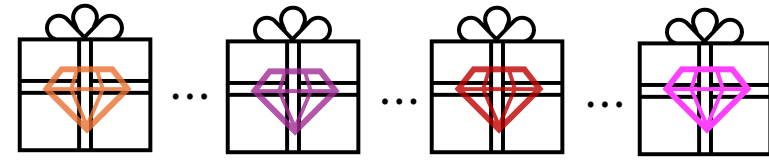
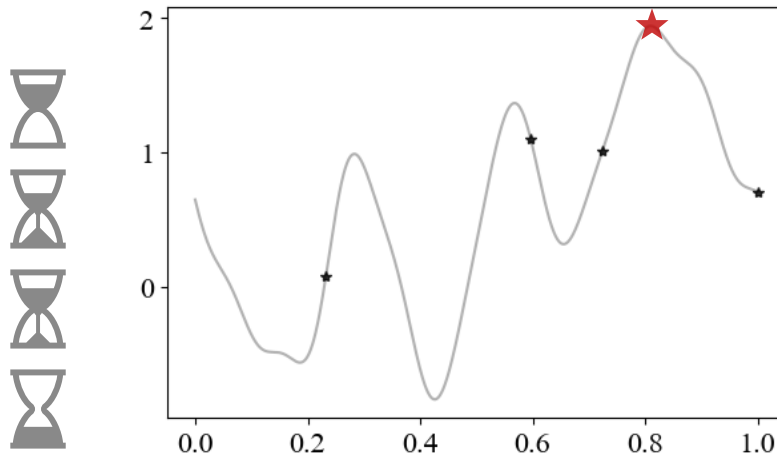
How to translate?



Optimal policy: Gittins index



# Bayesian Optimization $\Rightarrow$ Pandora's Box



Continuous



Discrete

Correlated



Independent

Hard budget constraint



Cost per sample

Is Gittins index good?

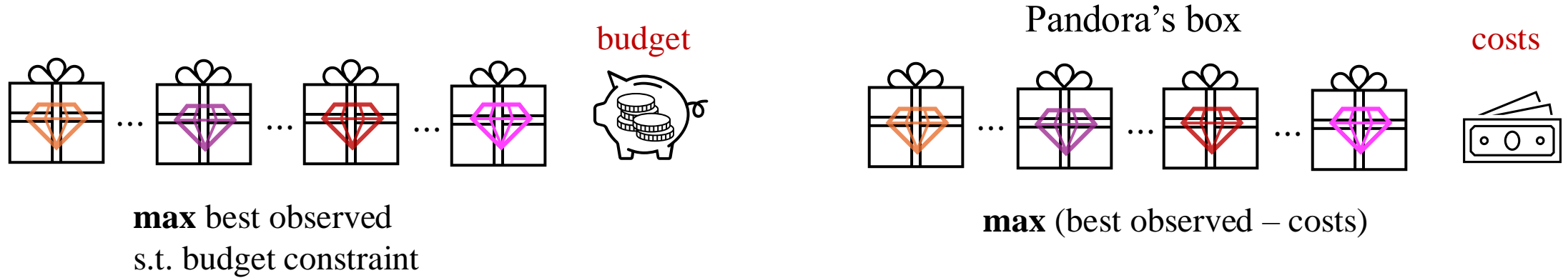
How to translate?



Optimal policy: Gittins index

Our contributions!

# How to translate?



Expected budget constraint



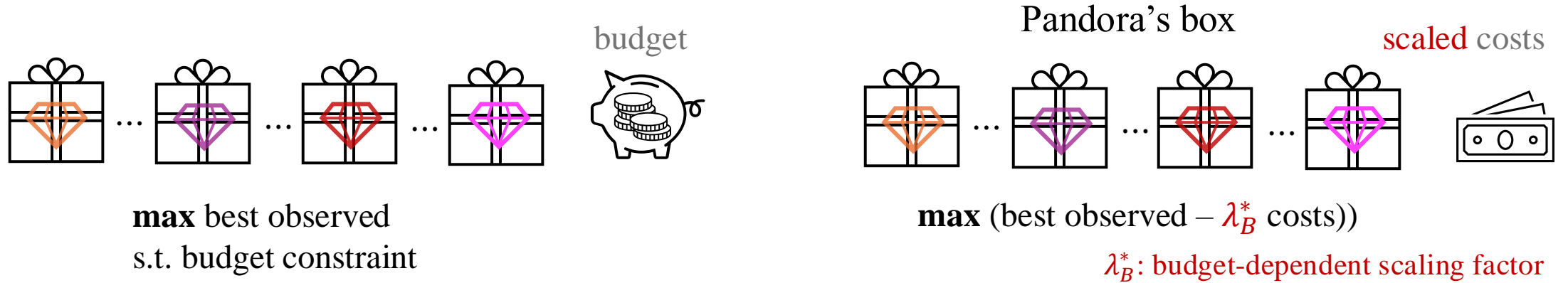
Cost per sample

Optimal policy?



