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

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

ECGI'24

Bayesian Optimization

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

$\in$ decision-making under uncertainty

Applications:
Hyperparameter tuning
Drug/material discovery
Experiment design

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Bayesian Optimization

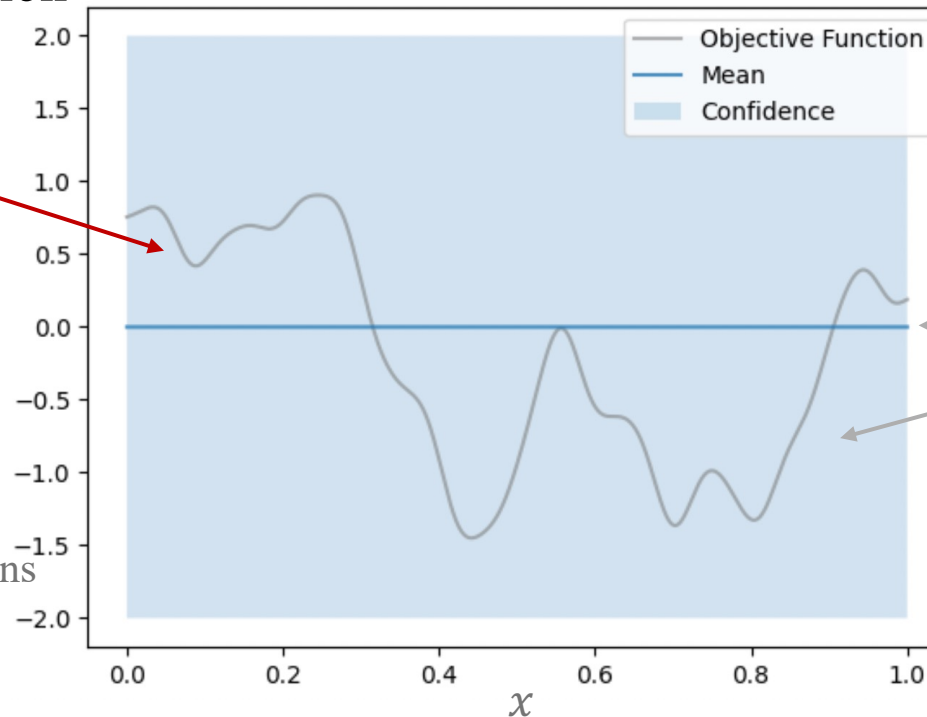**Goal:** optimize expensive-to-evaluate black-box function

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

Gaussian process: infinite-dimensional generalization of multivariate normal distributions

