

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

Bayesian Optimization

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

∈ decision-making under uncertainty

Applications:

Hyperparameter tuning
Drug/material discovery
Experiment design

Bayesian Optimization

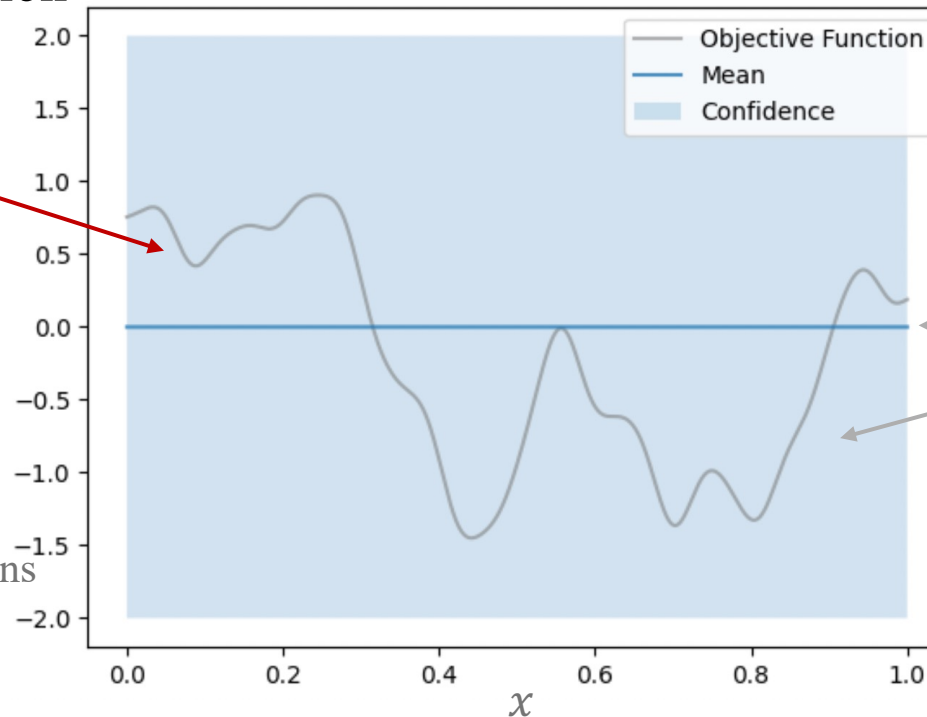
Goal: optimize expensive-to-evaluate **black-box** function

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

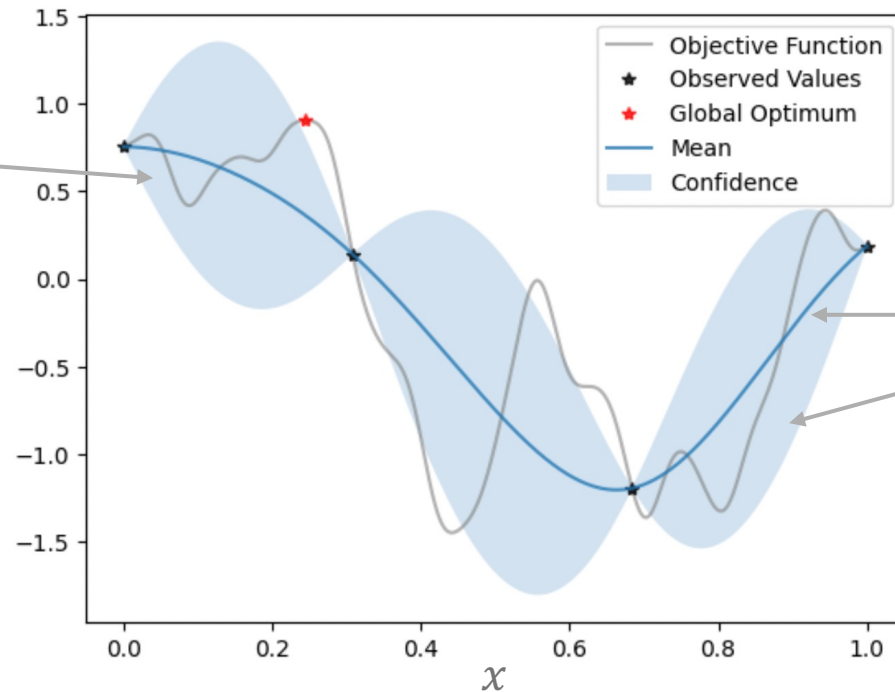
variance: confidence/uncertainty

Bayesian Optimization

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



Applications:

Hyperparameter tuning
Drug/material discovery
Experiment design

x : hyperparameter/configuration

mean: prediction

variance: confidence/uncertainty

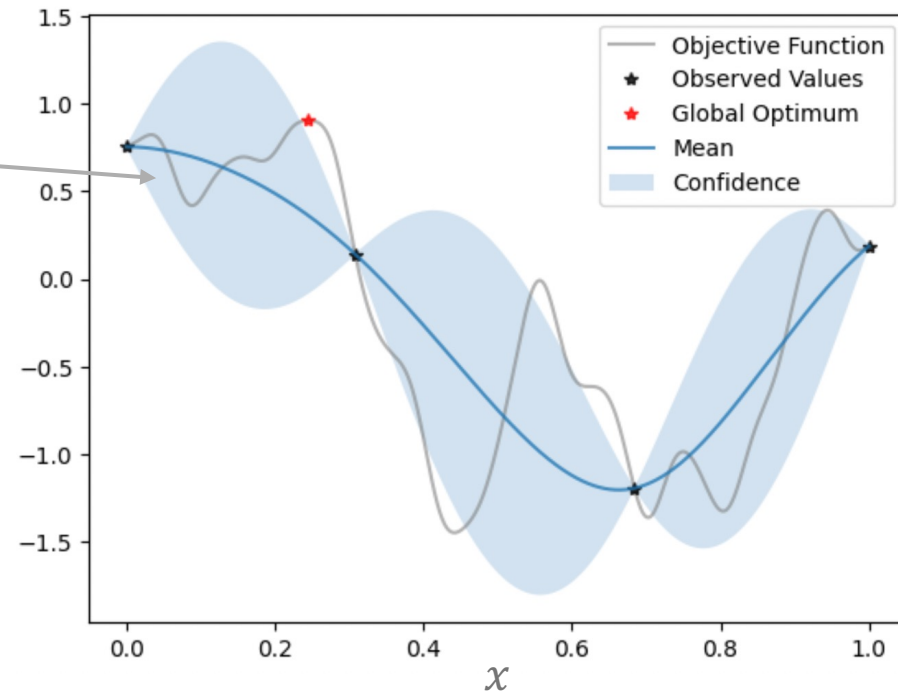
Objective: find global optimum $x^* = \operatorname{argmax}_{x \in \mathcal{X}} f(x)$

Decision: evaluate a set of points

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

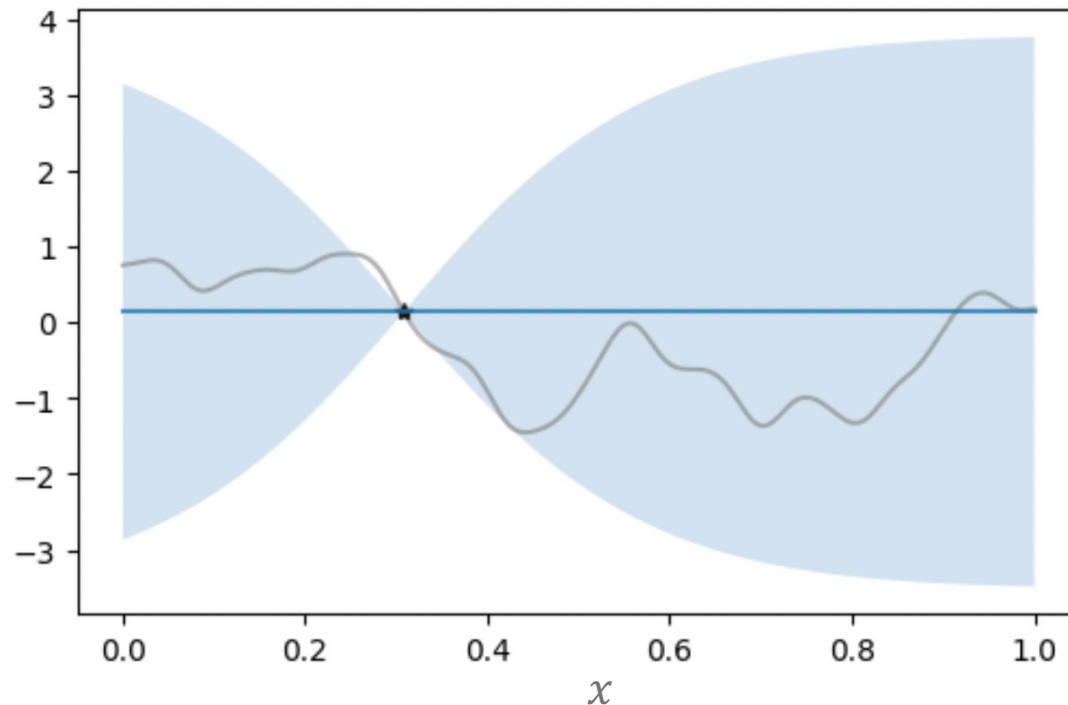
Objective: find global optimum $x^* = \operatorname{argmax}_{x \in \mathcal{X}} f(x)$