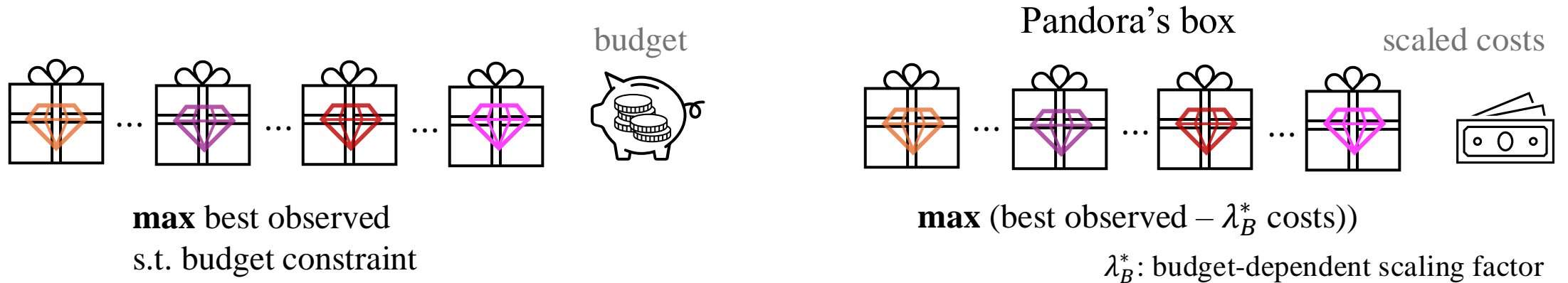
Optimal policy: Gittins index

# Expected budget constraint $\Leftrightarrow$ Cost per sample



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

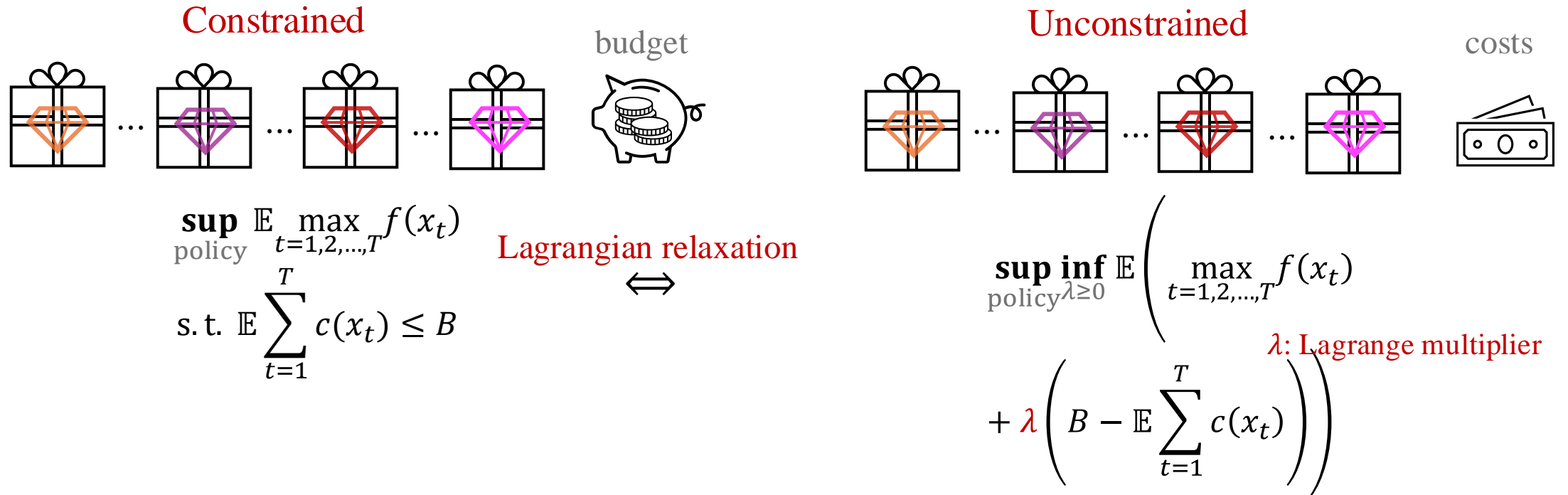
# Expected budget constraint $\Leftrightarrow$ Cost per sample



Reward distribution	Reference
finite support	[Aminian, Manshadi, Niazadeh'24]
general support	our work

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

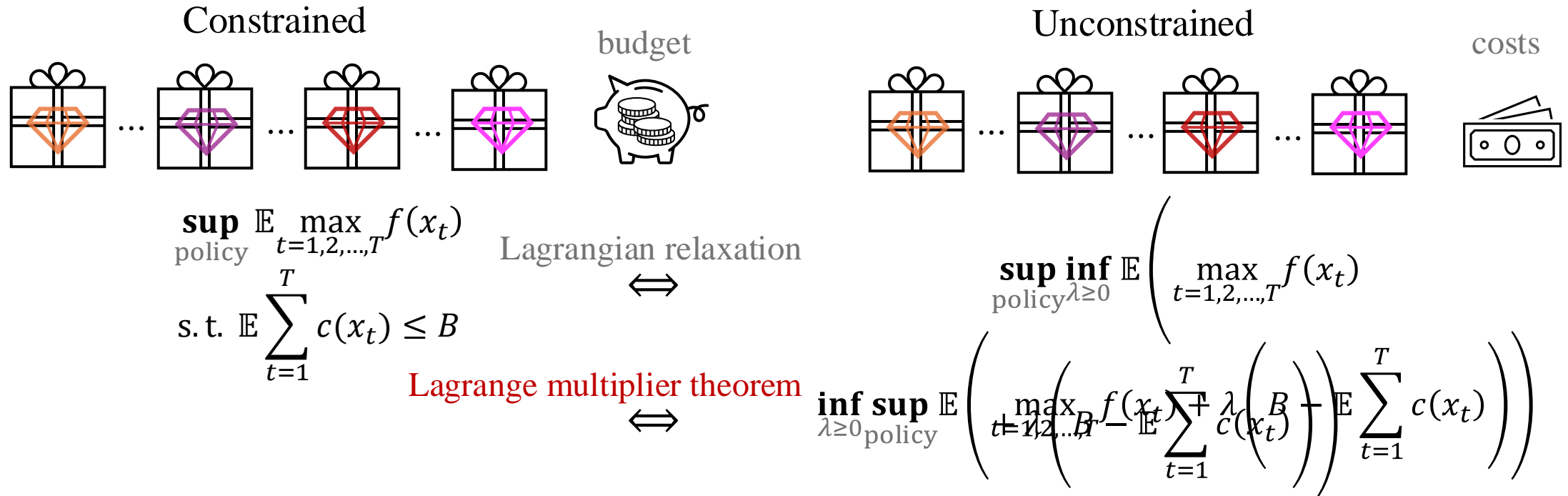
# Expected budget constraint $\Leftrightarrow$ Cost per sample



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

Extension to [Aminian, Manshadi, Niazadeh'24]