$\in$ decision-making under uncertainty

Applications:
Hyperparameter tuning
Drug/material discovery
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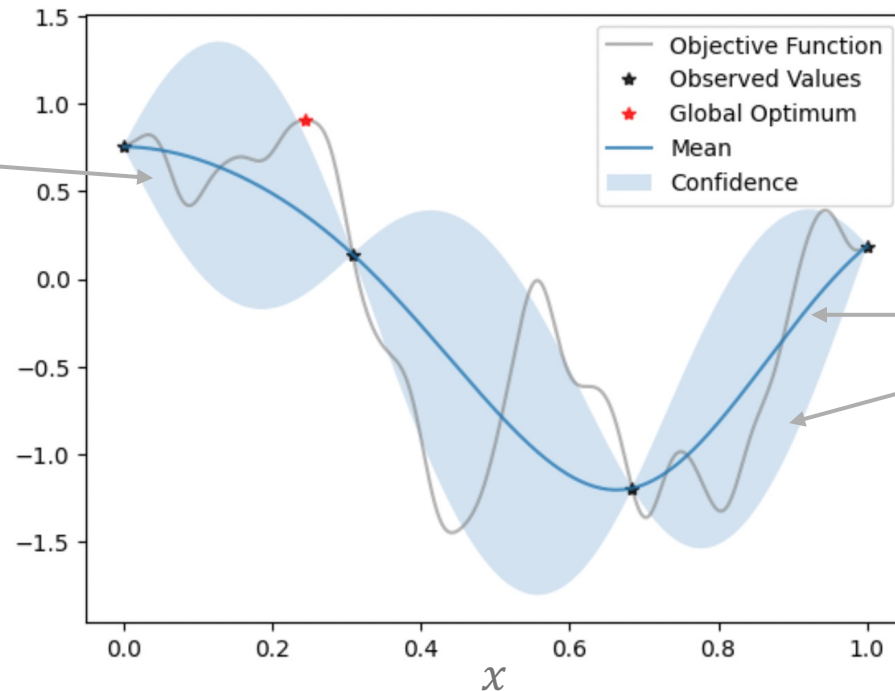x: hyperparameter/configuration
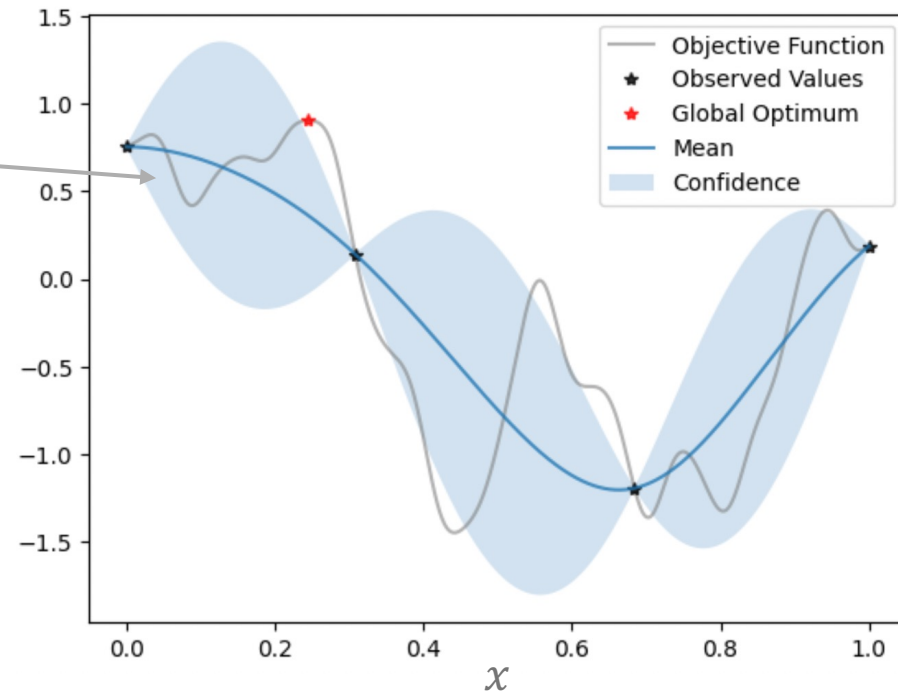
mean: prediction

variance: confidence/uncertainty

Bayesian Optimization

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x: hyperparameter/configuration