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

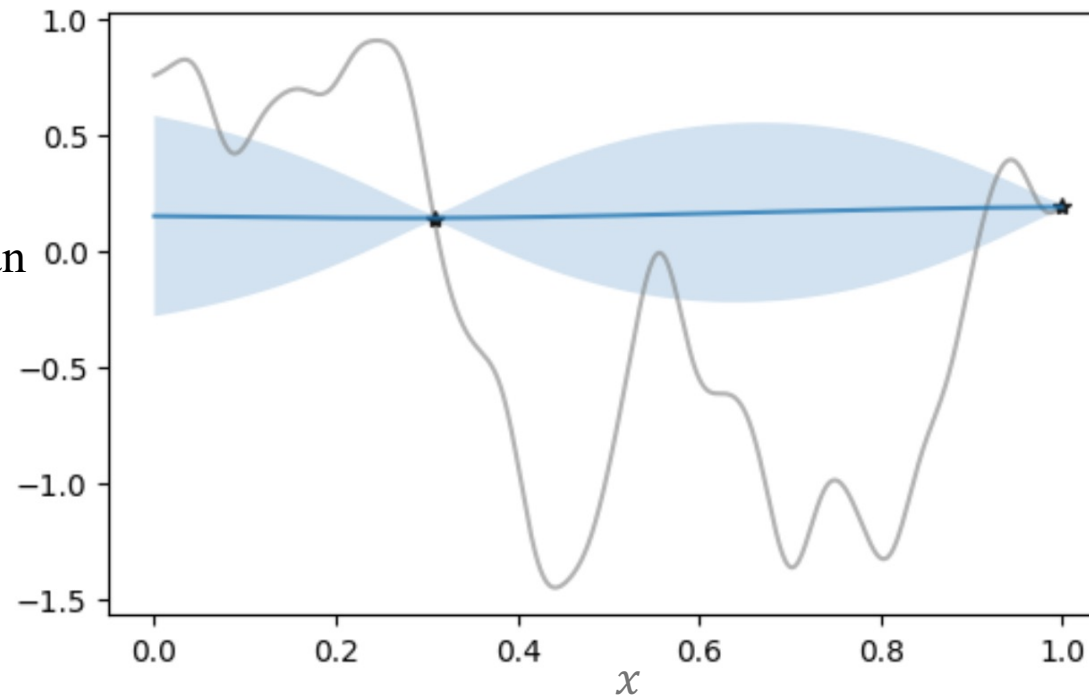
adaptively

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

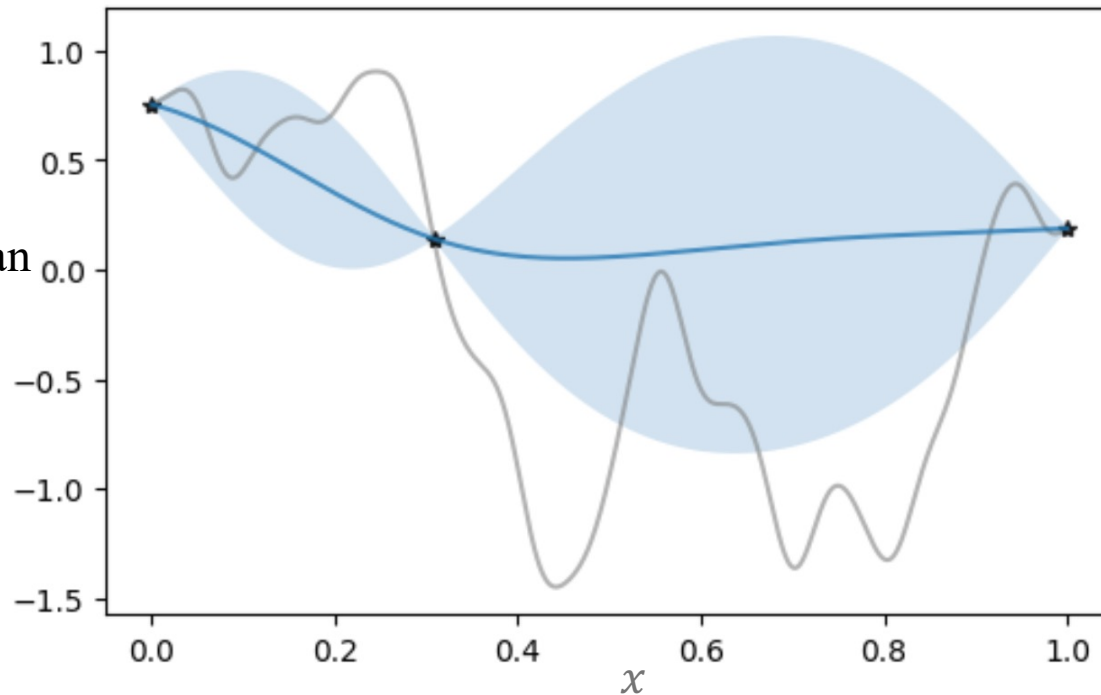
x : hyperparameter/configuration

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

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

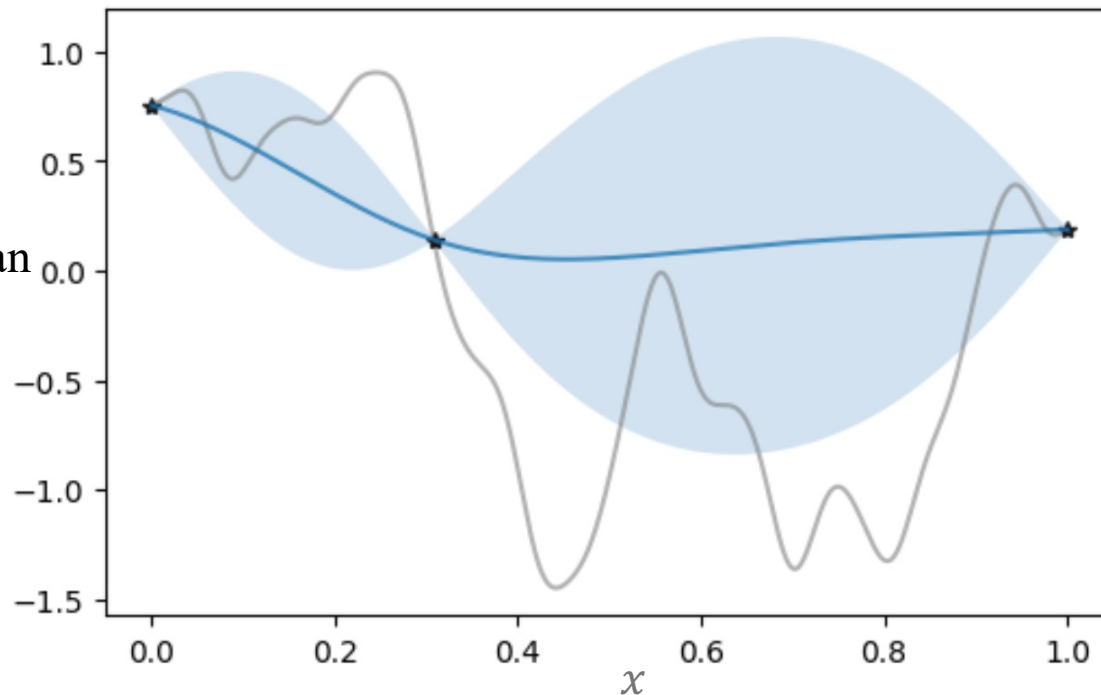
adaptively

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

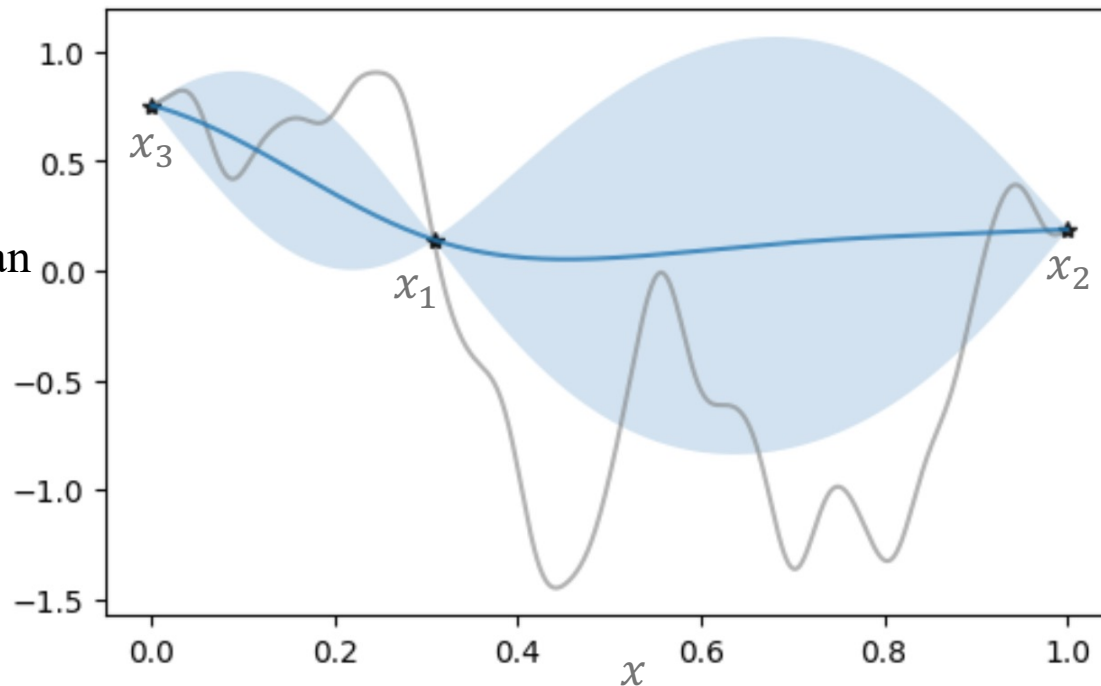
$x_1, x_2, \dots, x_T \in \mathcal{X}$

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

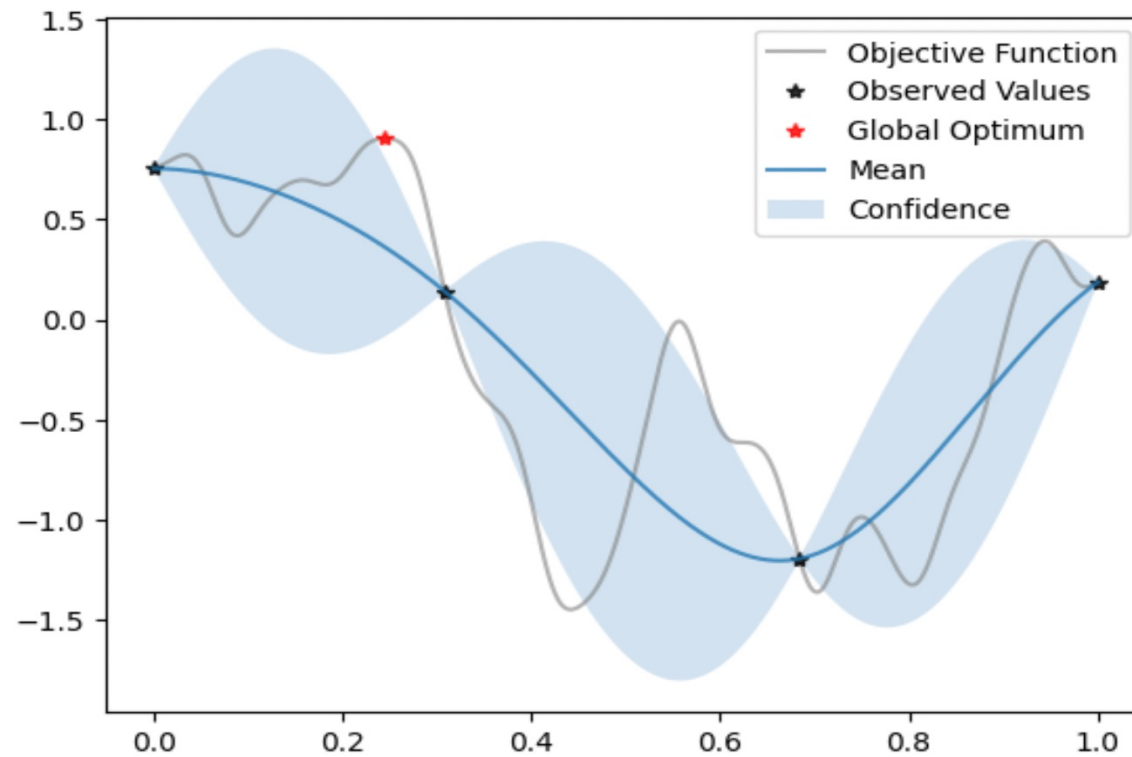
$$\sup_{\text{policy}} \mathbb{E} \max_{t=1,2,\dots,T} f(x_t)$$

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

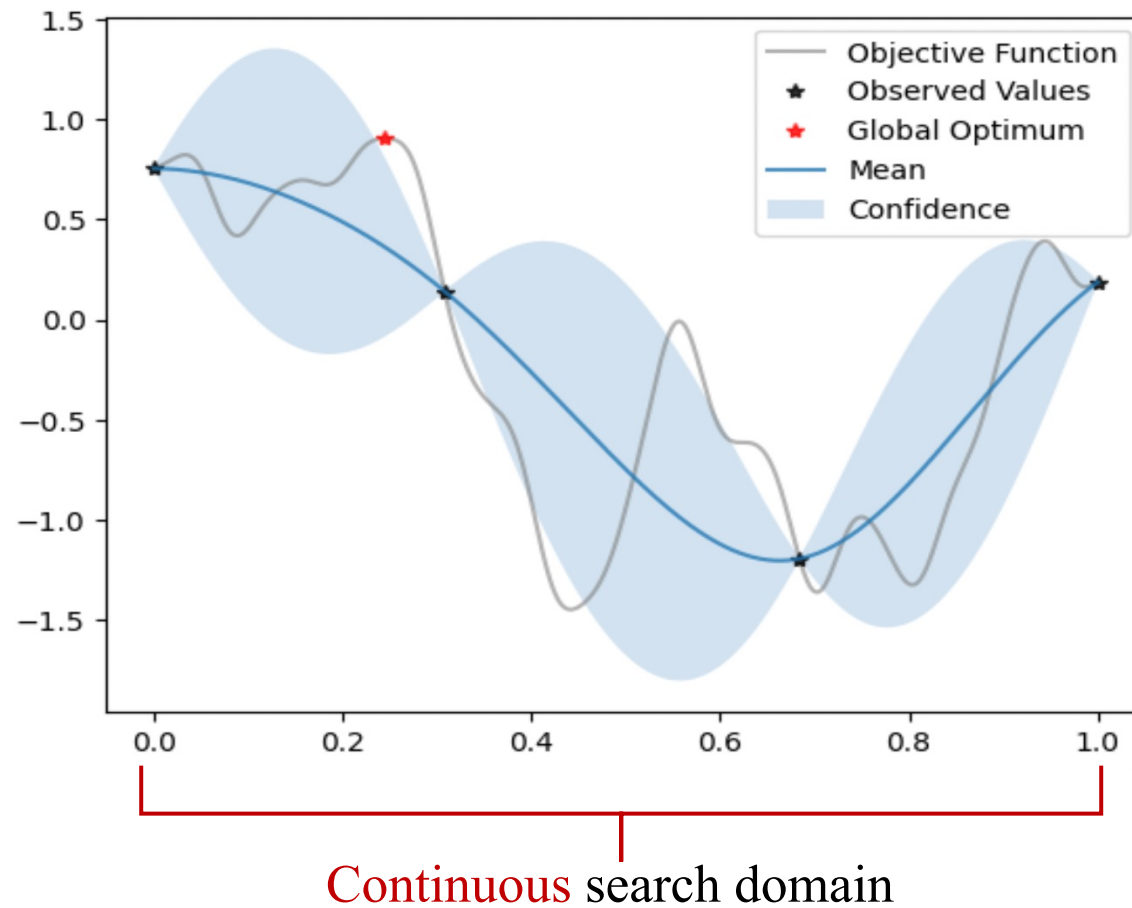
$$x_1, x_2, \dots, x_T \in \mathcal{X}$$

T : time budget

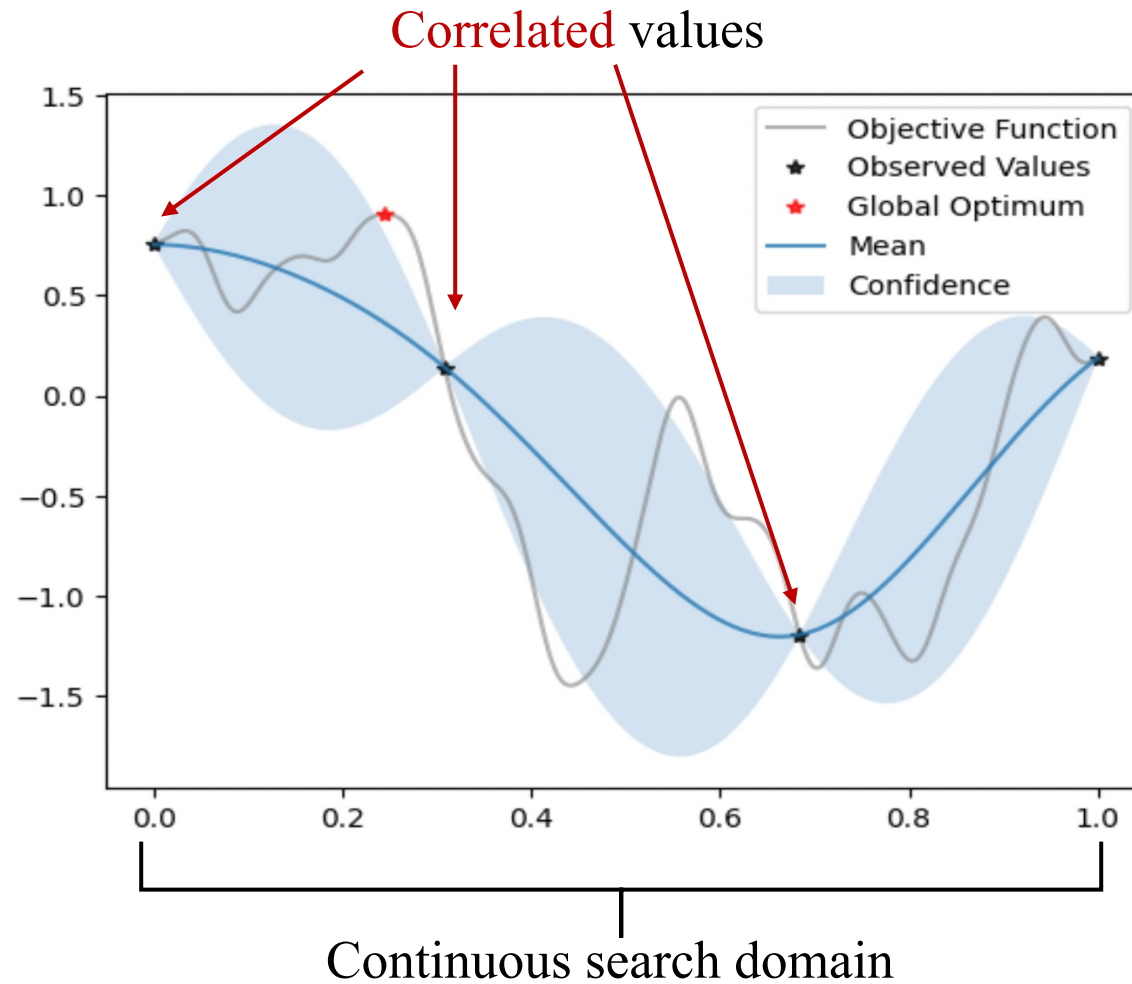
Why is it hard?



Why is it hard?



Why is it hard?



Why is it hard?

Hard budget **constraint**

~~$t=1$~~



~~$t=2$~~



~~$t=3$~~

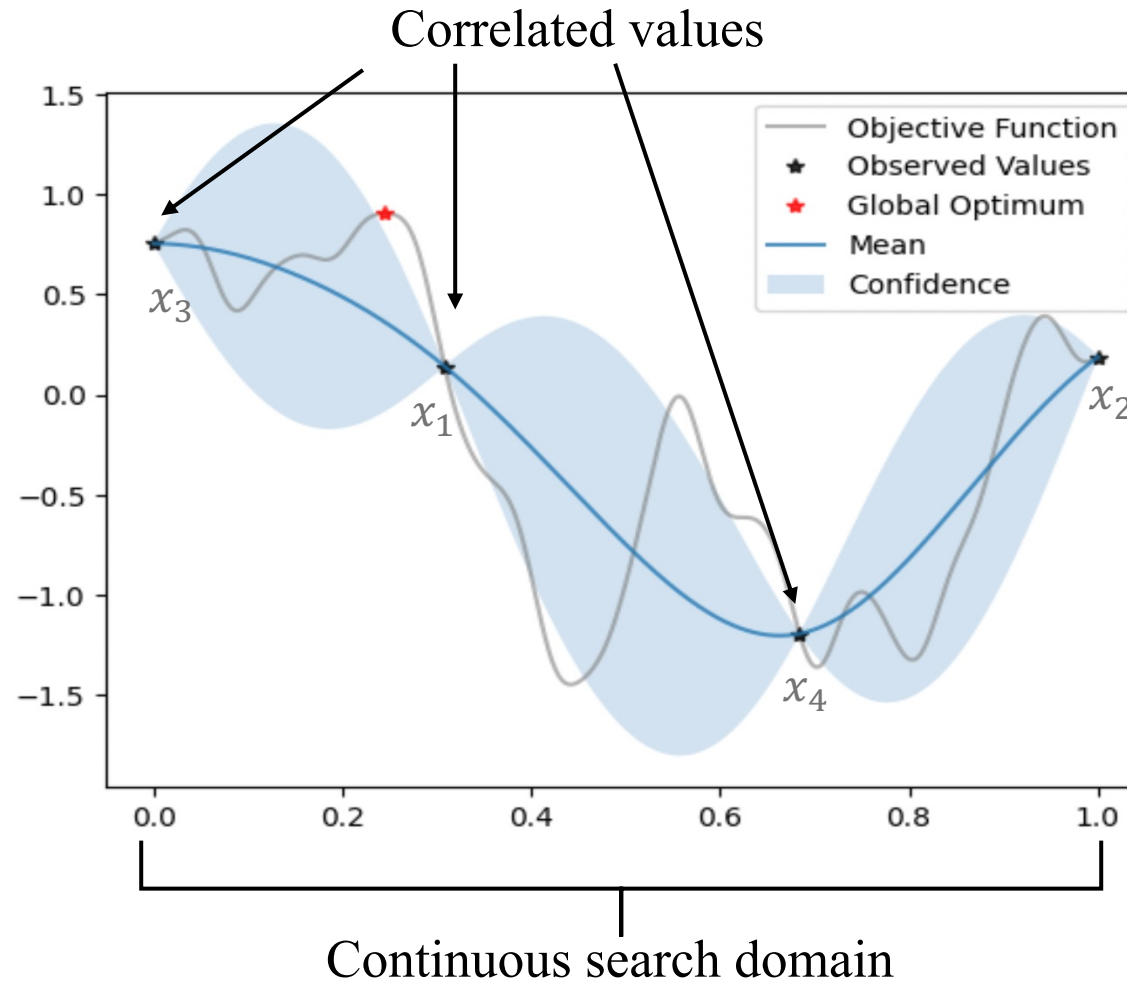


~~$t=4$~~



\vdots

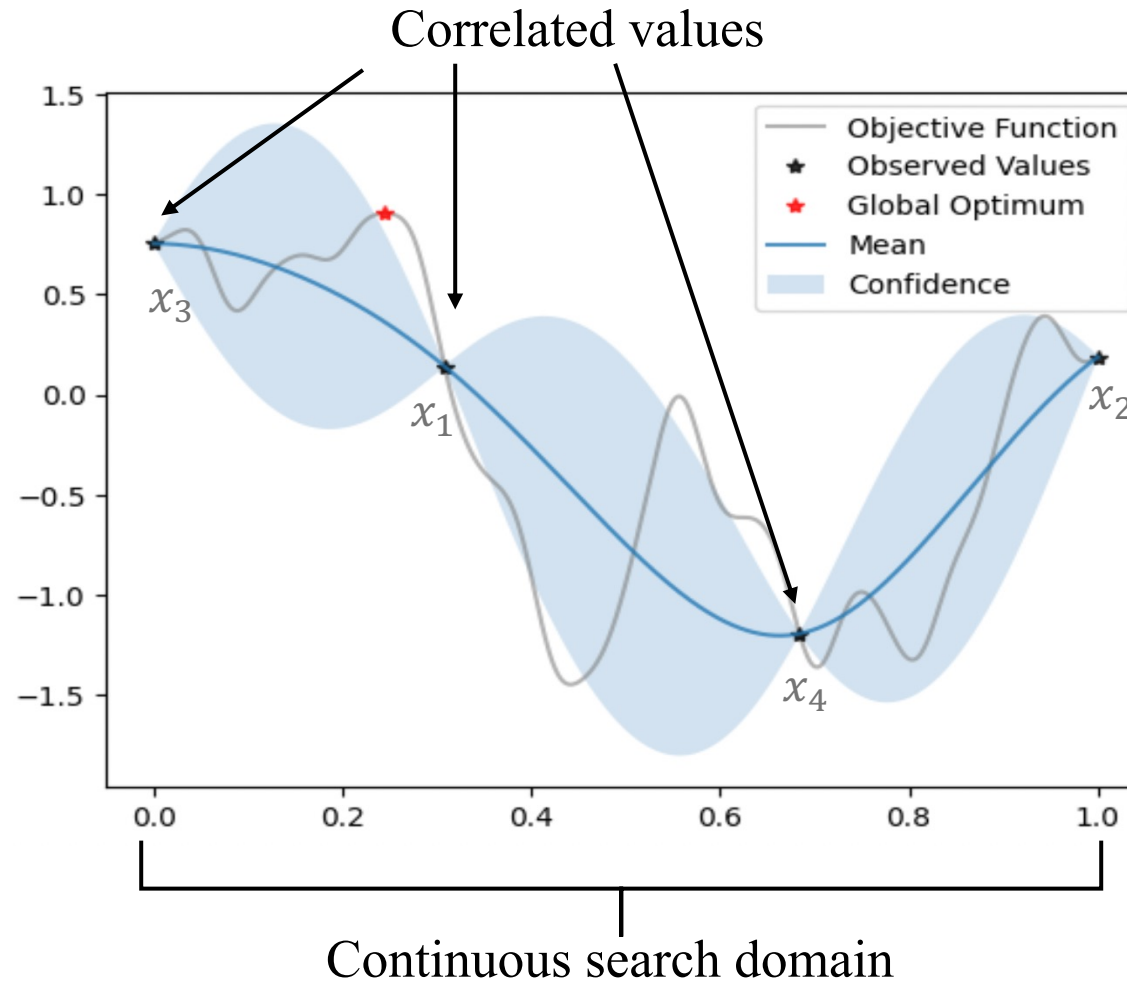
$t = T$



Why is it hard?

Hard budget constraint

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



Evaluation **costs** handling







uniform

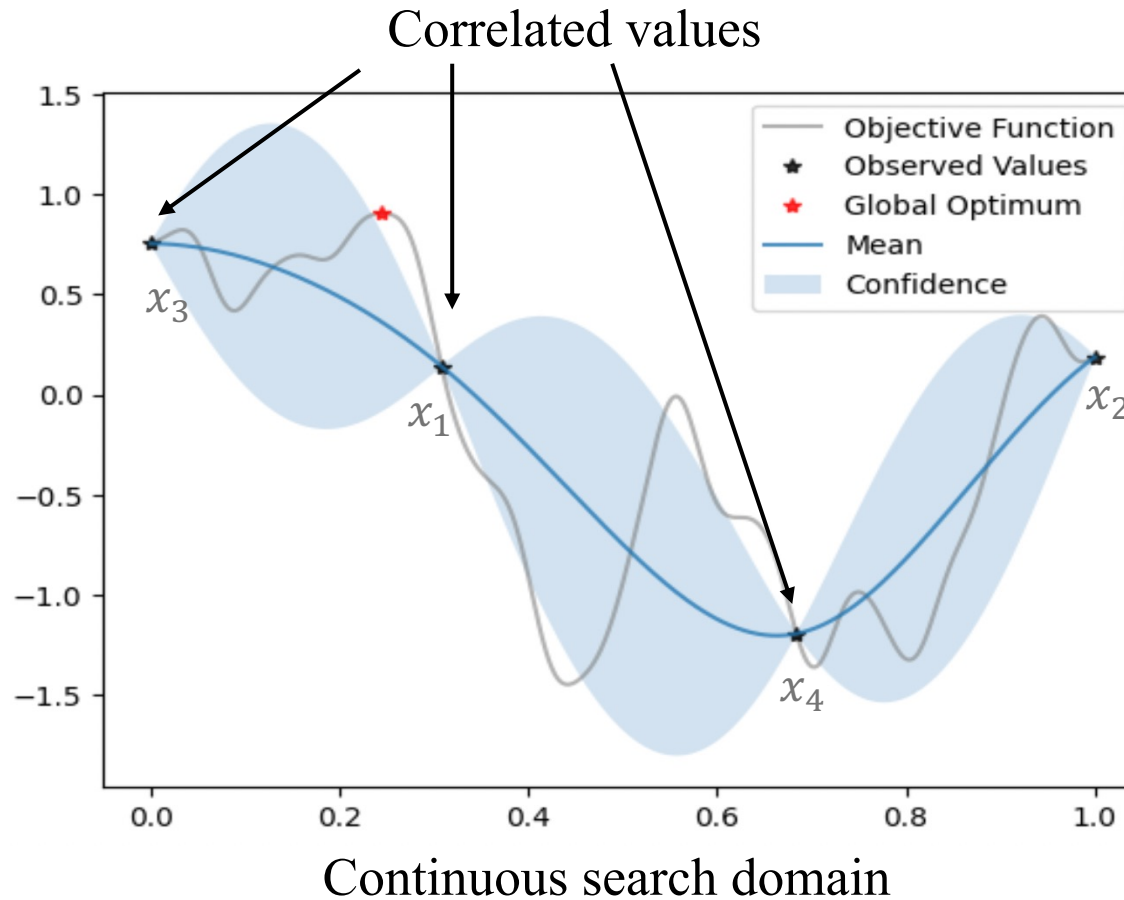


heterogeneous

Why is it hard?