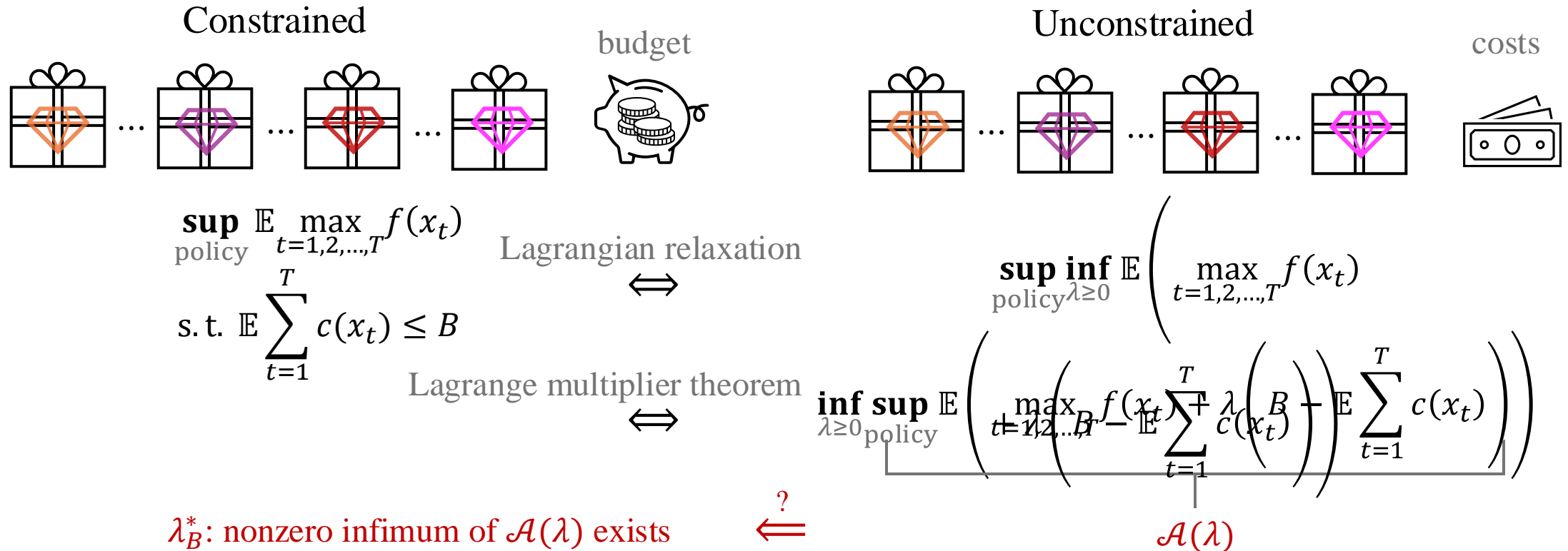
# Expected budget constraint $\Leftrightarrow$ Cost per sample



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

Extension to [Aminian, Manshadi, Niazadeh'24]

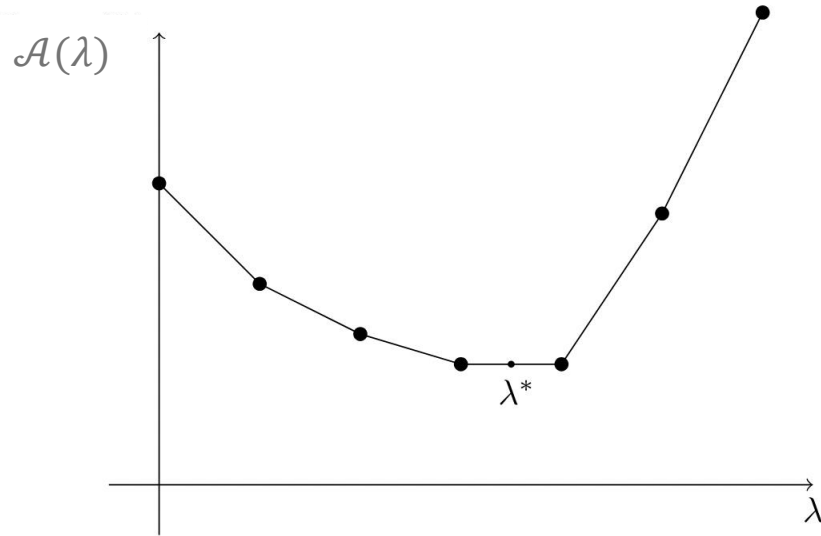
# Expected budget constraint $\Leftrightarrow$ Cost per sample



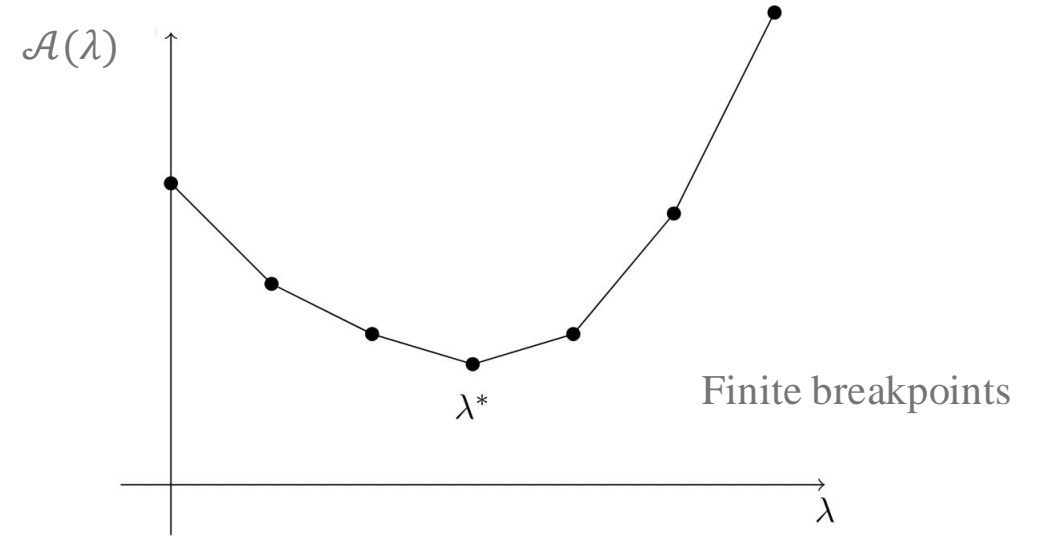
Optimal policy: Gittins solution to Pandora's box with scaled costs  $\Leftarrow$  Optimal policy: Gittins index

Extension to [Aminian, Manshadi, Niazadeh'24]

# Expected budget constraint $\Leftrightarrow$ Cost per sample



(a) Degenerate case, differentiable at  $\lambda^*$ .



(b) Non-degenerate case, breakpoint at  $\lambda^*$ .