mean: prediction

variance: confidence/uncertainty

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

Decision: evaluate a set of points

Bayesian Optimization

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

Applications:
Hyperparameter tuning
Drug/material discovery
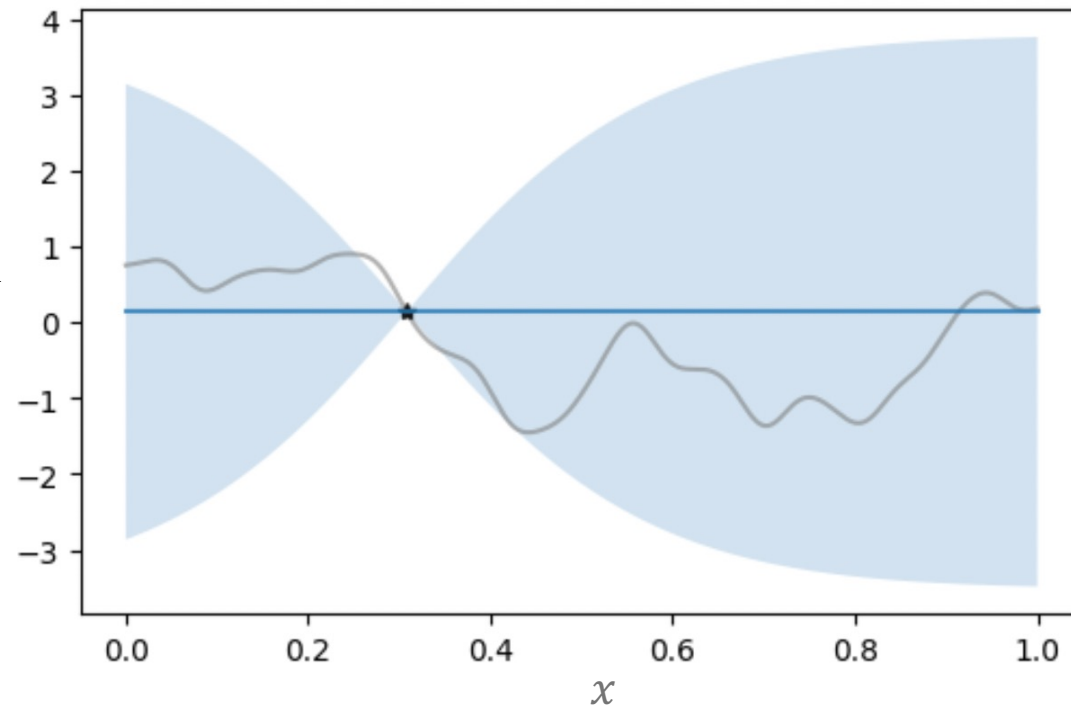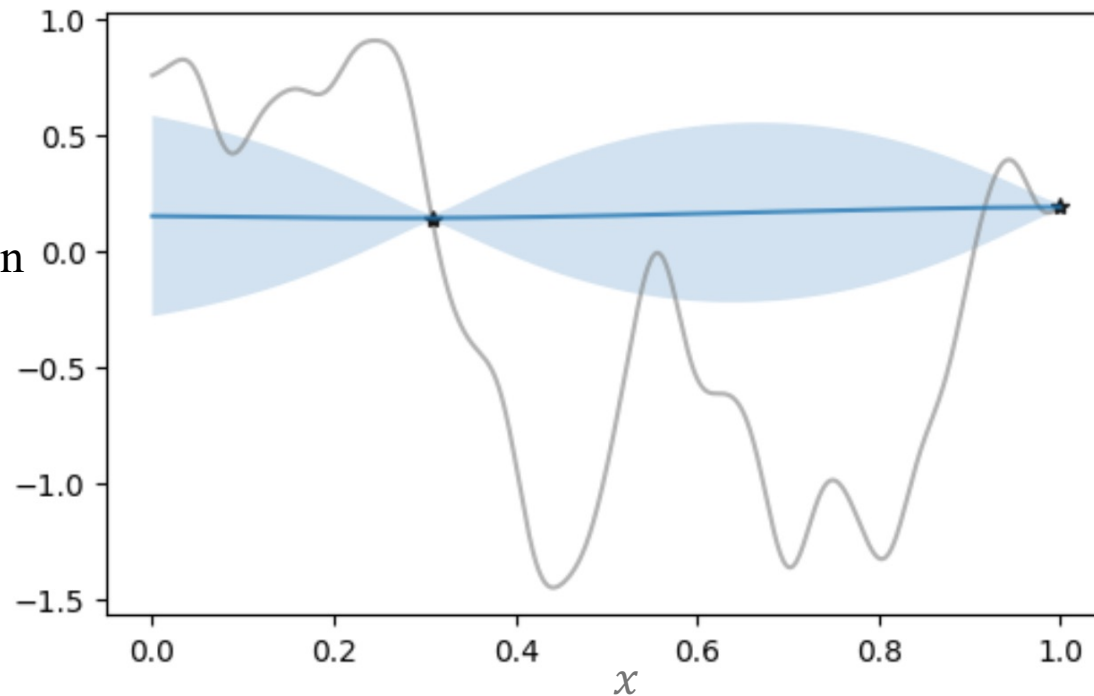Experiment design

x: hyperparameter/configuration

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Applications:

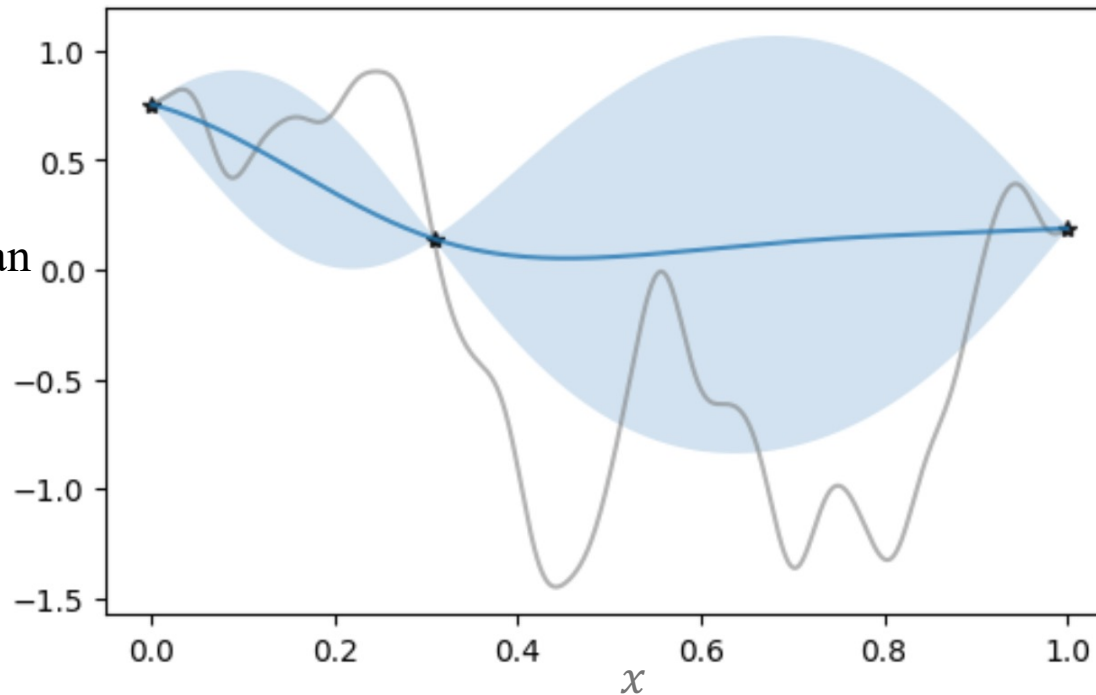Hyperparameter tuning
Drug/material discovery
Experiment design

x: hyperparameter/configuration

adaptively

Decision: evaluate a set of points

Bayesian Optimization

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

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Applications:
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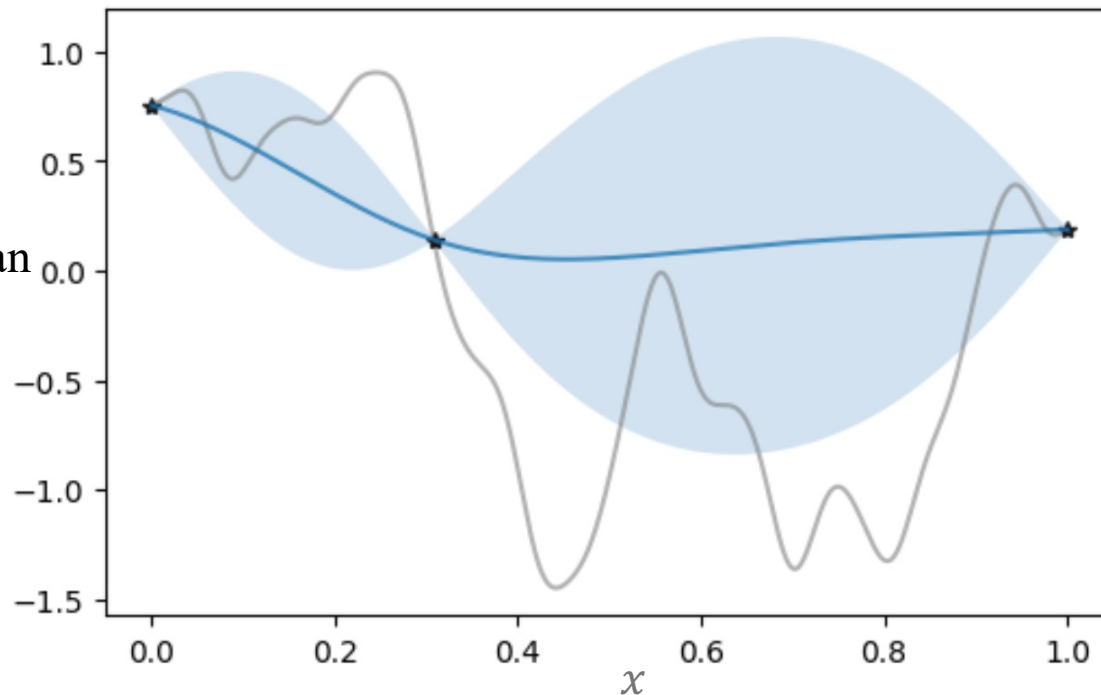
x: hyperparameter/configuration