Hard budget constraint

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



Evaluation costs handling



uniform



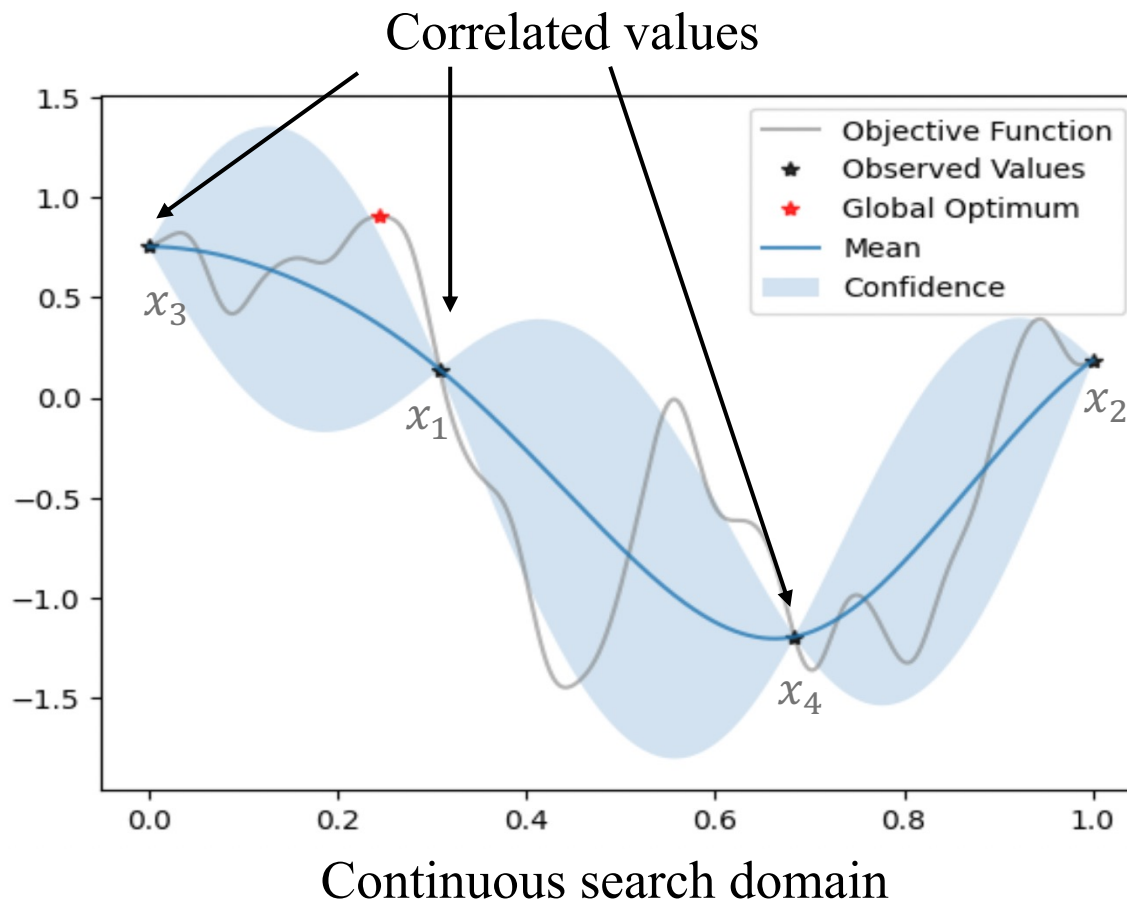
heterogeneous

\Rightarrow Optimal policy unknown!

Why is it hard?

Hard budget constraint

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



Evaluation costs handling



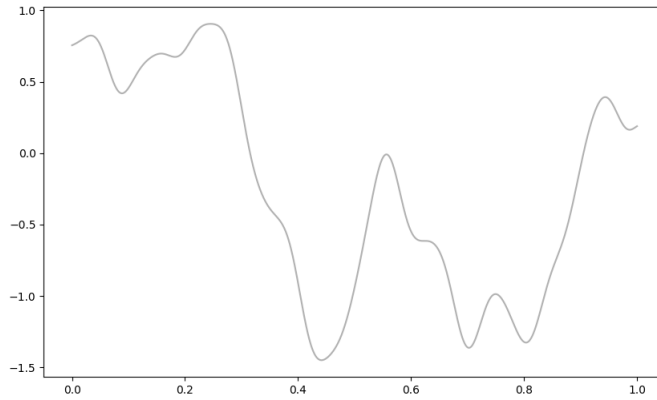
uniform



heterogeneous

Can we convert it to a solvable problem?

Bayesian Optimization

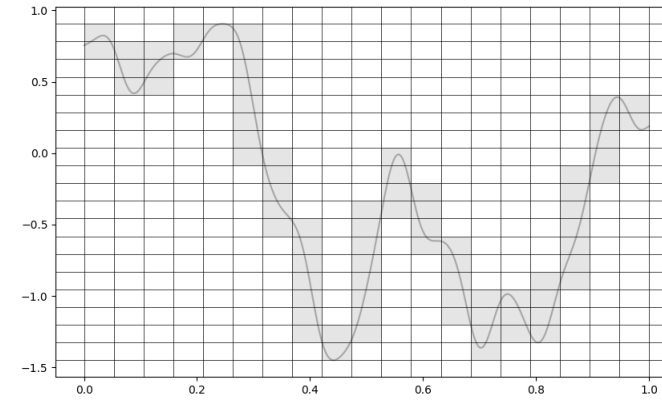
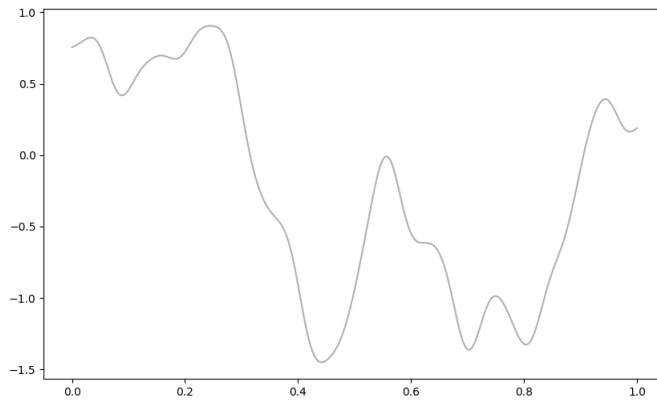


Continuous

Correlated

Hard budget constraint

Bayesian Optimization



Continuous

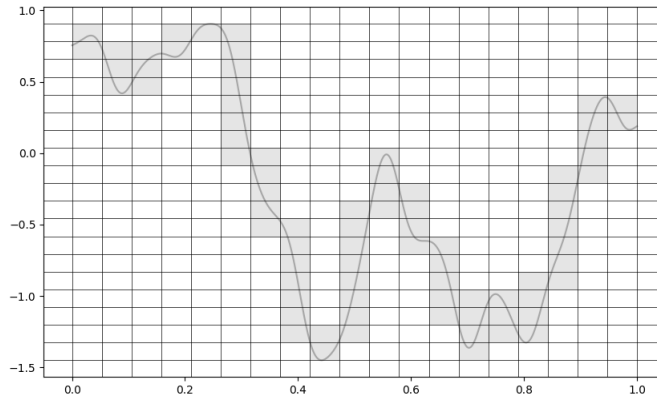


Discrete

Correlated

Hard budget constraint

Bayesian Optimization



Continuous

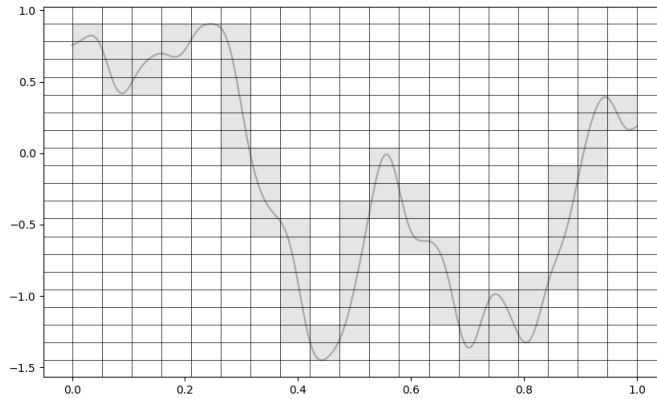


Discrete

Correlated

Hard budget constraint

Bayesian Optimization



Continuous



Discrete

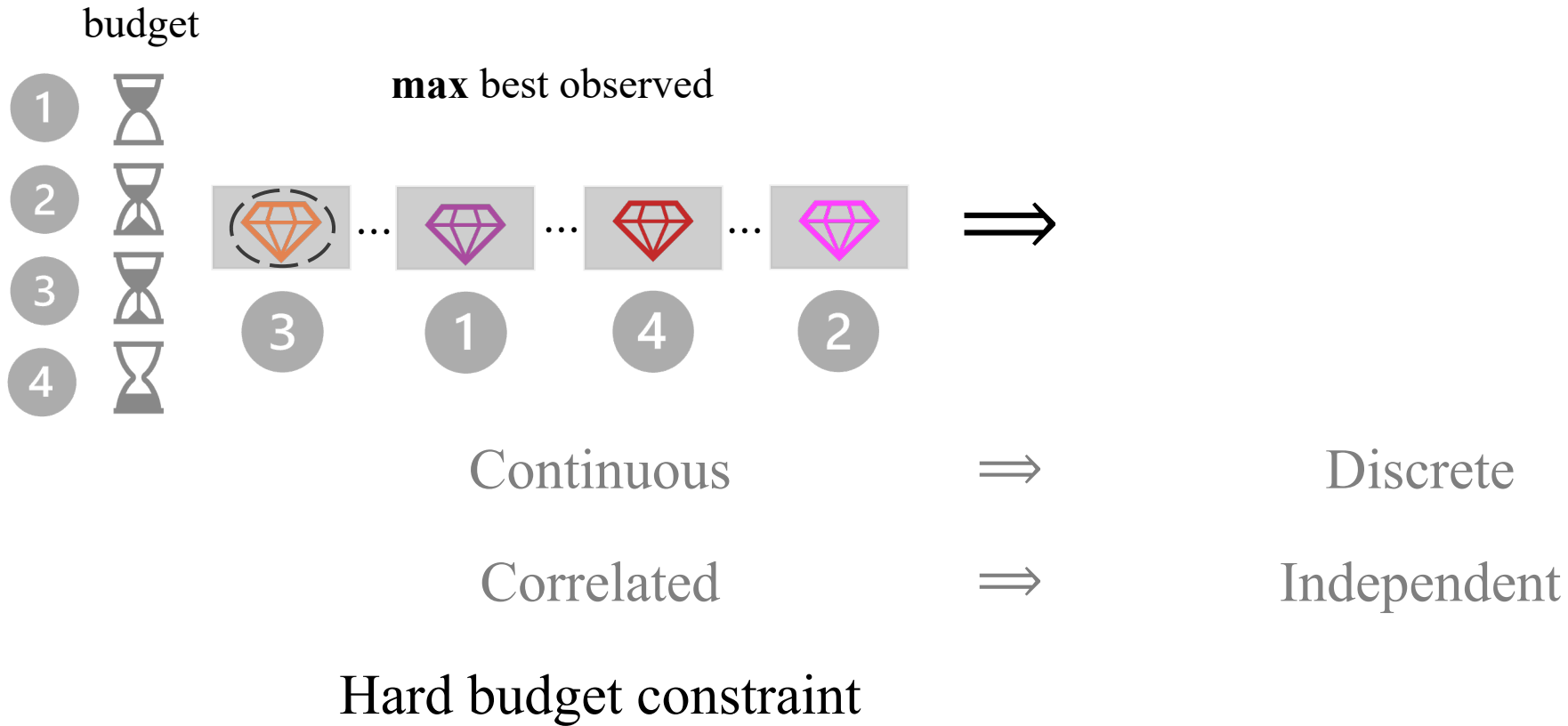
Correlated



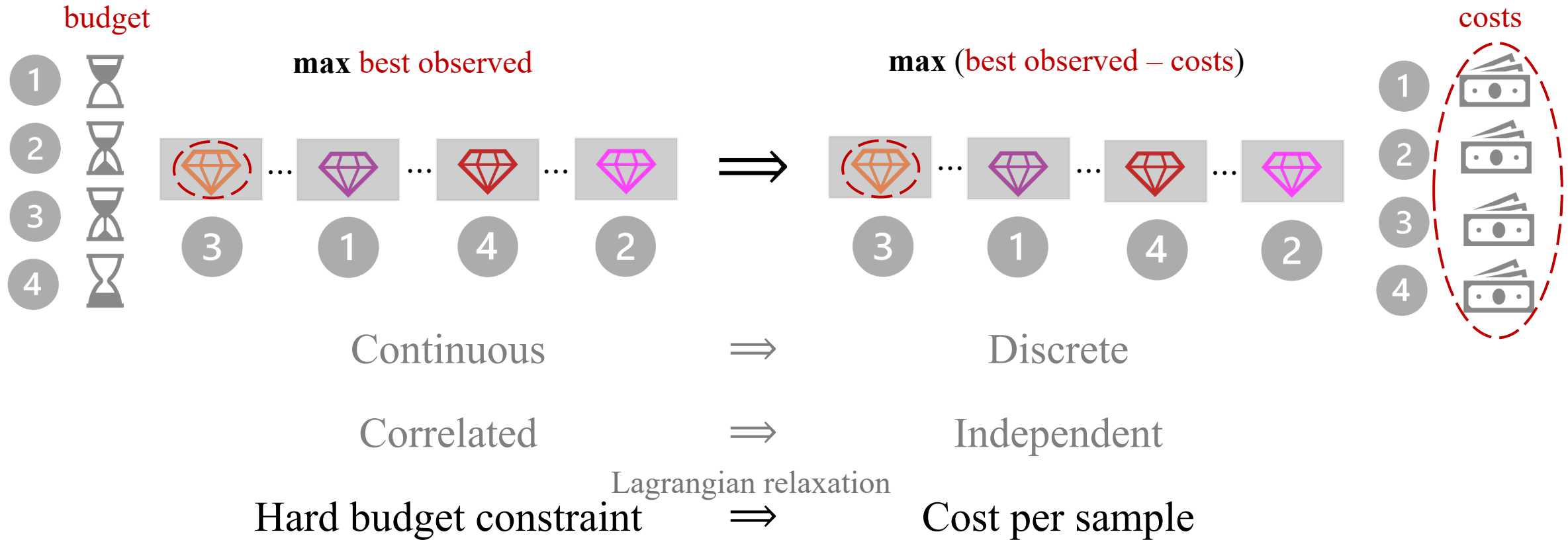
Independent

Hard budget constraint

Bayesian Optimization

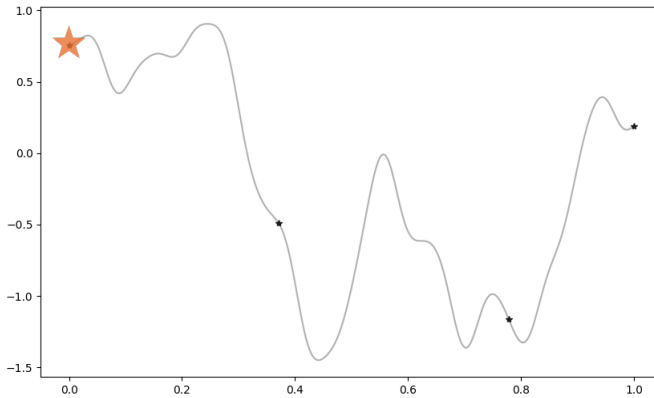


Bayesian Optimization

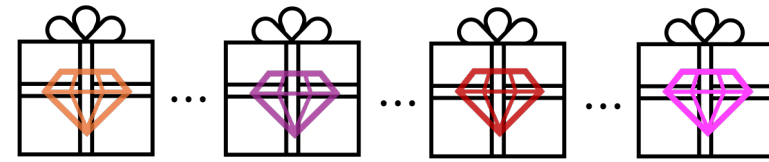
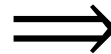


Bayesian Optimization \Rightarrow Pandora's Box

[Weitzman'79]



Continuous



Discrete



Independent

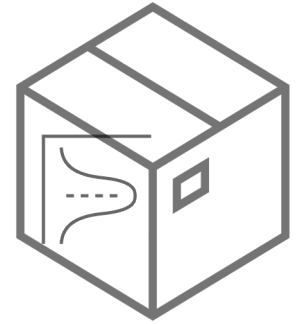
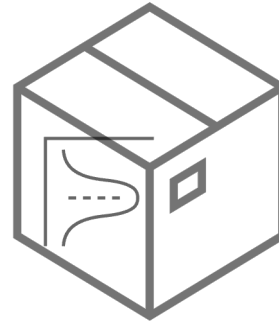
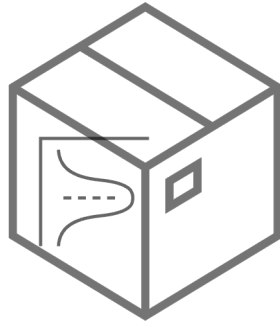
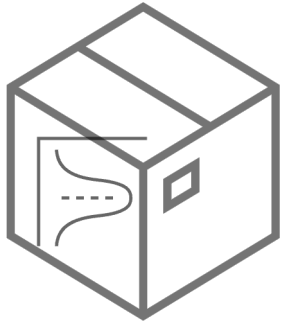