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

Envelope Theorem

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

$\Leftrightarrow$

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

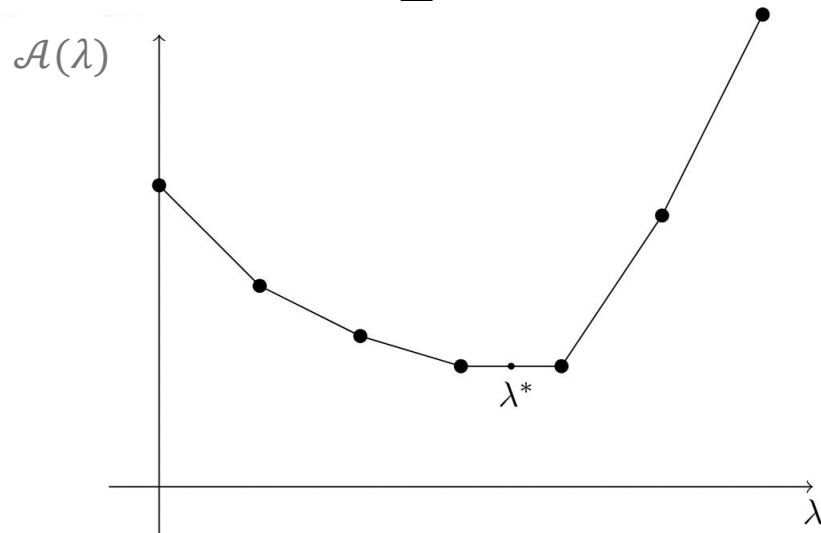
Optimal policy: Gittins solution to  
Pandora's box with scaled costs

$\Leftrightarrow$

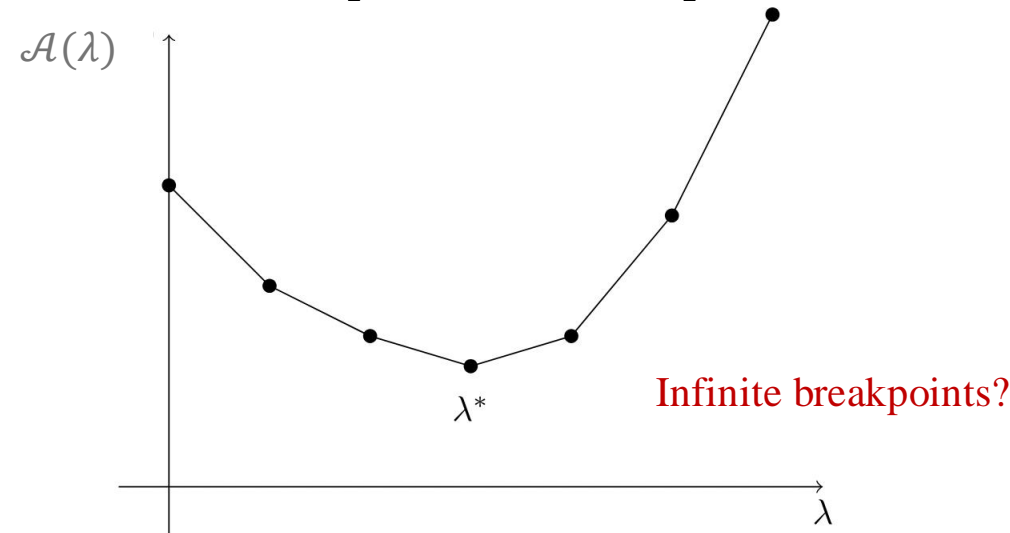
Optimal policy: Gittins index



# Expected budget constraint $\Leftrightarrow$ Cost per sample



(a) Degenerate case, differentiable at  $\lambda^*$ .



(b) Non-degenerate case, breakpoint at  $\lambda^*$ .

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

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

$\Leftrightarrow$

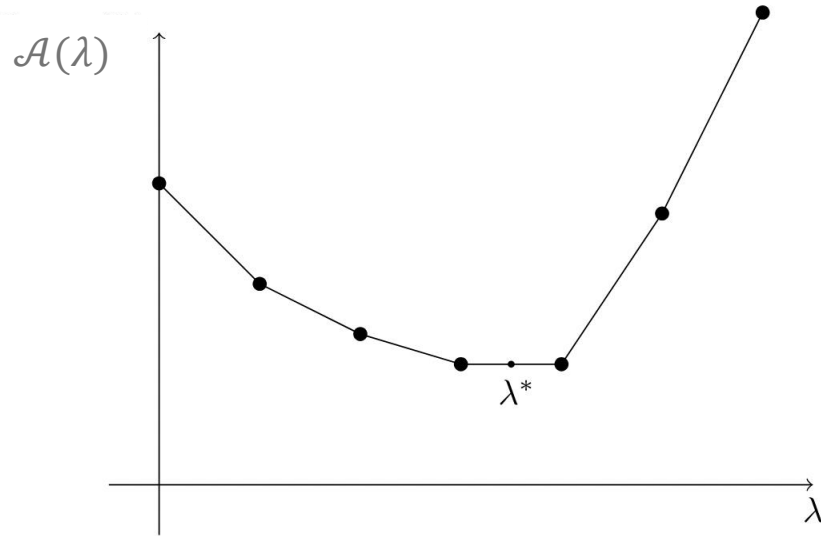
$\mathcal{A}(\lambda)$ : convex (possibly non-differentiable) in  $\lambda$

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

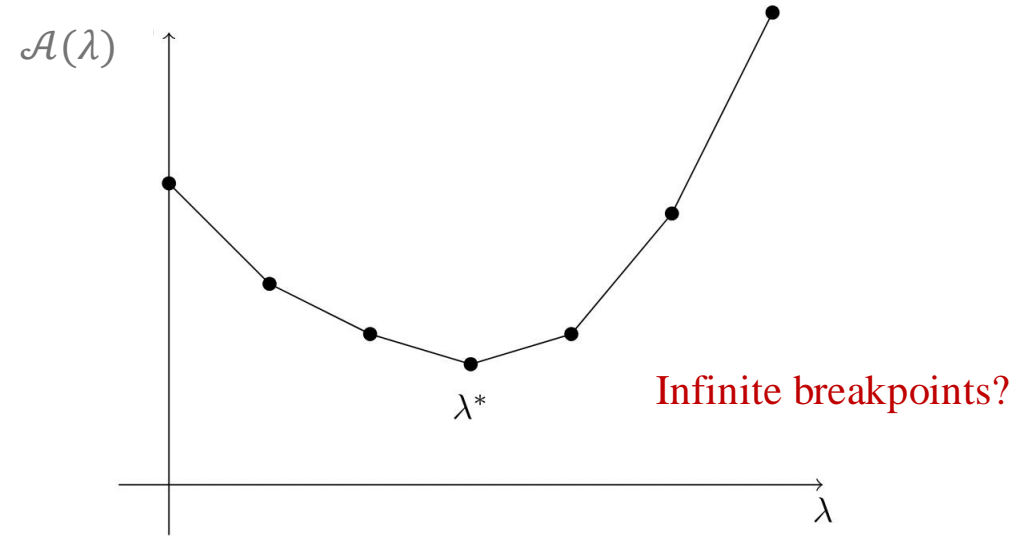
$\Leftrightarrow$

Optimal policy: Gittins index

# Expected budget constraint $\Leftrightarrow$ Cost per sample



(a) Degenerate case, differentiable at  $\lambda^*$ .