adaptively
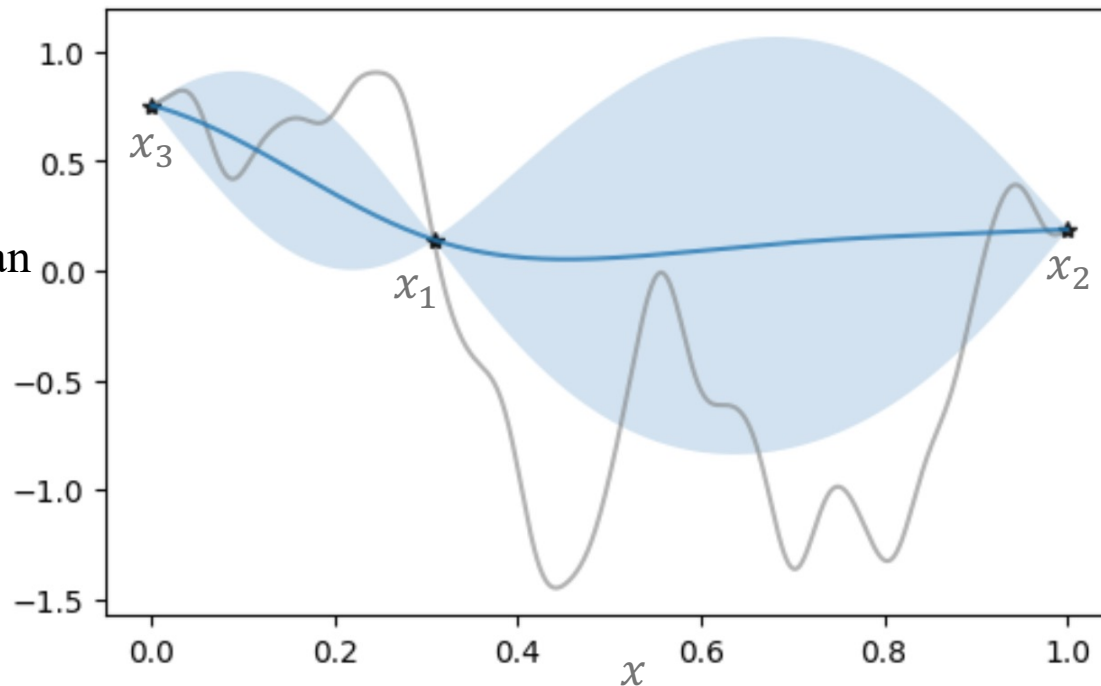
Decision: evaluate a set of points

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x: hyperparameter/configuration

Decision: adaptively evaluate a set of points

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

T: time budget

Bayesian Optimization

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

An unknown random function $f : \mathcal{X} \to \mathbb{R}$ 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