Hard budget constraint

Cost per sample

Pandora's Box

$t = 0$

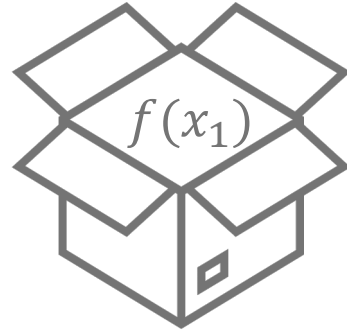
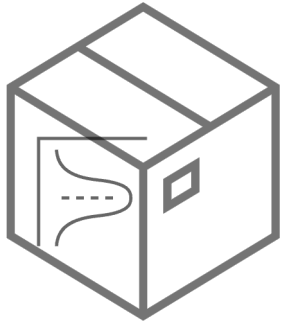


Objective: maximize net utility

Decision: adaptively evaluate a random number of boxes

Pandora's Box

$t = 1$



$c(x_1)$

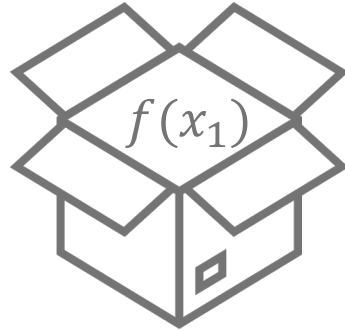
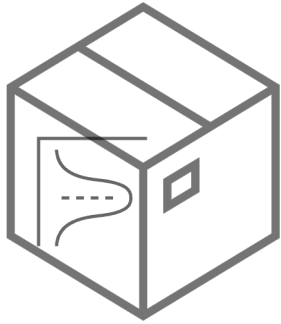


Objective: maximize net utility

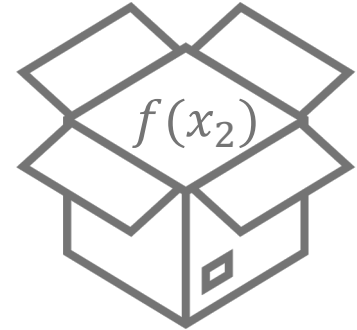
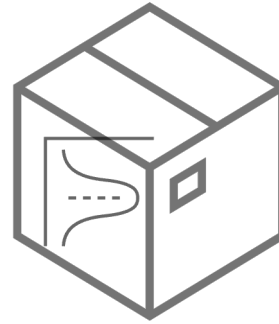
Decision: adaptively evaluate a random number of boxes

Pandora's Box

$t = 2$



$c(x_1)$



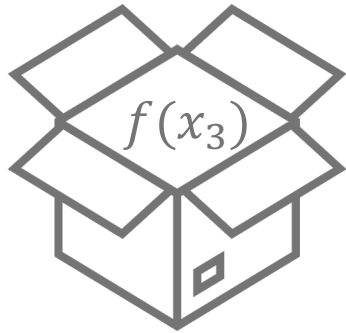
$c(x_2)$

Objective: maximize net utility

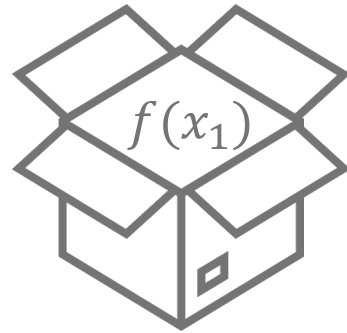
Decision: adaptively evaluate a random number of boxes

Pandora's Box

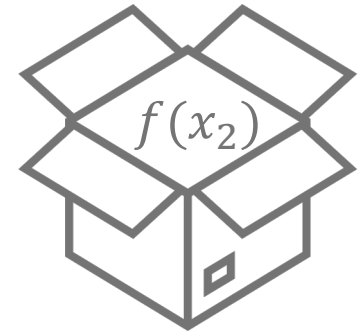
$t = 3$



$c(x_3)$



$c(x_1)$



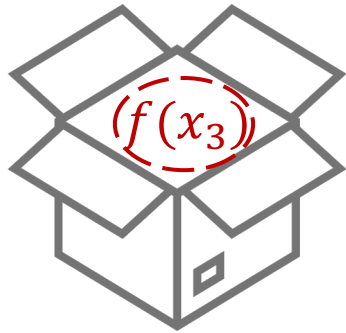
$c(x_2)$

Objective: maximize net utility

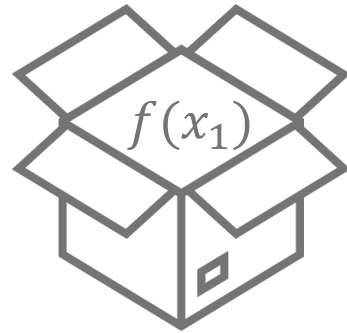
Decision: adaptively evaluate a random number of boxes

Pandora's Box

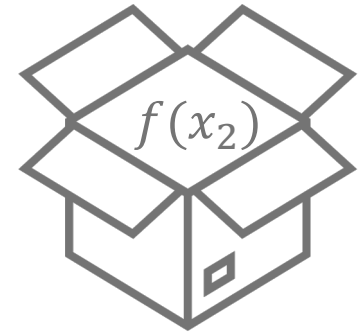
$t = 3$



$c(x_3)$



$c(x_1)$



$c(x_2)$

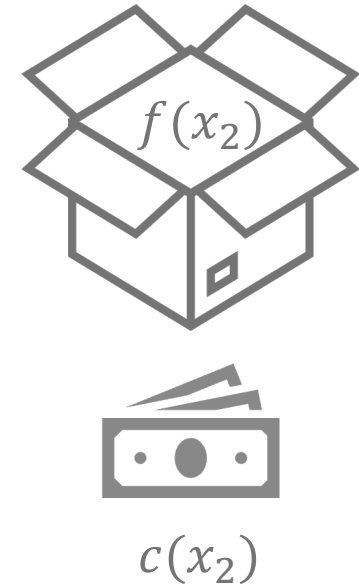
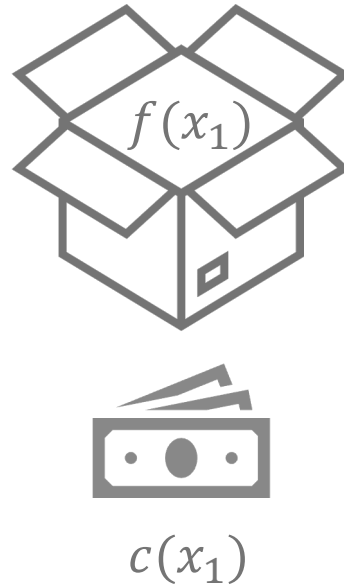
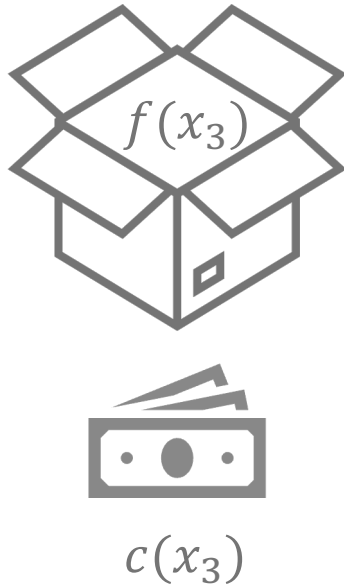
Objective: maximize **net utility**

Decision: adaptively evaluate a random number of boxes

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

Pandora's Box

$t = 3$



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

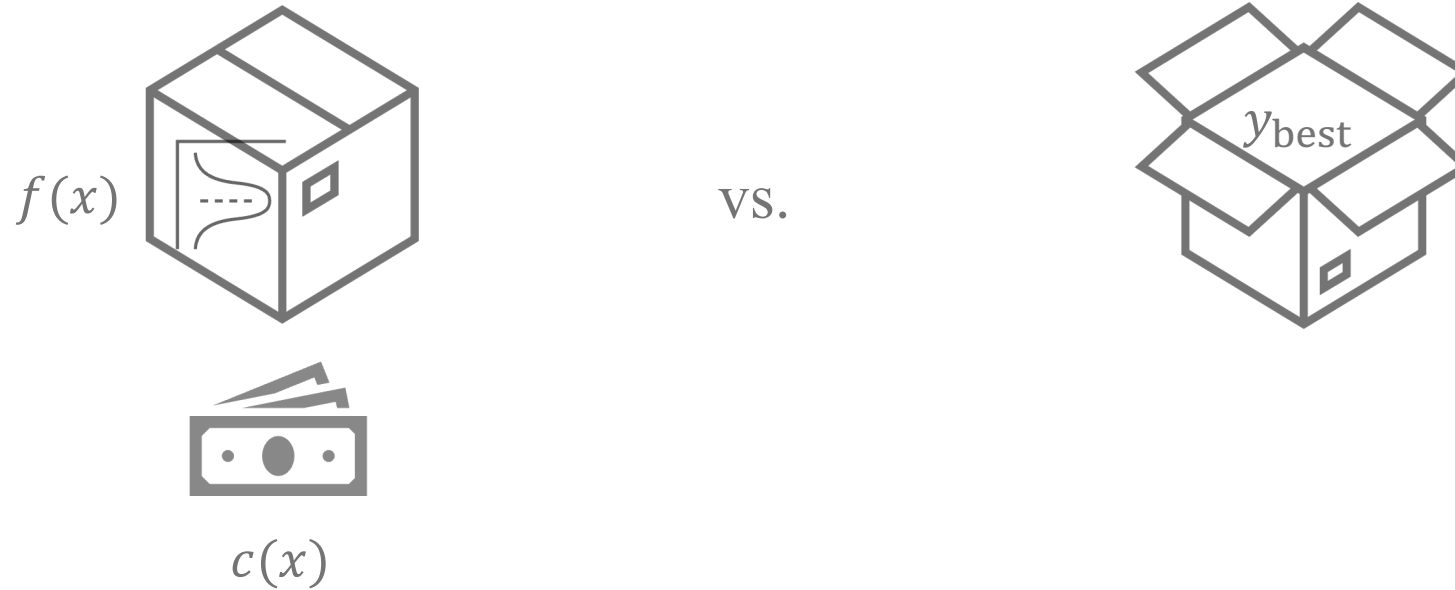
$$x_1, x_2, \dots, x_T \in \mathcal{X}$$

\mathcal{X} : discrete

T : random stopping time

Naïve Greedy policy can fail [Singla'18]

Naïve Greedy policy

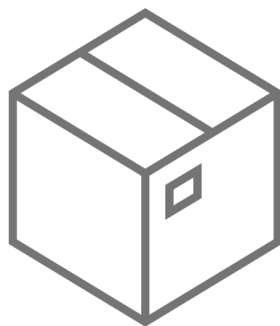
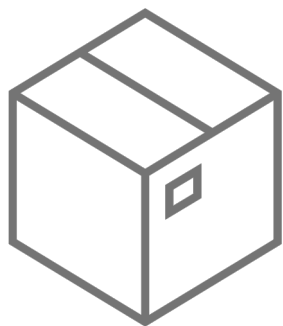


Inspection rule: $\operatorname{argmax}_x (\operatorname{El}_f(x; y_{\text{best}}) - c(x))$ **Stopping rule:** $\operatorname{El}_f(x; y_{\text{best}}) \leq c(x), \forall x \in \mathcal{X}$
expected improvement - cost expected improvement \leq cost

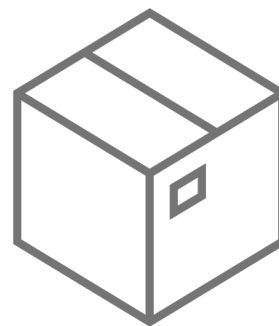
y_{best} : current best observed value

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

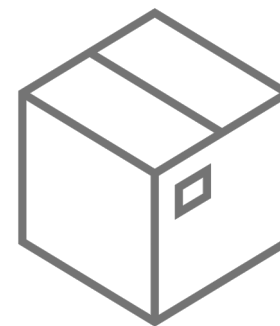
Naïve Greedy policy can fail [Singla'18]



...



...



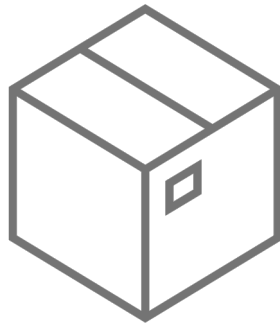
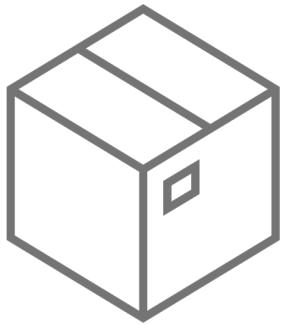
$$\begin{aligned} f(1) &= 200 \text{ w.p. } 1 \\ c(1) &= 198 \end{aligned}$$

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

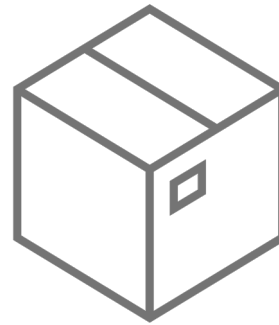
Naïve Greedy policy can fail [Singla'18]

$t = 0$

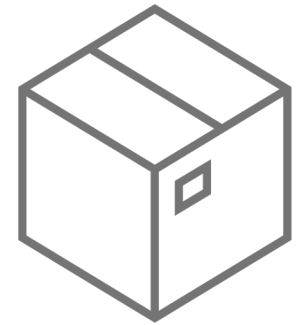
$y_{\text{best}} = 0$



...



...



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

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

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

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

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

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

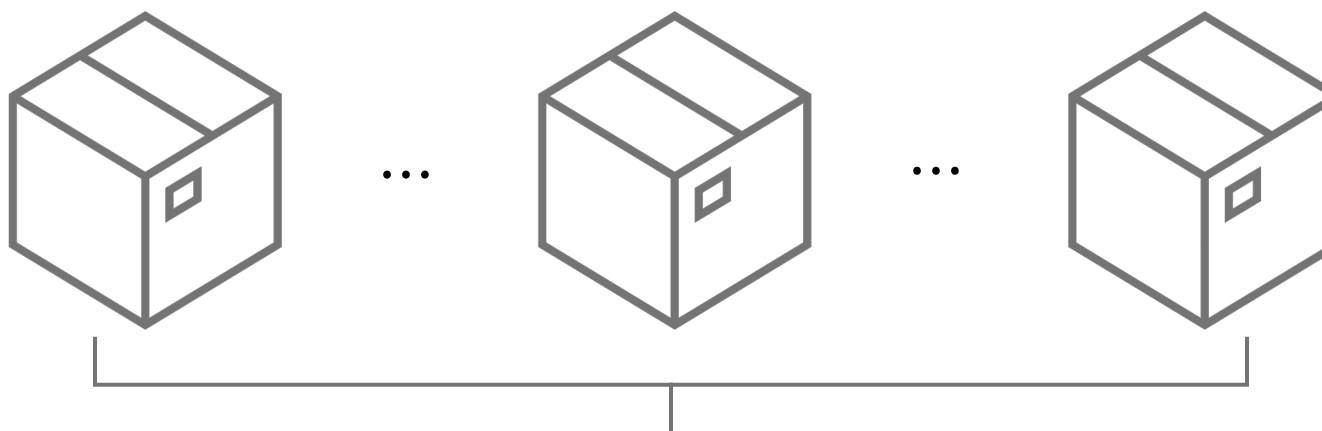
Naïve Greedy policy can fail [Singla'18]

$t = 1$

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



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



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

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

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

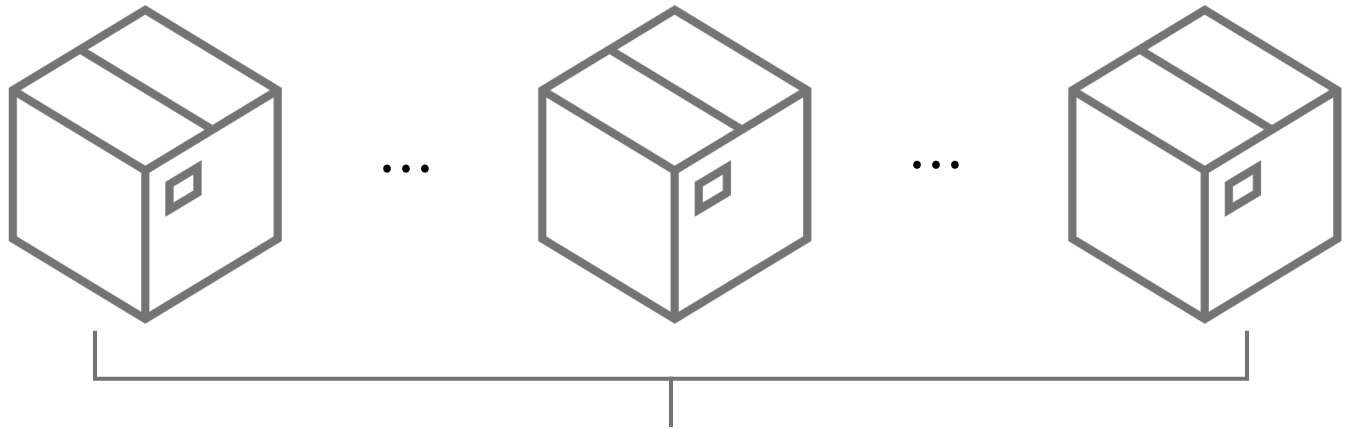
$$\text{EI}_f(x; y) := \mathbb{E}[(f(x) - y)^+]$$

Naïve Greedy policy can fail [Singla'18]

$t = 1$



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



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

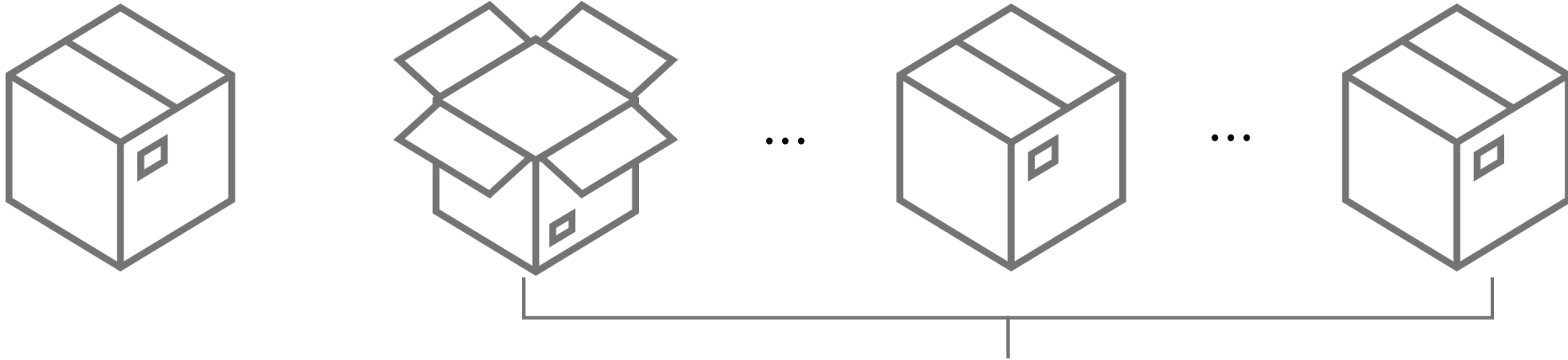
Inspection rule: $\operatorname{argmax}_x (\operatorname{El}_f(x; y_{\text{best}}) - c(x))$ **Stopping rule:** $\operatorname{El}_f(x; y_{\text{best}}) \leq c(x), \forall x \in \mathcal{X}$