(b) Non-degenerate case, breakpoint at  $\lambda^*$ .

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

Our work: sharp Envelope Theorem

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

$\Leftrightarrow$

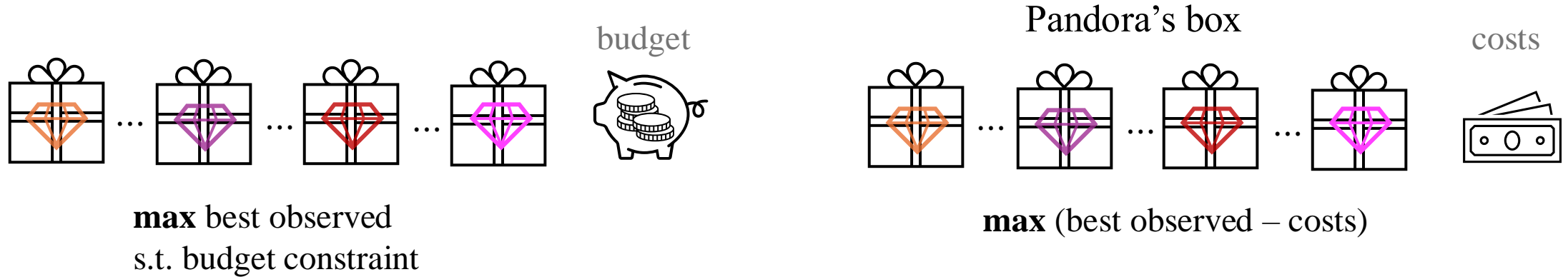
$\mathcal{A}(\lambda)$ : convex (possibly non-differentiable) in  $\lambda$

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

$\Leftrightarrow$

Optimal policy: Gittins index

# How to translate?



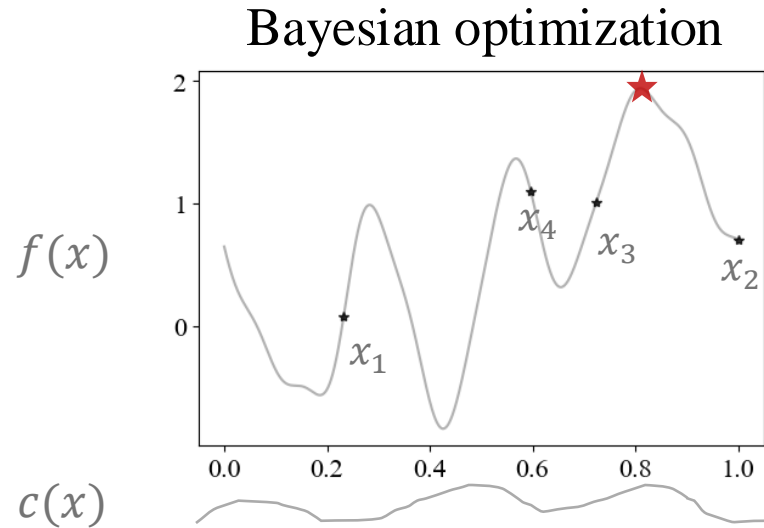
Hard budget constraint

$\Leftarrow$

Cost per sample

$$\operatorname{argmax}_x \alpha^*(x) \text{ s.t. } \operatorname{El}_f(x; \alpha^*(x)) = \lambda_B^* c(x) \Leftarrow \operatorname{argmax}_x \alpha^*(x) \text{ s.t. } \operatorname{El}_f(x; \alpha^*(x)) = c(x)$$

# How to translate?

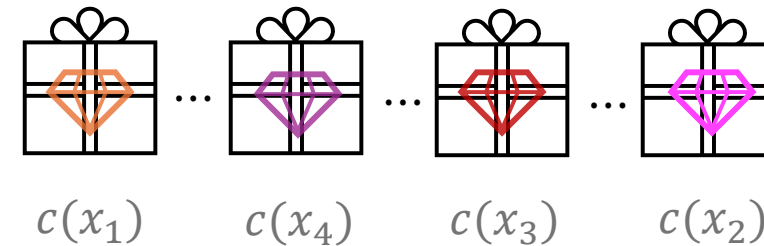


Continuous

Correlated

Hard budget constraint

Budget-constrained  
Pandora's box



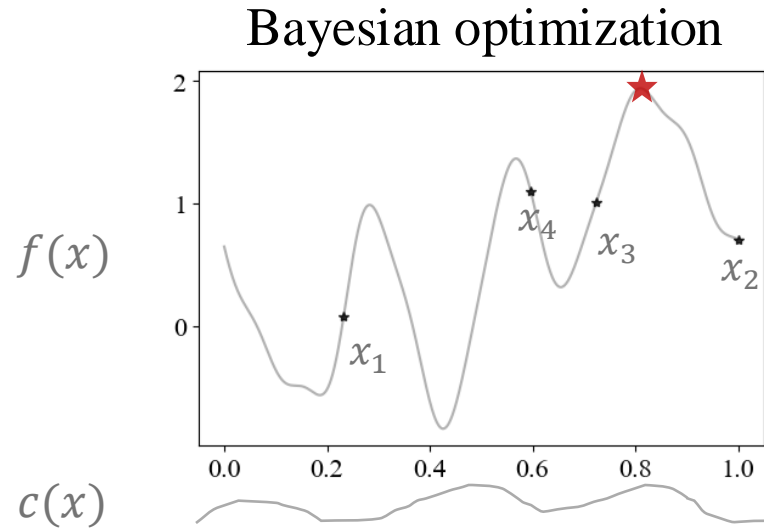
Discrete

Independent

Cost per sample

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

# How to translate?

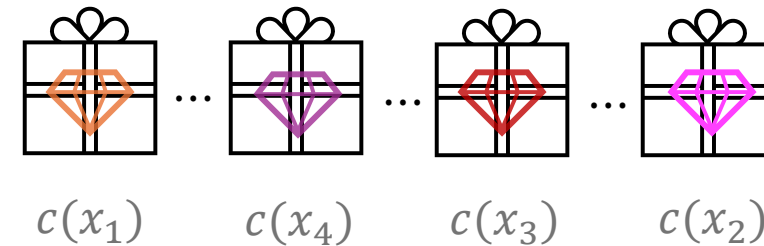


Continuous

Correlated

Hard budget constraint

Budget-constrained  
Pandora's box



Discrete

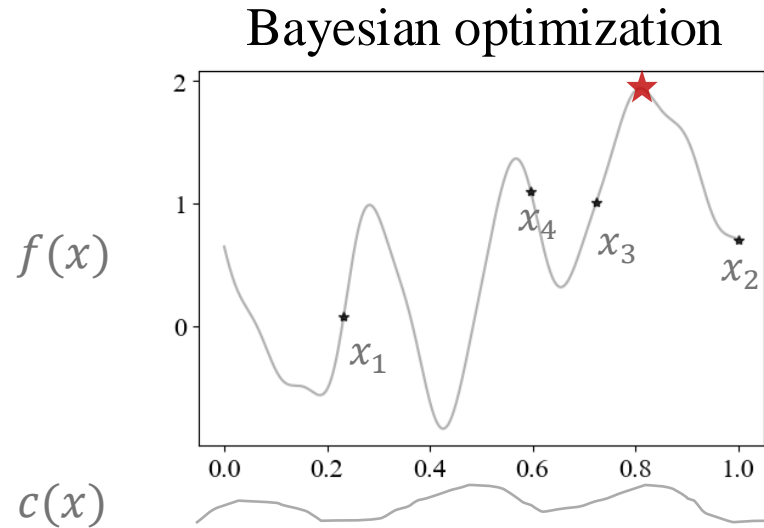
Independent

Cost per sample

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

$D$ : observed data

# How to translate?

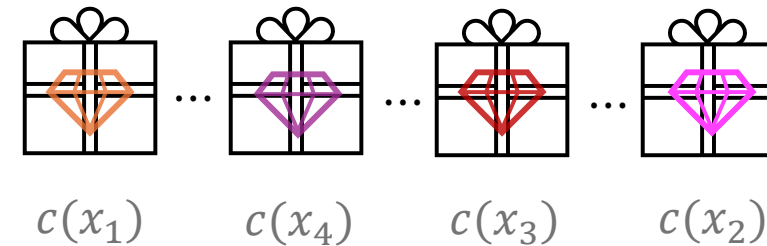


Continuous

Correlated

Hard budget constraint

Budget-constrained  
Pandora's box



Discrete

Independent

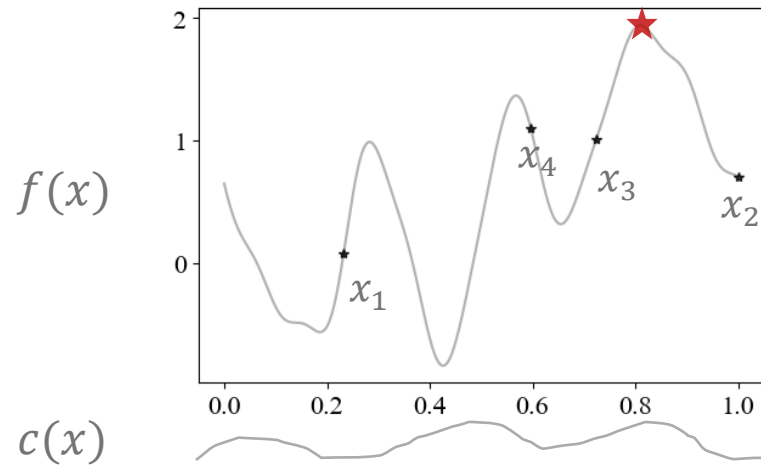
Cost per sample

$$\operatorname{argmax}_x \alpha^*(x) \text{ s.t. } \underbrace{\operatorname{EI}_{f|D}(x; \alpha^*(x))}_{\text{popular one-step heuristic: EI policy}} = \lambda_B^* c(x) \iff \operatorname{argmax}_x \alpha^*(x) \text{ s.t. } \operatorname{EI}_f(x; \alpha^*(x)) = \lambda_B^* c(x)$$

popular one-step  
heuristic: EI policy

# How to translate?

Bayesian optimization



Continuous

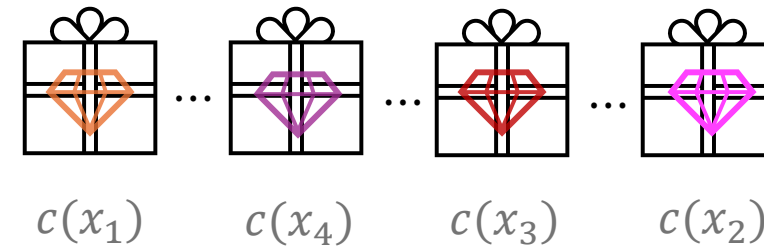
Correlated

Hard budget constraint

$$\operatorname{argmax}_x \alpha^*(x) \text{ s.t. } \underbrace{\operatorname{EI}_{f|D}(x; \alpha^*(x))}_{\text{ratio of EI and cost: EIPC policy}} = \lambda_B^* c(x)$$

ratio of EI and cost: EIPC policy

Budget-constrained  
Pandora's box



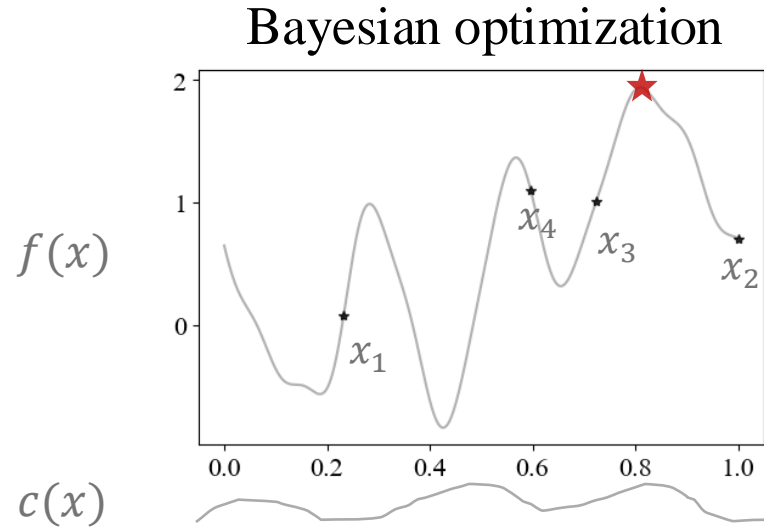
Discrete

Independent

Cost per sample

$$\operatorname{argmax}_x \alpha^*(x) \text{ s.t. } \operatorname{EI}_f(x; \alpha^*(x)) = \lambda_B^* c(x)$$