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

Naïve Greedy policy can fail [Singla'18]

$t \approx 100$

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



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

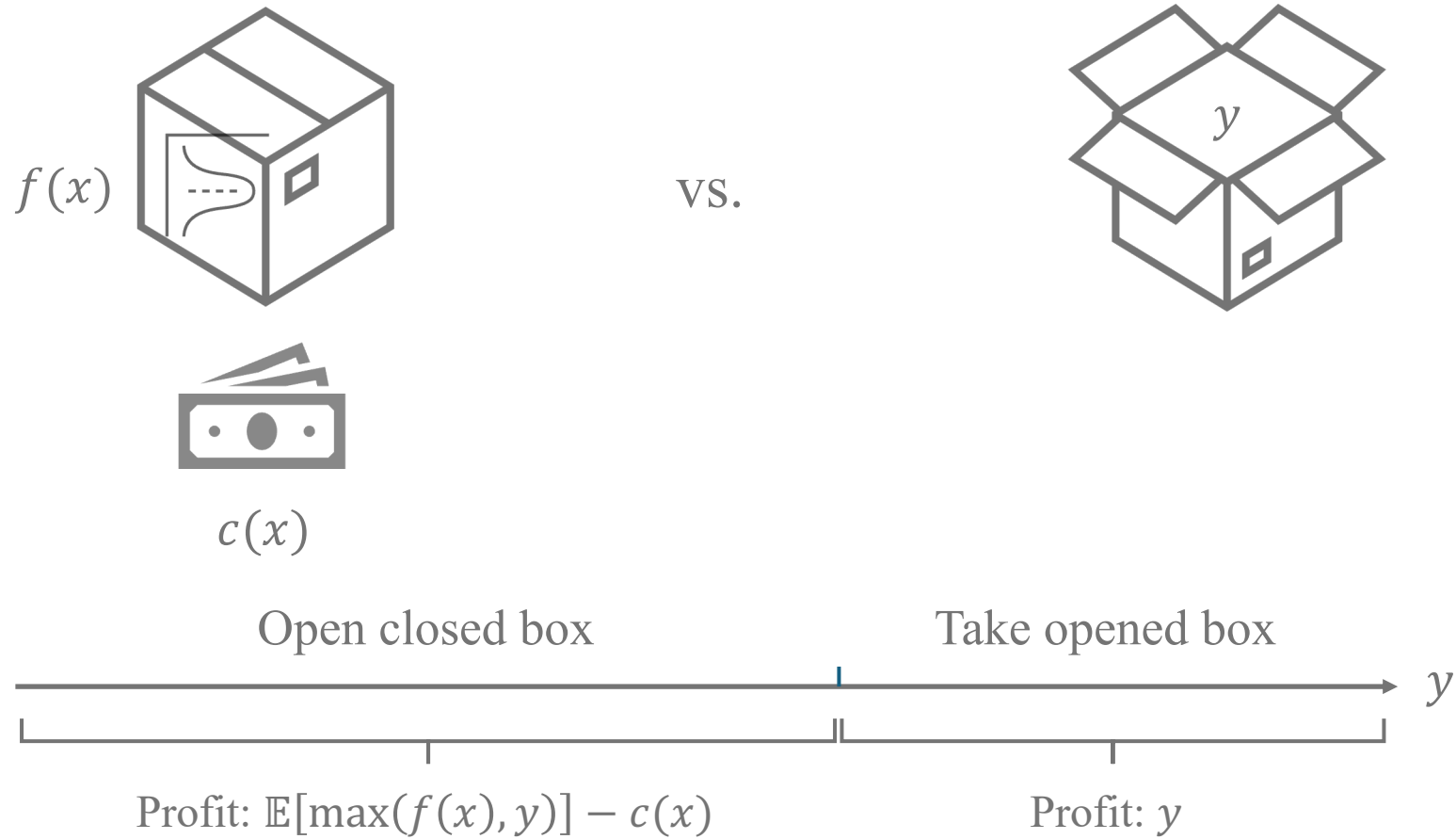
$$f(x) = \begin{cases} 200 & \text{w.p. } 0.01 \\ 0 & \text{otherwise} \end{cases}, c(x) = 1, x \in \{2, 3, \dots, 1000\}$$

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

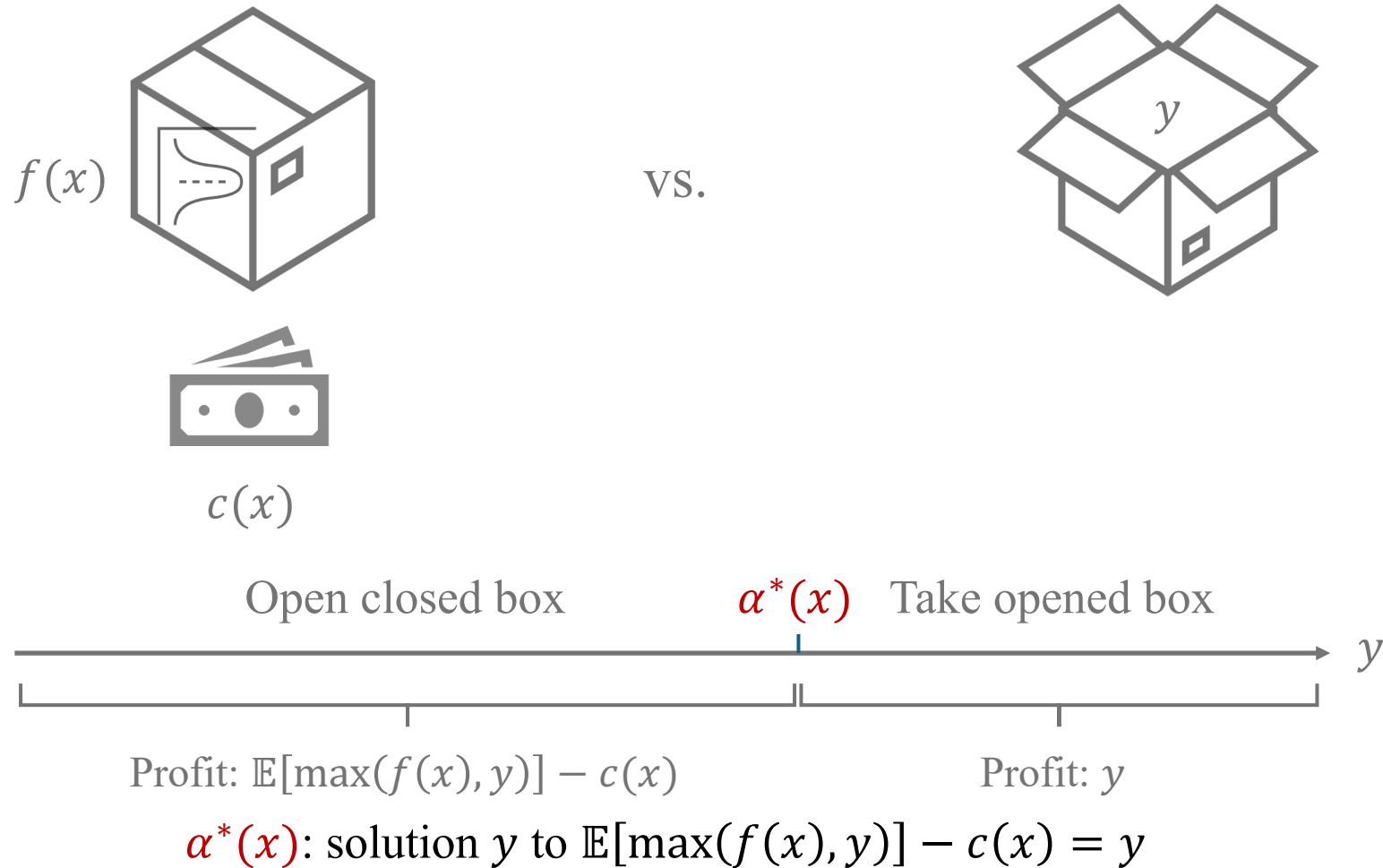
Stopping rule: $y_{\text{best}} = 200$

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

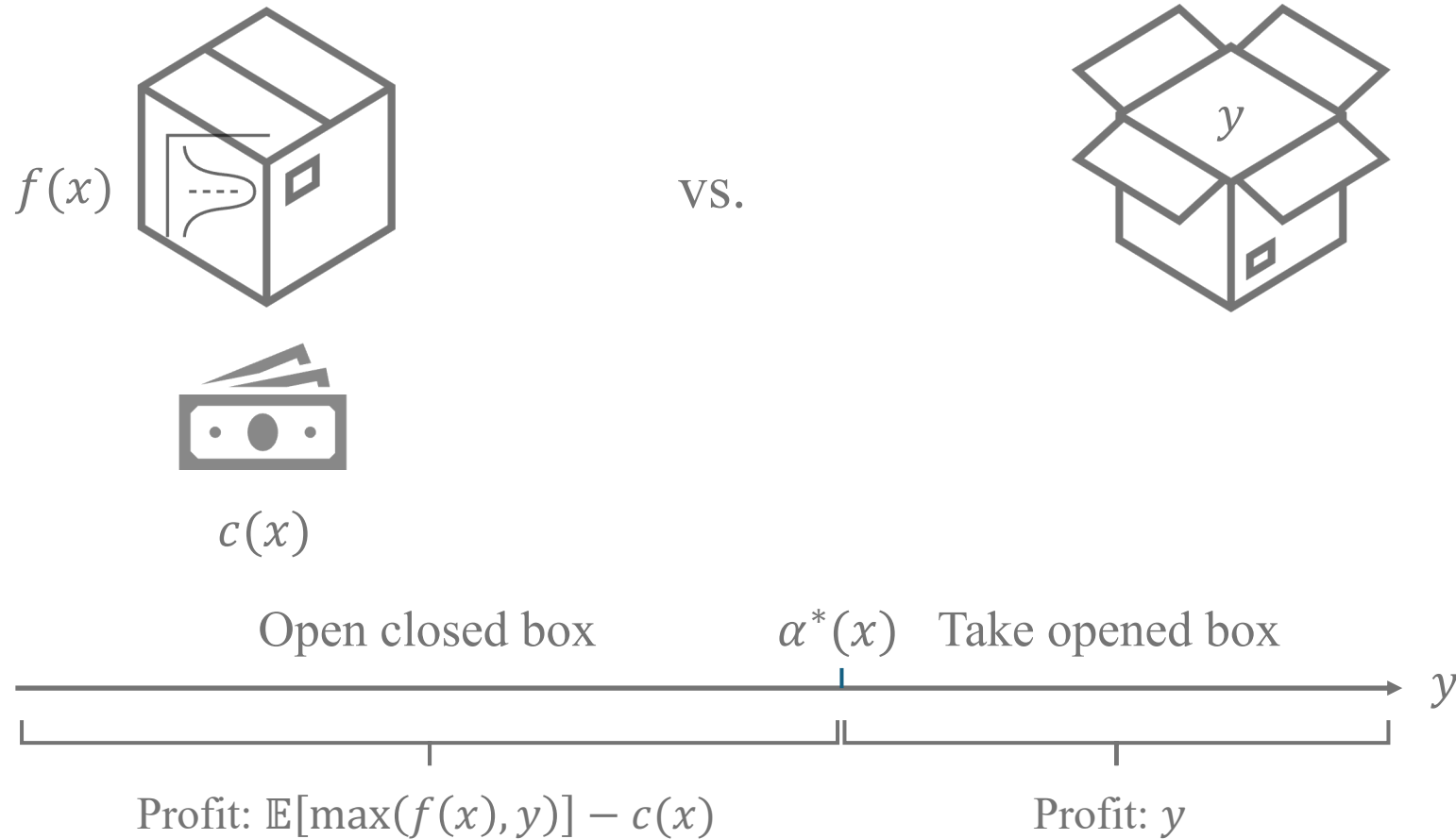
1.5-box Problem



1.5-box Problem

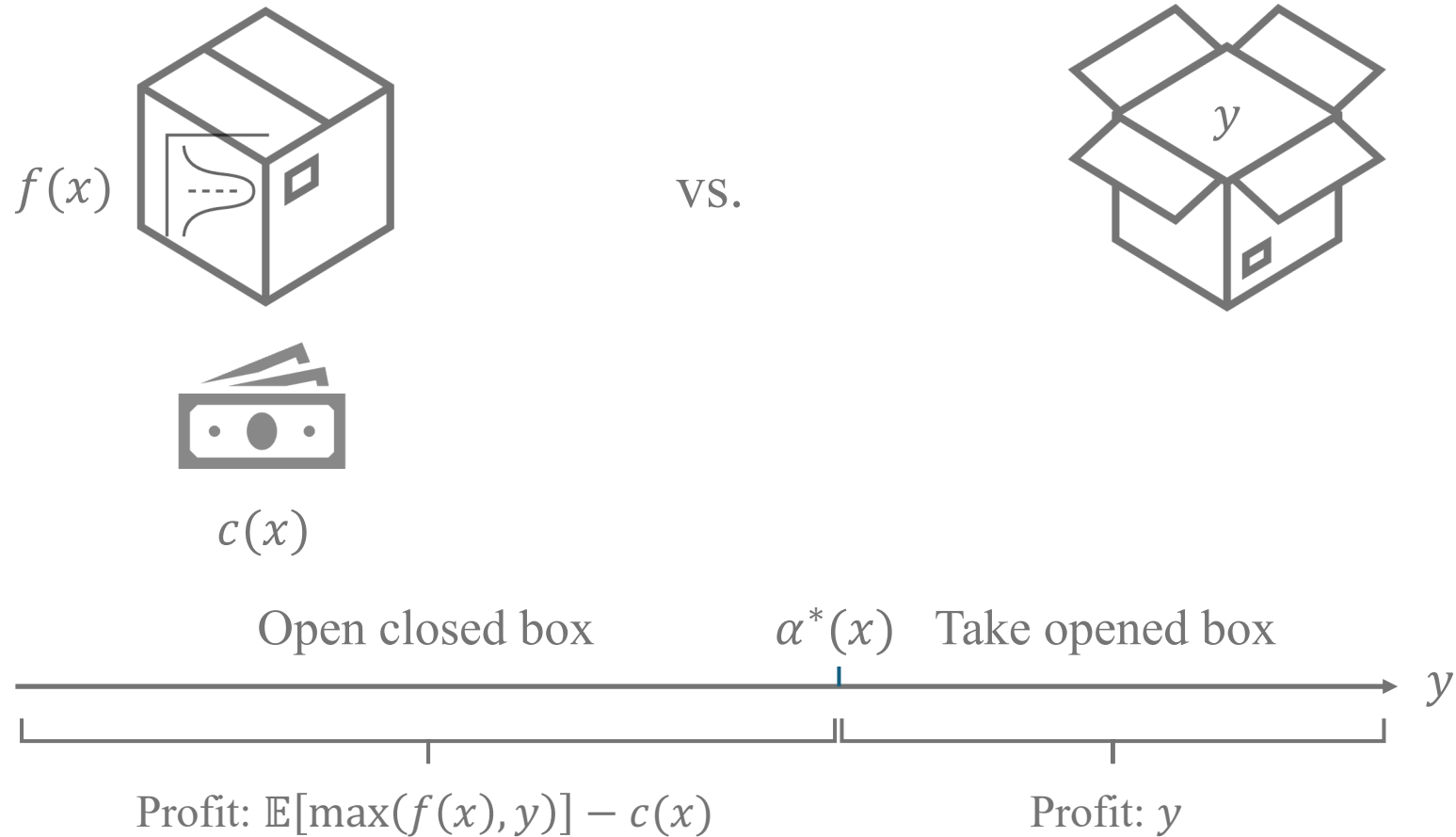


1.5-box Problem



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

1.5-box Problem

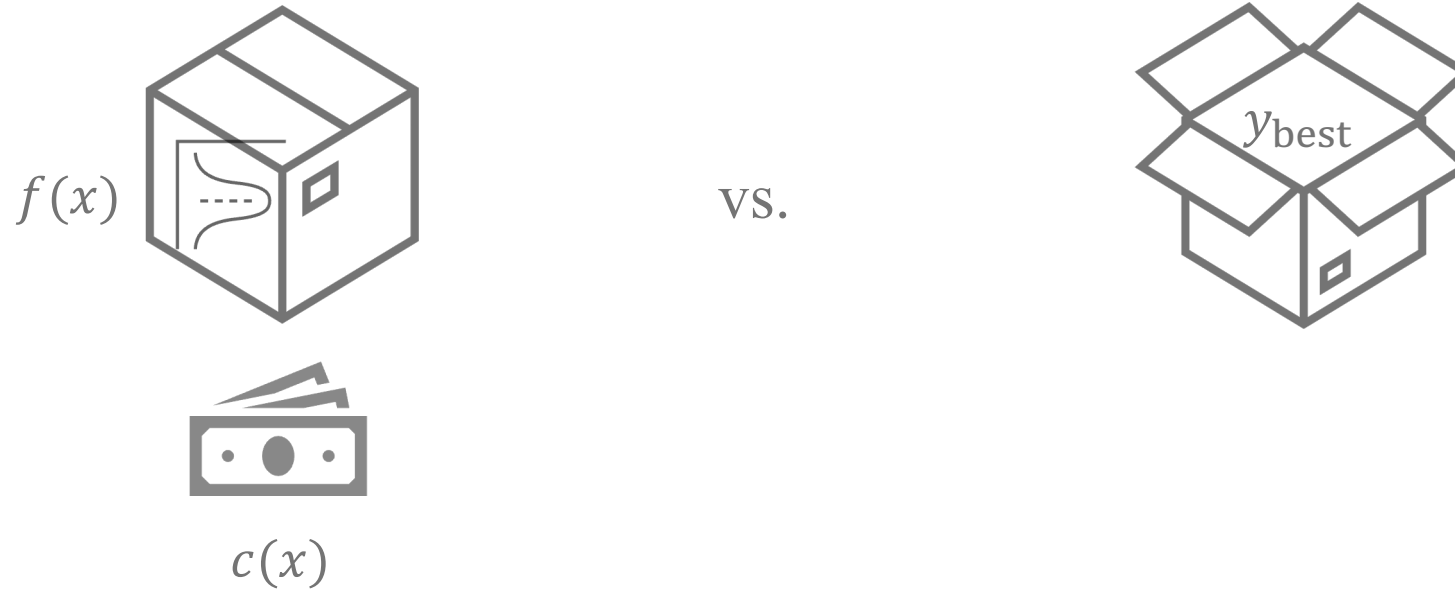


$\alpha^*(x)$: solution y to $\mathbb{E}[(f(x) - y)^+] = c(x)$

$\alpha^*(x)$: 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

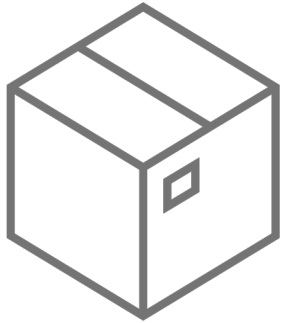
Gittins index \leq current best

y_{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

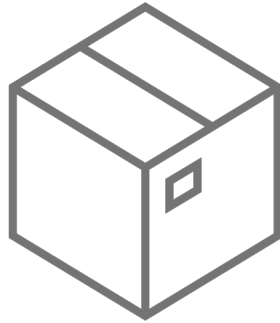
$t = 0$



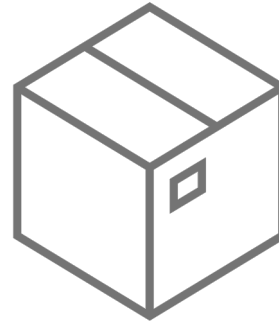
$$f(1) = 200 \text{ w.p. } 1$$

$$c(1) = 198$$

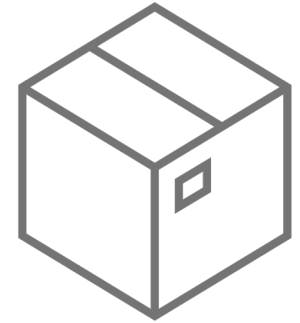
$$200 - ? = 198$$



...