# How to translate?

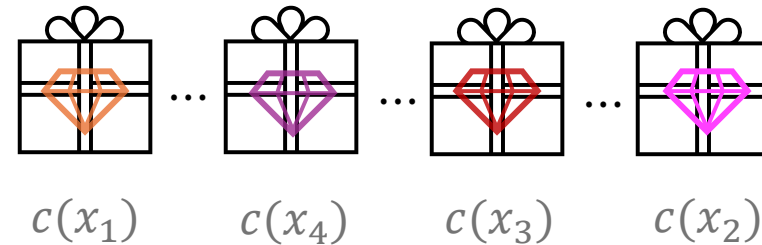


Continuous

Correlated

Hard budget constraint

Budget-constrained  
Pandora's box



Discrete

Independent

Cost per sample

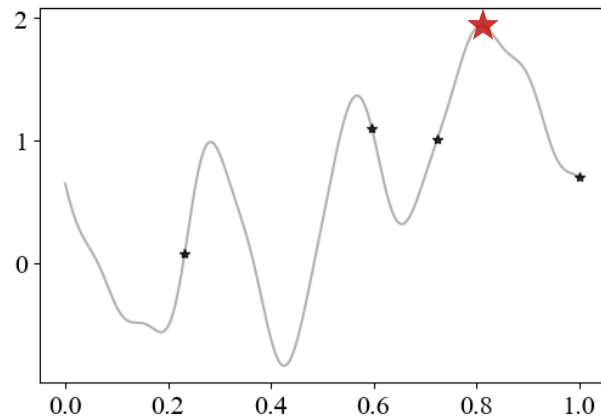
$$\operatorname{argmax}_x \alpha^*(x) \text{ s.t. } \operatorname{EI}_{f|D}(x; \alpha^*(x)) = \lambda_B^* c(x) \iff \operatorname{argmax}_x \alpha^*(x) \text{ s.t. } \operatorname{EI}_f(x; \alpha^*(x)) = \lambda_B^* c(x)$$

EI and EIPC policy can be arbitrarily worse [Astudillo, Jiang, Balandat, Bakshy, Frazier'21]

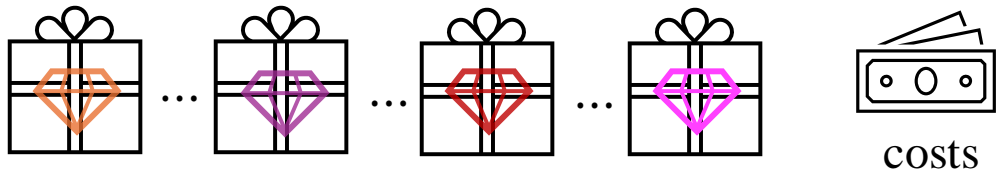


# Our Contributions

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



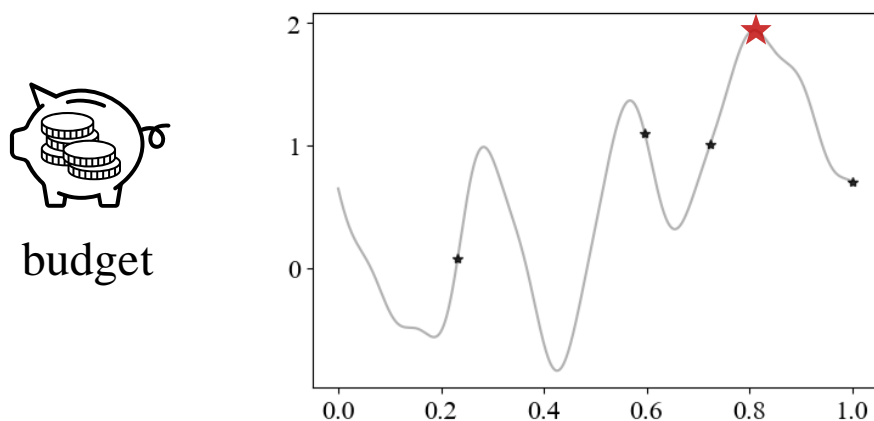
?