...



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

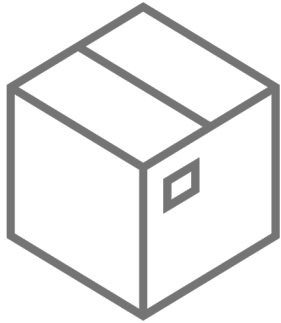
$$(200 - ?) * 0.01 = 1$$

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

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

Optimal policy: Gittins policy

$t = 0$



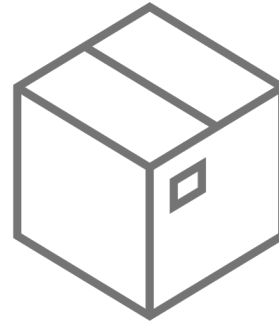
$$f(1) = 200 \text{ w.p. } 1$$

$$c(1) = 198$$

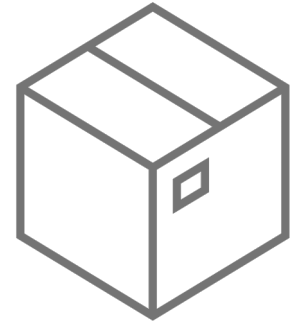
$$\alpha^*(1) = 2$$



...



...



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

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

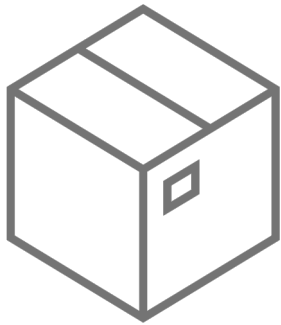
Inspection rule: $\operatorname{argmax}_x \alpha^*(x)$ s.t. $\operatorname{EI}_f(x; \alpha^*(x)) = c(x)$ **Stopping rule:** $\alpha^*(x) \leq y_{\text{best}}, \forall x \in \mathcal{X}$

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

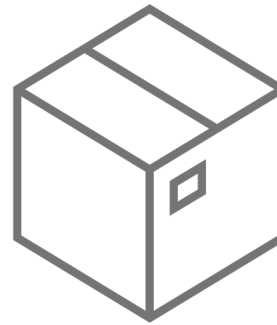
Optimal policy: Gittins policy

$t = 1$

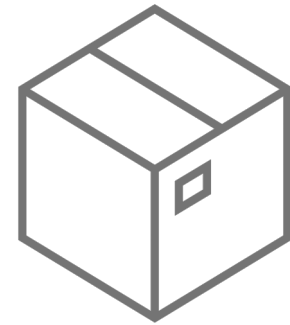
$y_{\text{best}} = 200 \text{ or } 0$



...



...



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

$$c(1) = 198$$

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

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

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

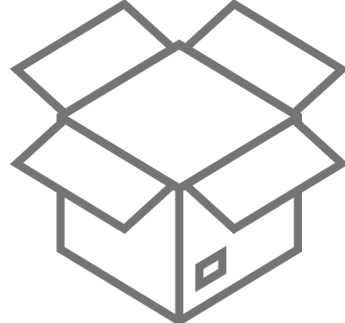
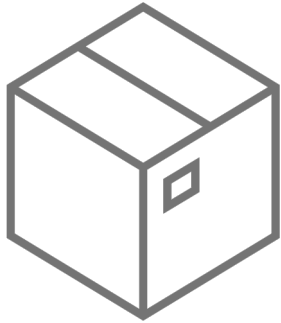
Inspection rule: $\operatorname{argmax}_x \alpha^*(x)$ s.t. $\operatorname{EI}_f(x; \alpha^*(x)) = c(x)$ **Stopping rule:** $\alpha^*(x) \leq y_{\text{best}}, \forall x \in \mathcal{X}$

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

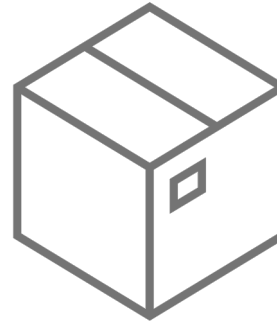
Optimal policy: Gittins policy

$t \approx 100$

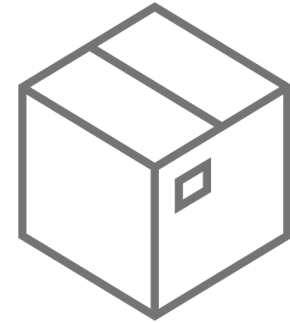
$y_{\text{best}} = 200$



...



...



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

$$c(1) = 198$$

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

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

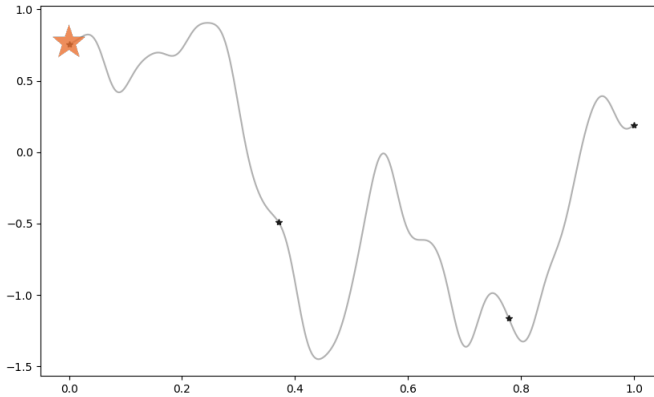
$$\alpha^*(x) = 100$$

Inspection rule: $\operatorname{argmax}_x \alpha^*(x)$ s.t. $\mathbb{E}_f(x; \alpha^*(x)) = c(x)$ **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

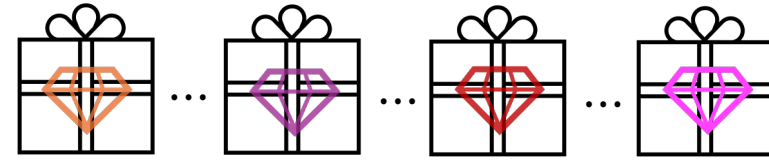
Special case of Markovian/
Bayesian multi-armed bandits



Continuous

Correlated

Hard budget constraint



Discrete



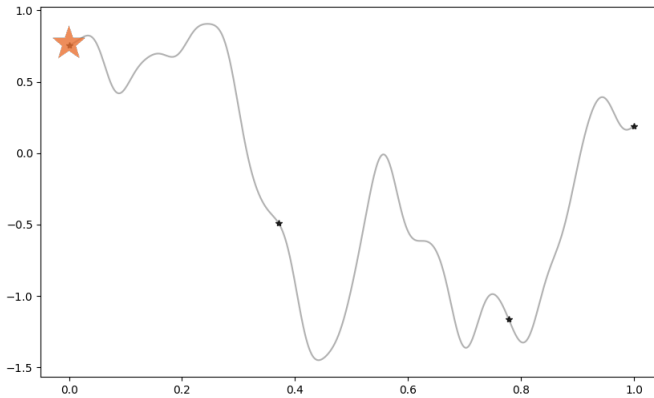
Independent



Cost per sample

Optimal policy: Gittins index [Weitzman'79]

Bayesian Optimization \Rightarrow Pandora's Box

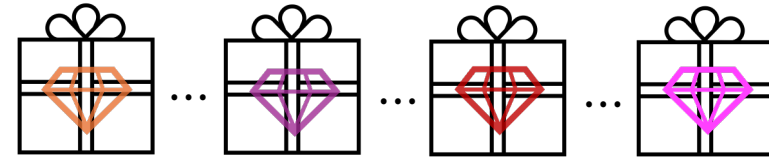
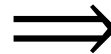


Continuous

Correlated

Hard budget constraint

Is Gittins index good?



Discrete

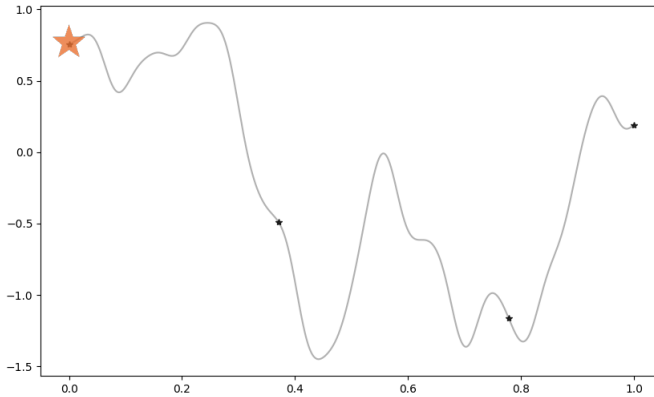
Independent

Cost per sample

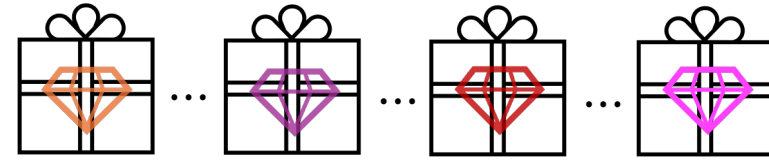
Optimal policy: Gittins index



Bayesian Optimization \Rightarrow Pandora's Box



Continuous



Discrete

Correlated



Independent

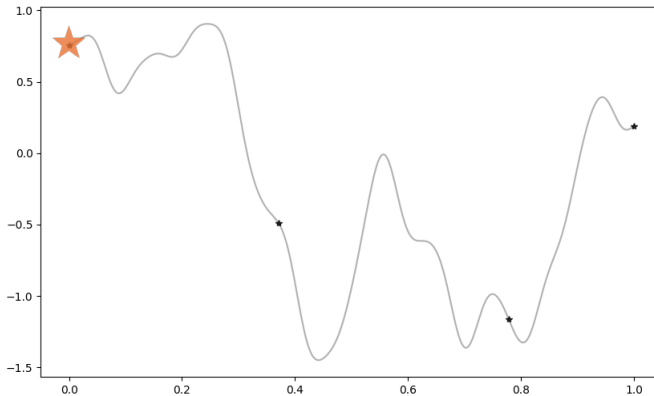
Hard budget constraint



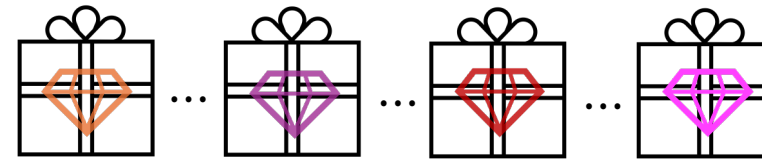
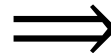
Cost per sample

Is Gittins index good? How to translate? \Leftarrow Optimal policy: Gittins index

Bayesian Optimization \Rightarrow Pandora's Box



Continuous



Discrete

Correlated



Independent

Hard budget constraint



Cost per sample

Is Gittins index good?

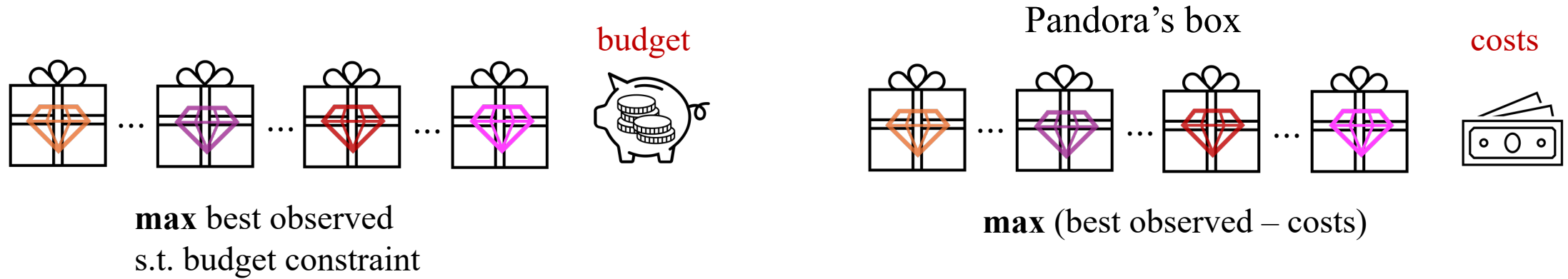
How to translate?



Optimal policy: Gittins index

Our contributions!

How to translate?



Expected budget constraint



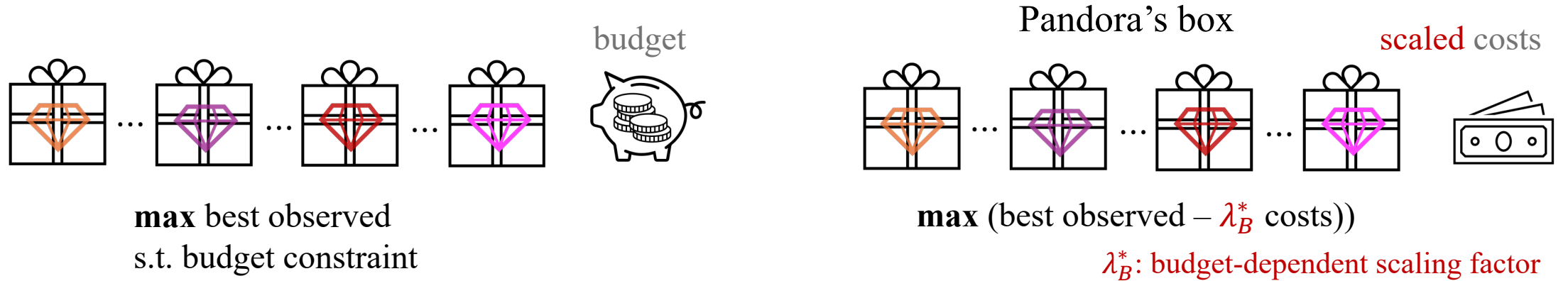
Cost per sample

Optimal policy?



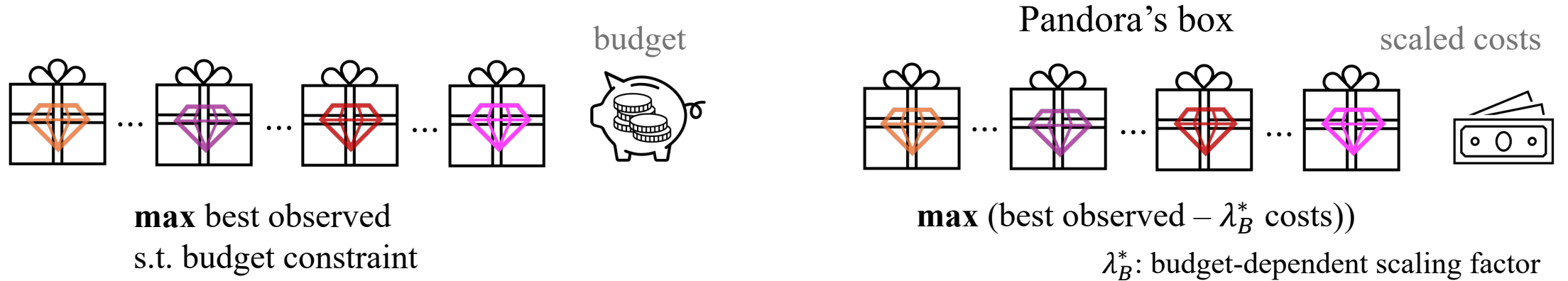
Optimal policy: Gittins index

Expected budget constraint \Leftrightarrow Cost per sample



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

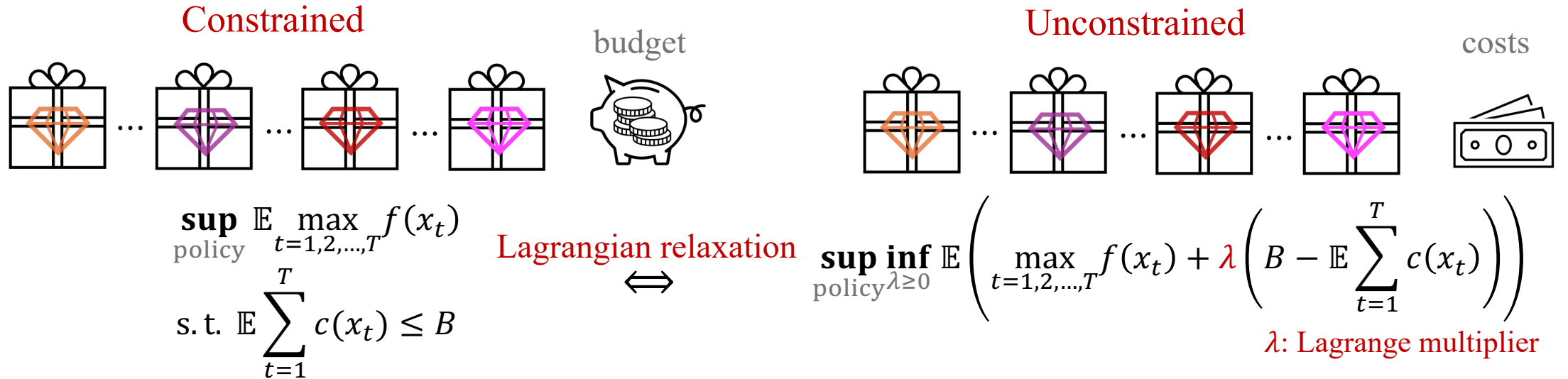
Expected budget constraint \Leftrightarrow Cost per sample



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

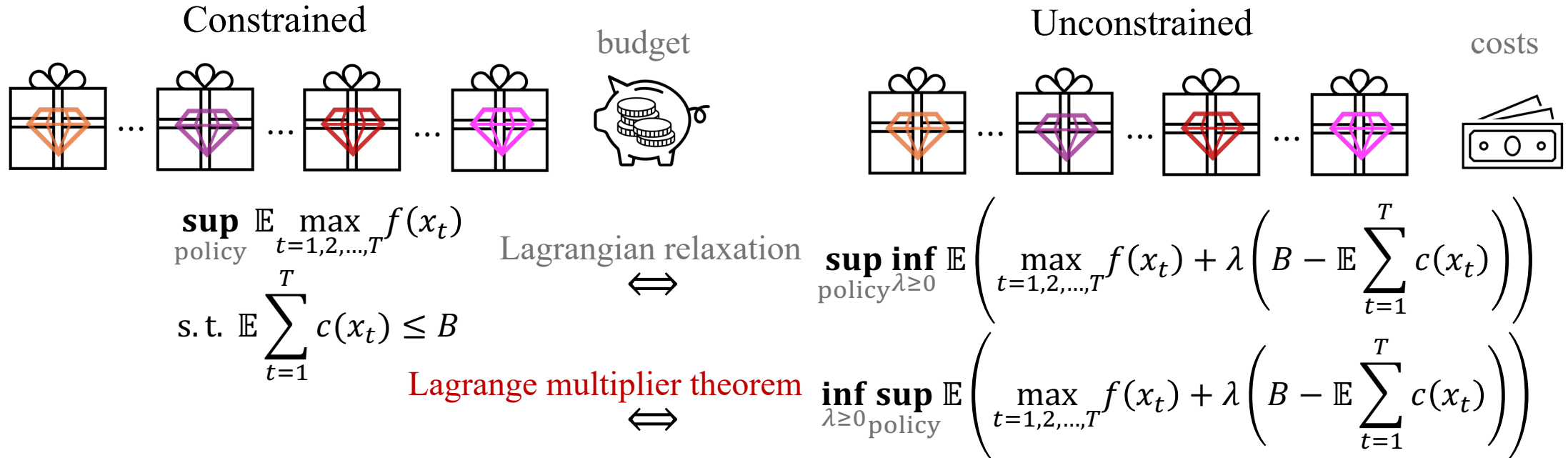
Expected budget constraint \Leftrightarrow Cost per sample



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

Extension to [Aminian, Manshadi, Niazadeh'24]

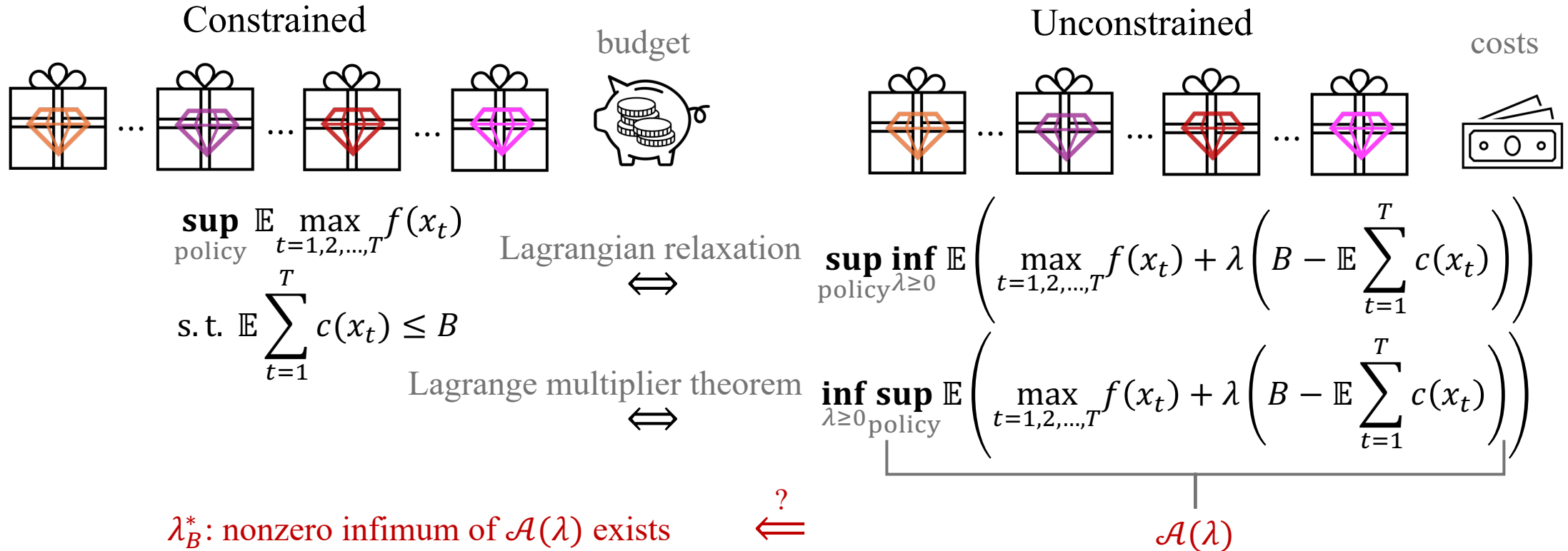
Expected budget constraint \Leftrightarrow Cost per sample



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

Extension to [Aminian, Manshadi, Niazadeh'24]

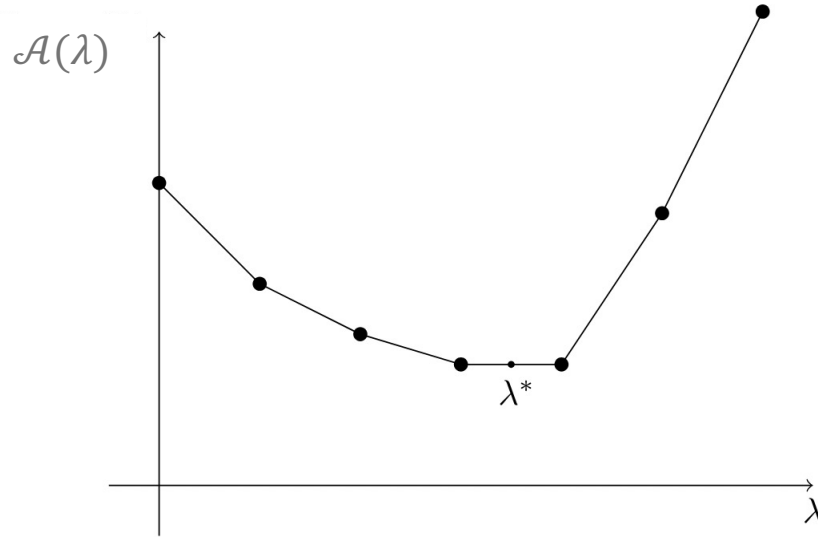
Expected budget constraint \Leftrightarrow Cost per sample



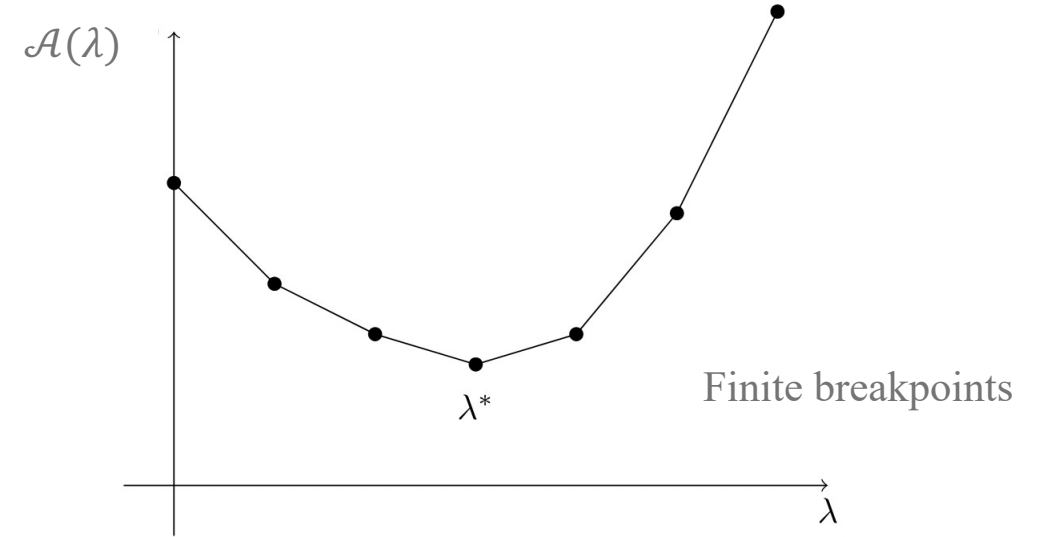
Optimal policy: Gittins solution to Pandora's box with scaled costs \Leftarrow Optimal policy: Gittins index

Extension to [Aminian, Manshadi, Niazadeh'24]

Expected budget constraint \Leftrightarrow Cost per sample



(a) Degenerate case, differentiable at λ^* .



(b) Non-degenerate case, breakpoint at λ^* .

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

Envelope Theorem

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

\Leftrightarrow

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

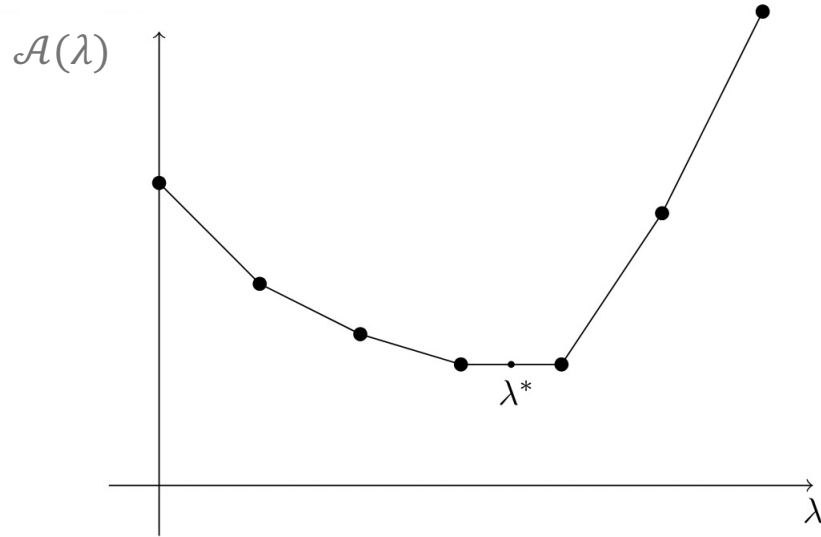
Optimal policy: Gittins solution to
Pandora's box with scaled costs

\Leftrightarrow

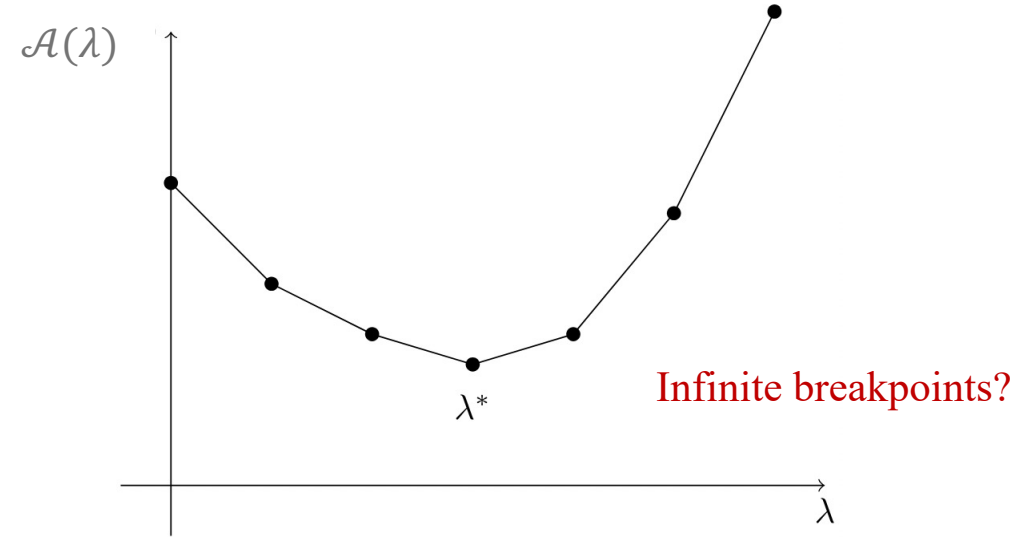
Optimal policy: Gittins index

Figure from [Aminian, Manshadi, Niazadeh'24]

Expected budget constraint \Leftrightarrow Cost per sample



(a) Degenerate case, differentiable at λ^* .



(b) Non-degenerate case, breakpoint at λ^* .

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

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

\Leftrightarrow

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

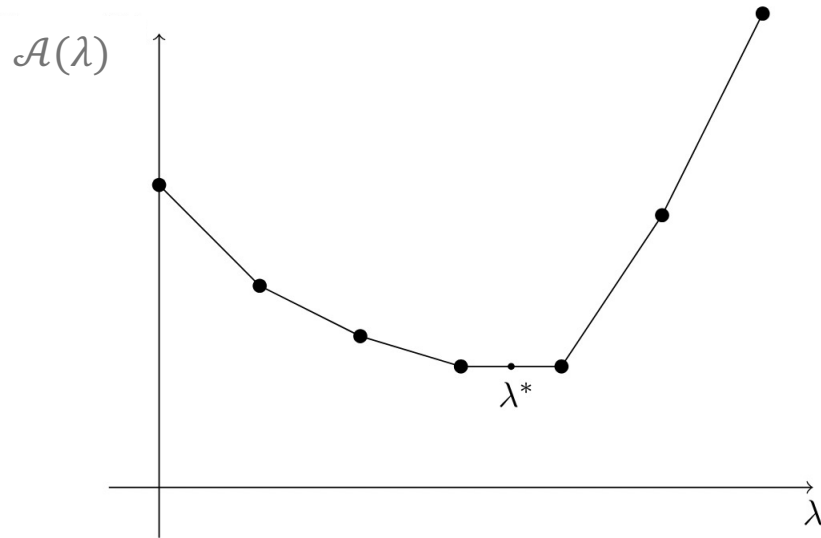
Optimal policy: Gittins solution to Pandora's box with scaled costs

\Leftrightarrow

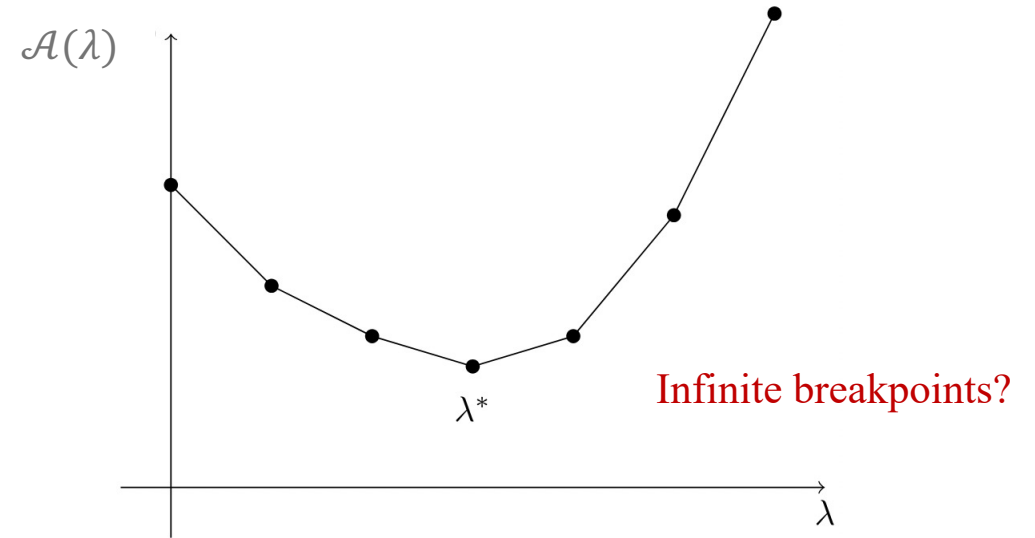
Optimal policy: Gittins index

Figure from [Aminian, Manshadi, Niazadeh'24]

Expected budget constraint \Leftrightarrow Cost per sample



(a) Degenerate case, differentiable at λ^* .



(b) Non-degenerate case, breakpoint at λ^* .

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

Our work: sharp Envelope Theorem

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

\Leftrightarrow

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

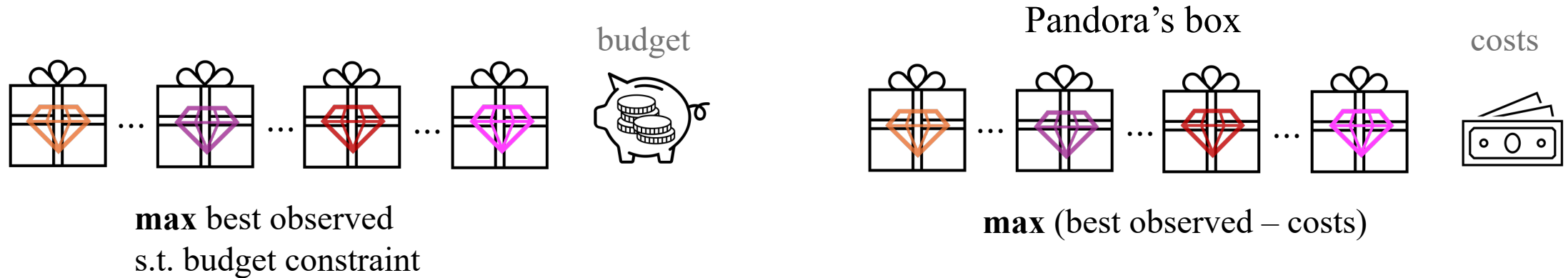
Optimal policy: Gittins solution to
Pandora's box with scaled costs

\Leftrightarrow

Optimal policy: Gittins index

Figure from [Aminian, Manshadi, Niazadeh'24]

How to translate?



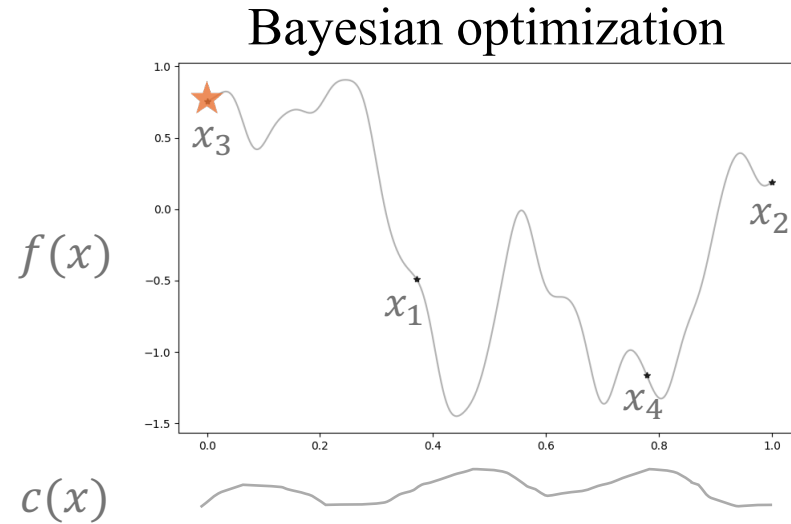
Hard budget constraint

\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?