Pandora's Box Gittins index

# Our Contributions

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



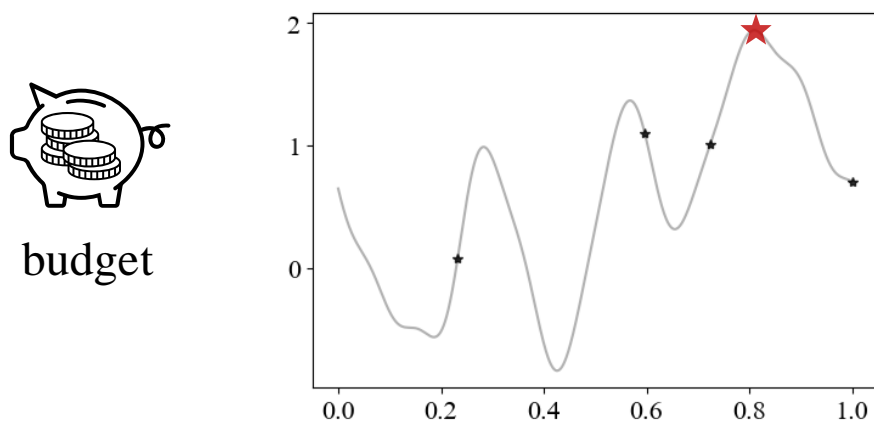
Our work



Pandora's Box Gittins index

# Our Contributions

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



budget



Our work

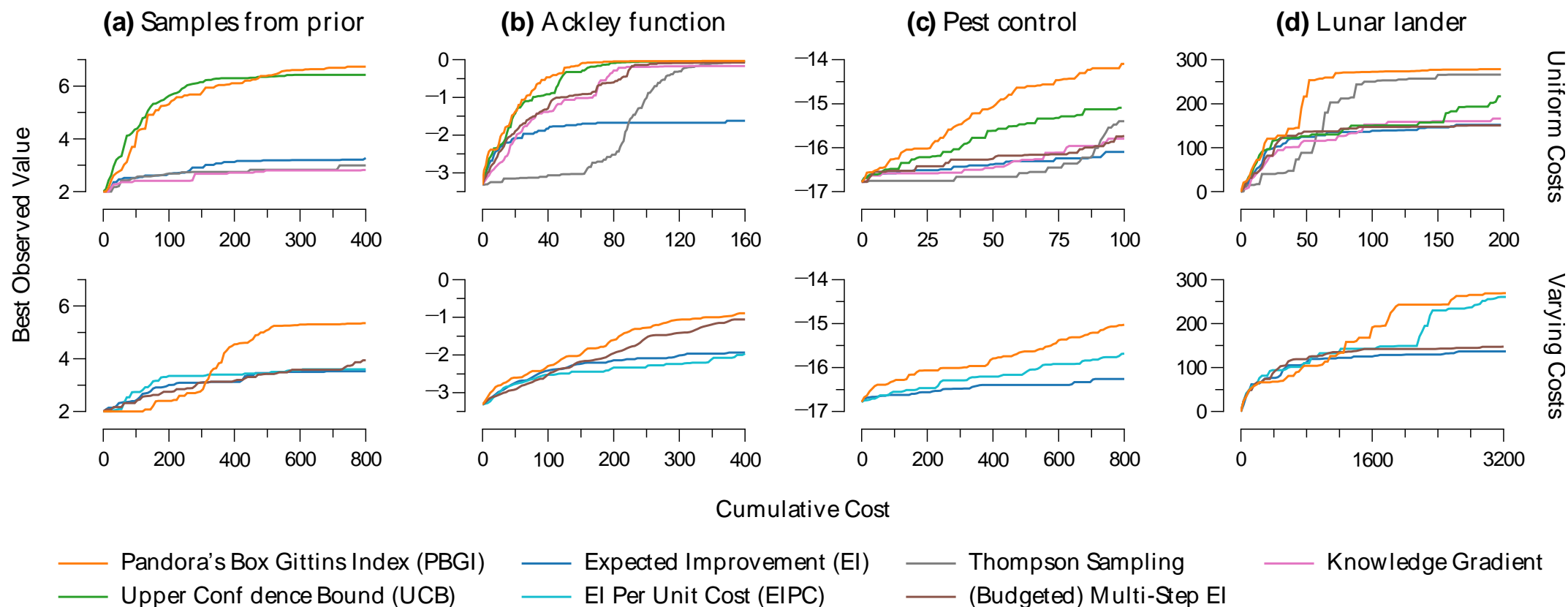


Pandora's Box Gittins index

# Experiment Results: PBGI vs Baselines

Synthetic

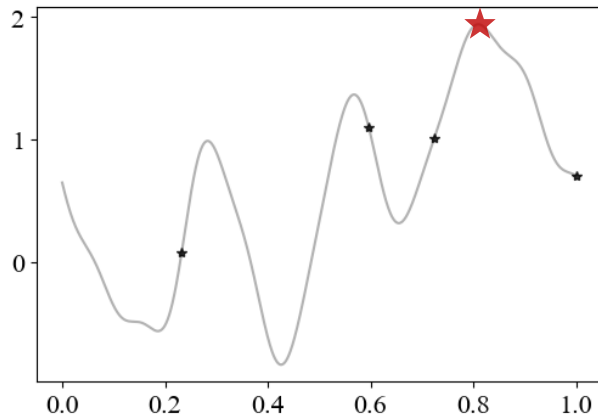
Empirical



EI and EIPC policy can be arbitrarily worse [Astudillo, Jiang, Balandat, Bakshy, Frazier'21]

# Conclusions

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



**Our work**

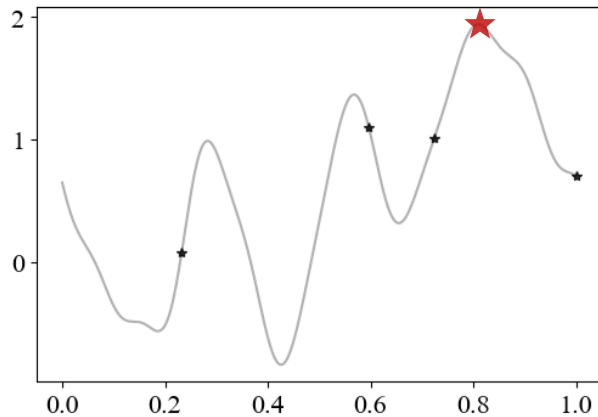


Pandora's Box Gittins index

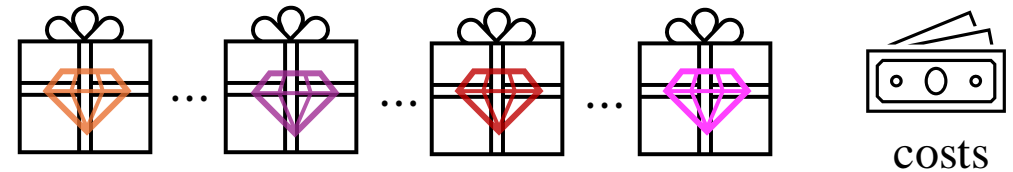
Check our preprint on arXiv!

# Conclusions

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



**Our work**

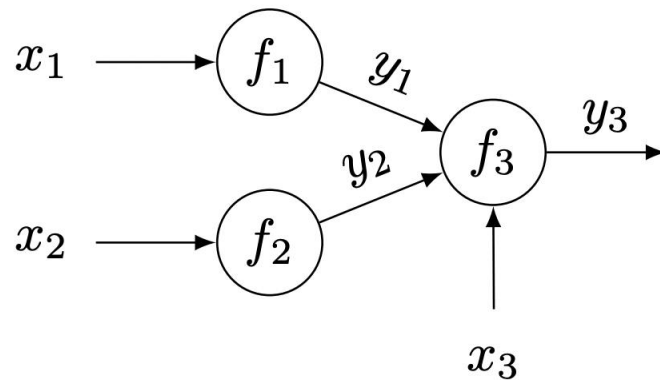


Pandora's Box Gittins index

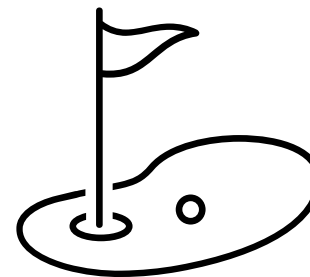
Check our preprint on arXiv!

# 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** (partial feedback, multi-fidelity, function network, etc.) via Gittins variants (Pandora's nested boxes, “golf”-style Markovian MAB, optional inspection, etc.)



?



“Golf” Gittins indices

[Dumitriu, Tetali, Winkler’03]