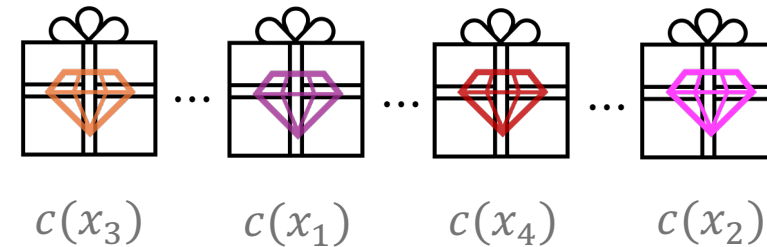


Continuous

Correlated

Hard budget constraint

Budget-constrained
Pandora's box



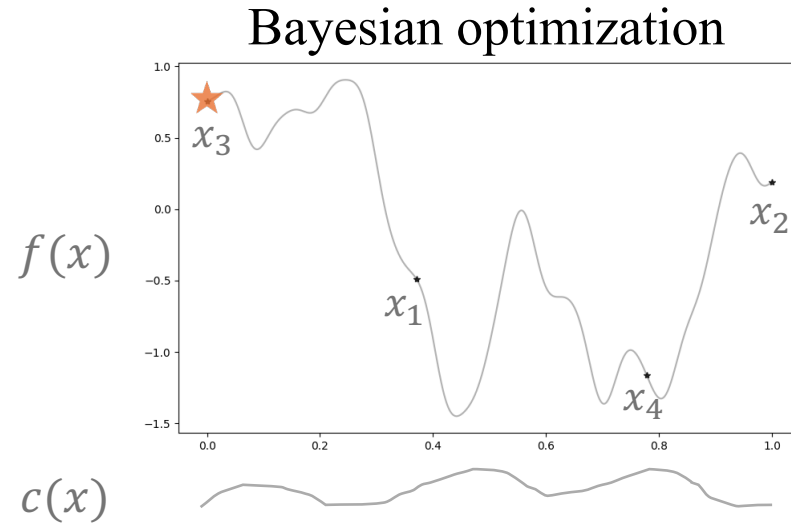
Discrete

Independent

Cost per sample

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

How to translate?

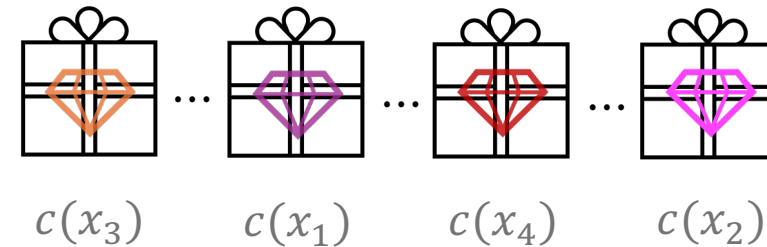


Continuous

Correlated

Hard budget constraint

Budget-constrained
Pandora's box



Discrete

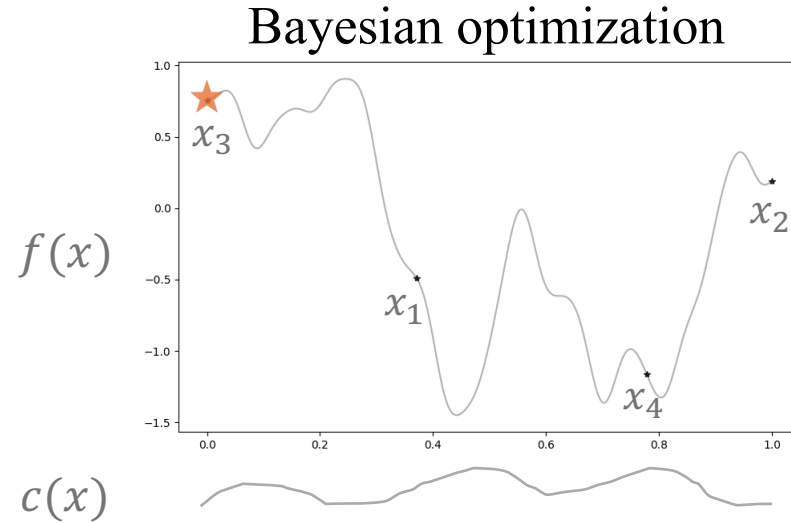
Independent

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?

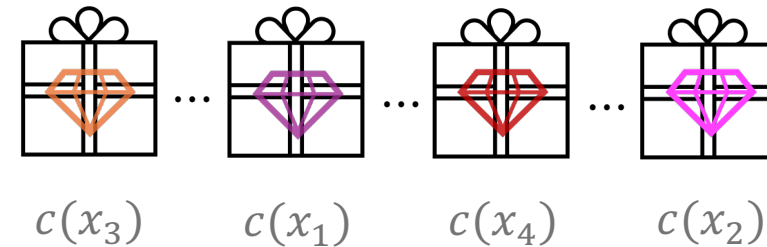


Continuous

Correlated

Hard budget constraint

Budget-constrained
Pandora's box



Discrete

Independent

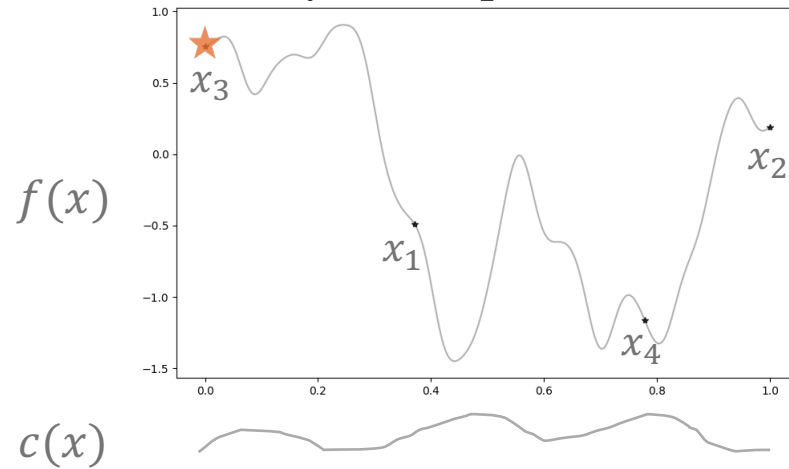
Cost per sample

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

popular one-step
heuristic: EI policy

How to translate?

Bayesian optimization



Continuous

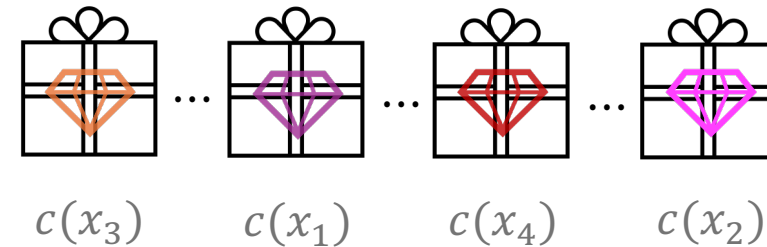
Correlated

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



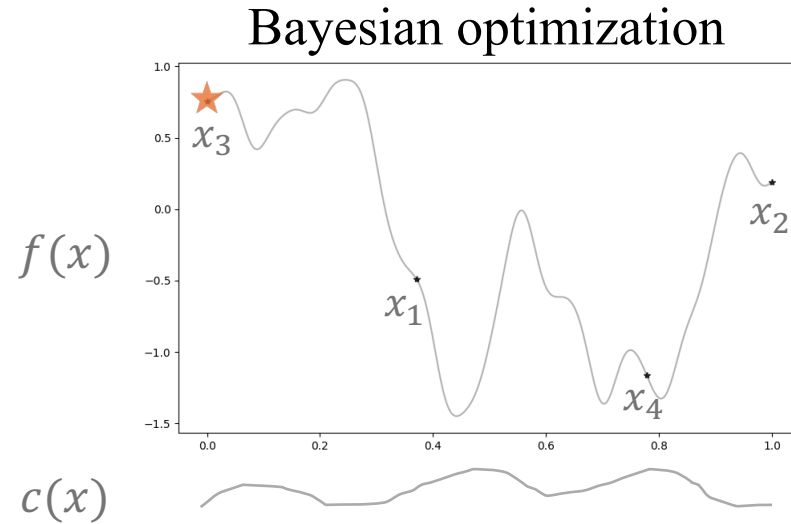
Discrete

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?

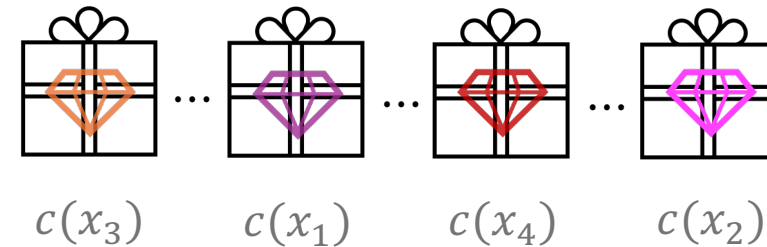


Continuous

Correlated

Hard budget constraint

Budget-constrained
Pandora's box



Discrete

Independent

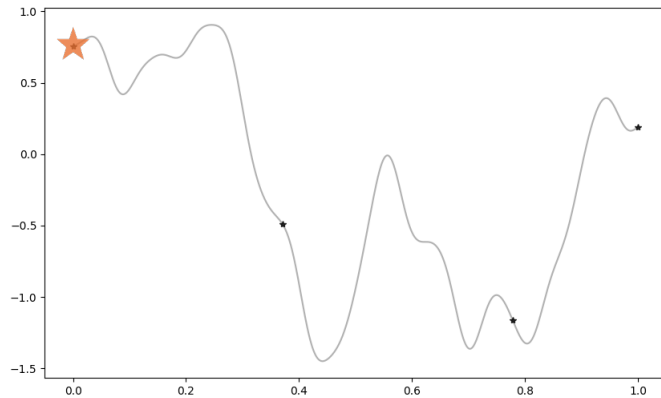
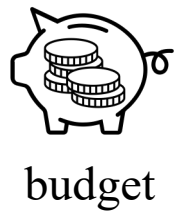
Cost per sample

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

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?



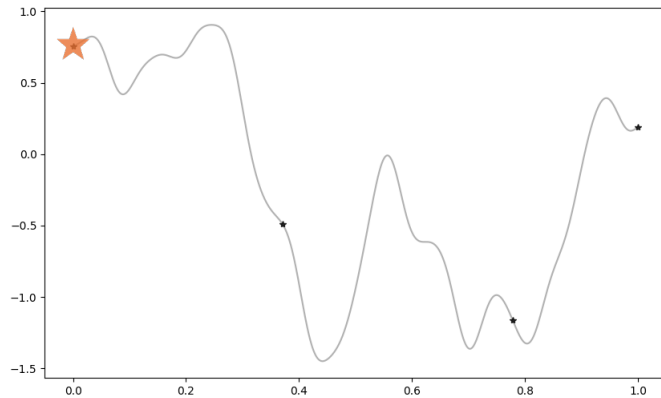
?



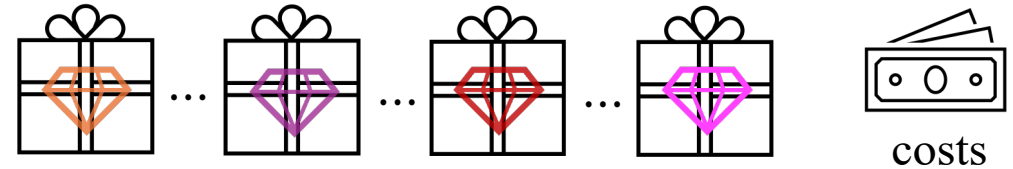
Pandora's Box Gittins index

Our Contributions

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



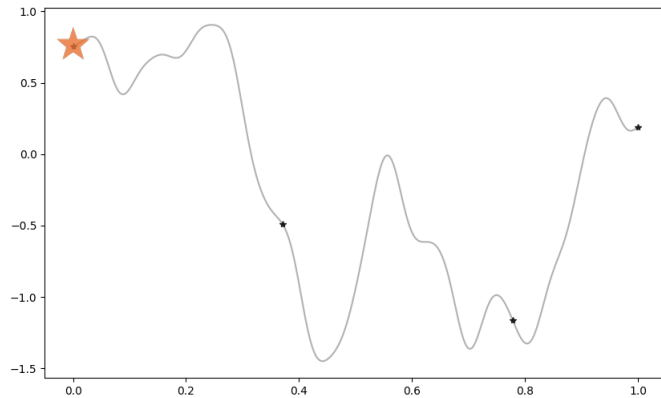
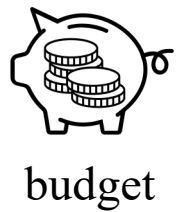
Our work



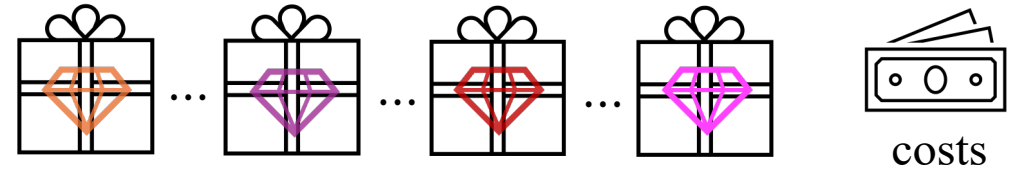
Pandora's Box Gittins index

Our Contributions

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



Our work

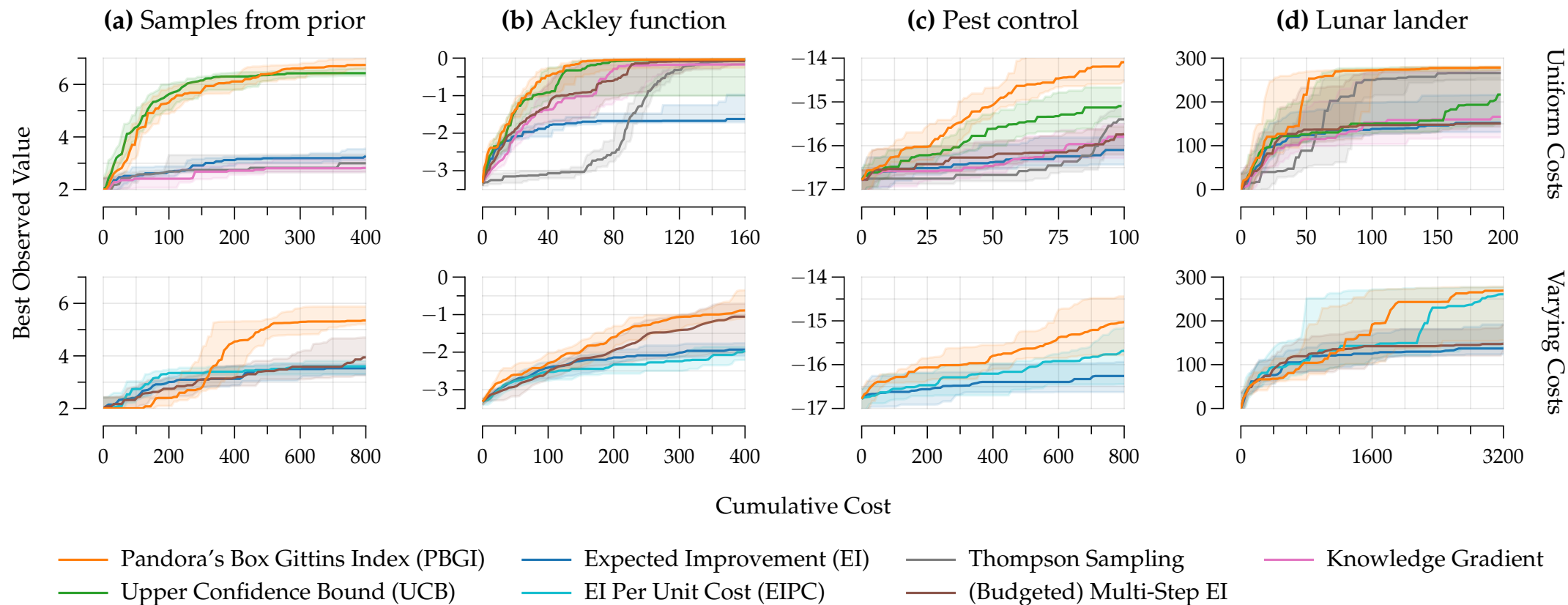


Pandora's Box Gittins index

Experiment Results: PBGI vs Baselines

Synthetic

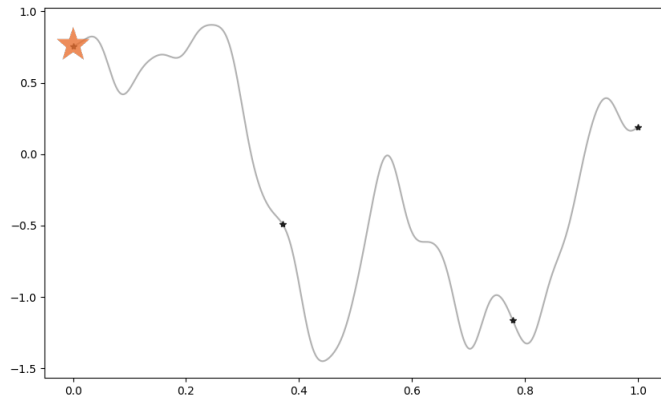
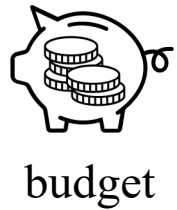
Empirical



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

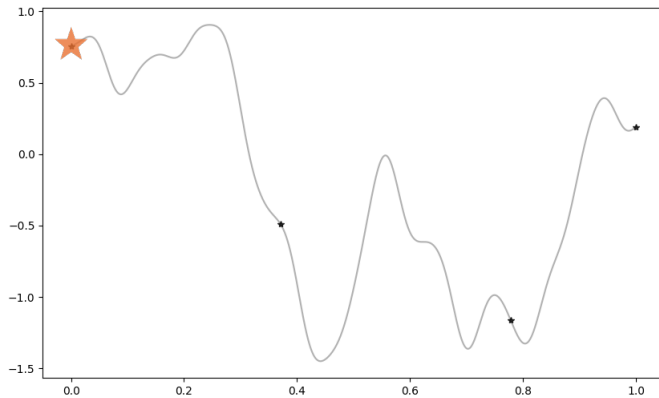
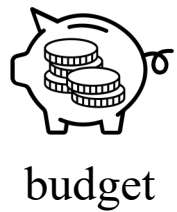


Pandora's Box Gittins index

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

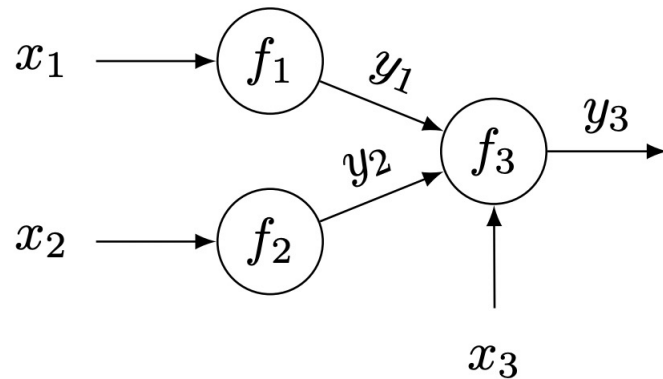


\Leftarrow Pandora's Box Gittins index

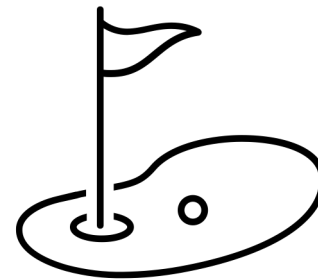
Check our preprint on arXiv!

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]