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

Decision: adaptively evaluate a set of points

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

T: time budget

Why is it hard?
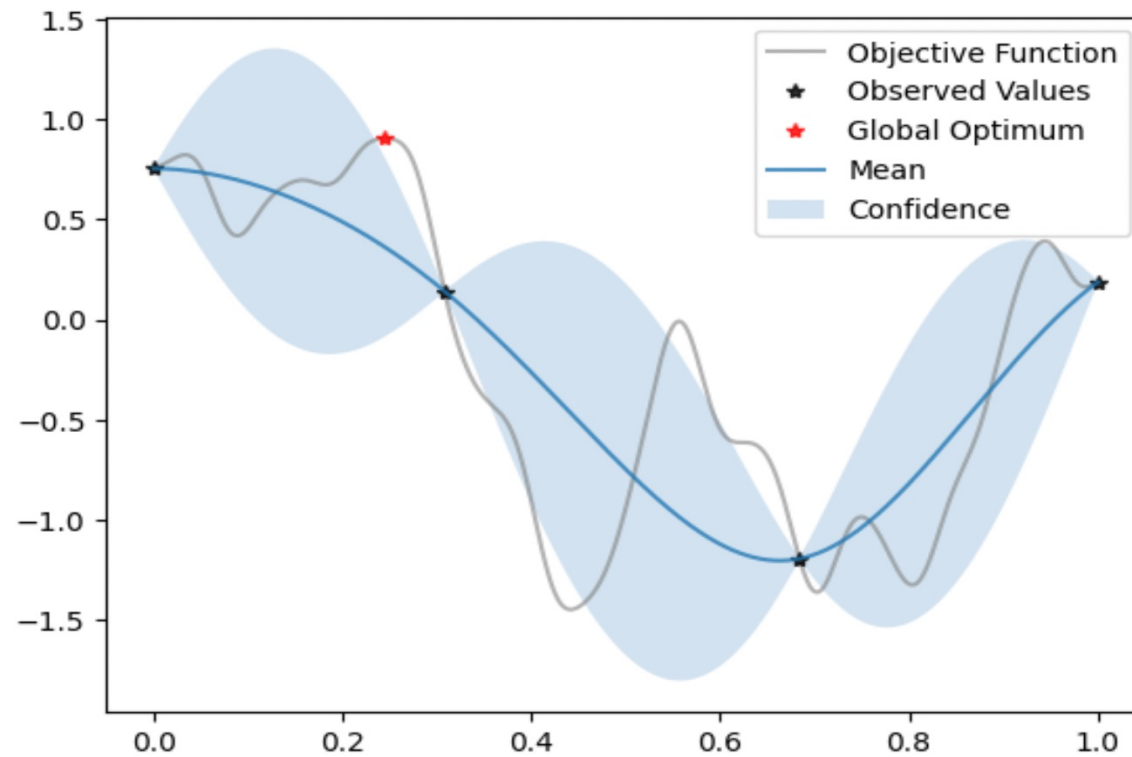
Why is it hard?
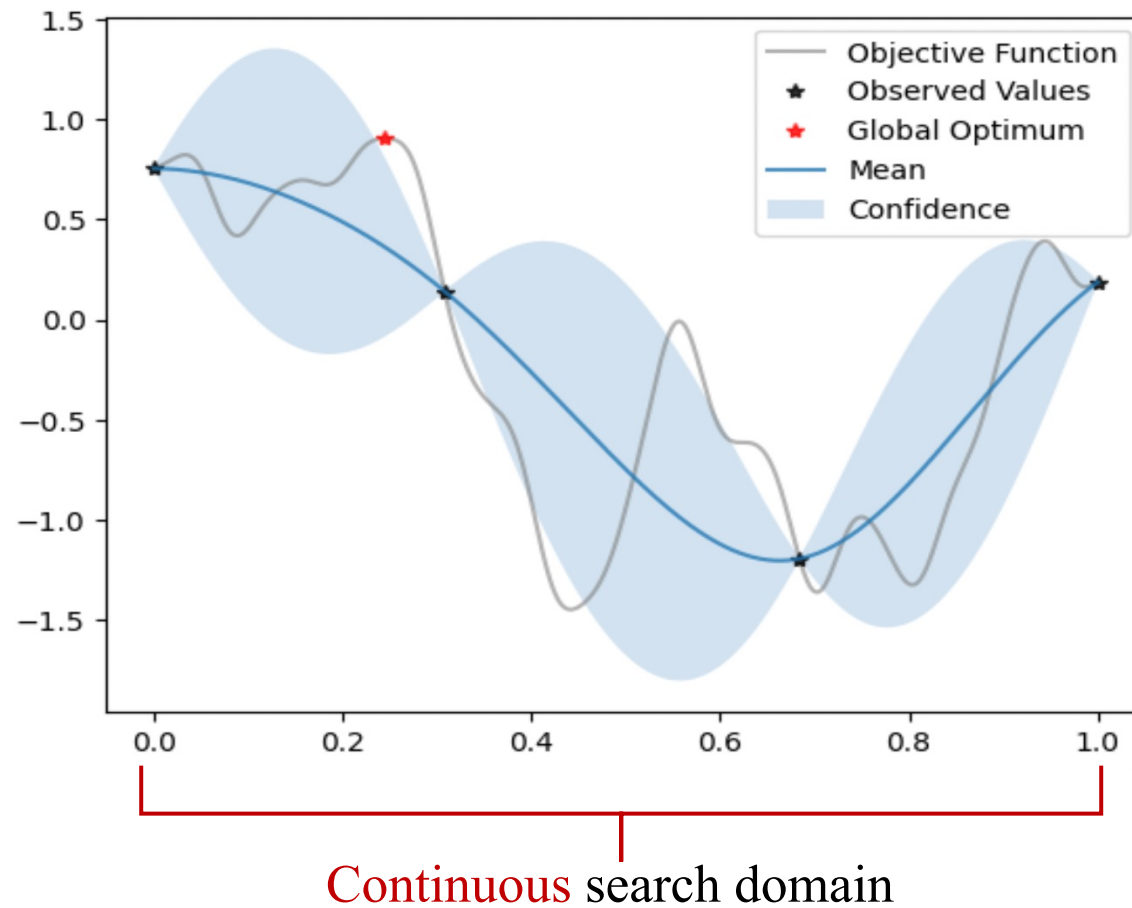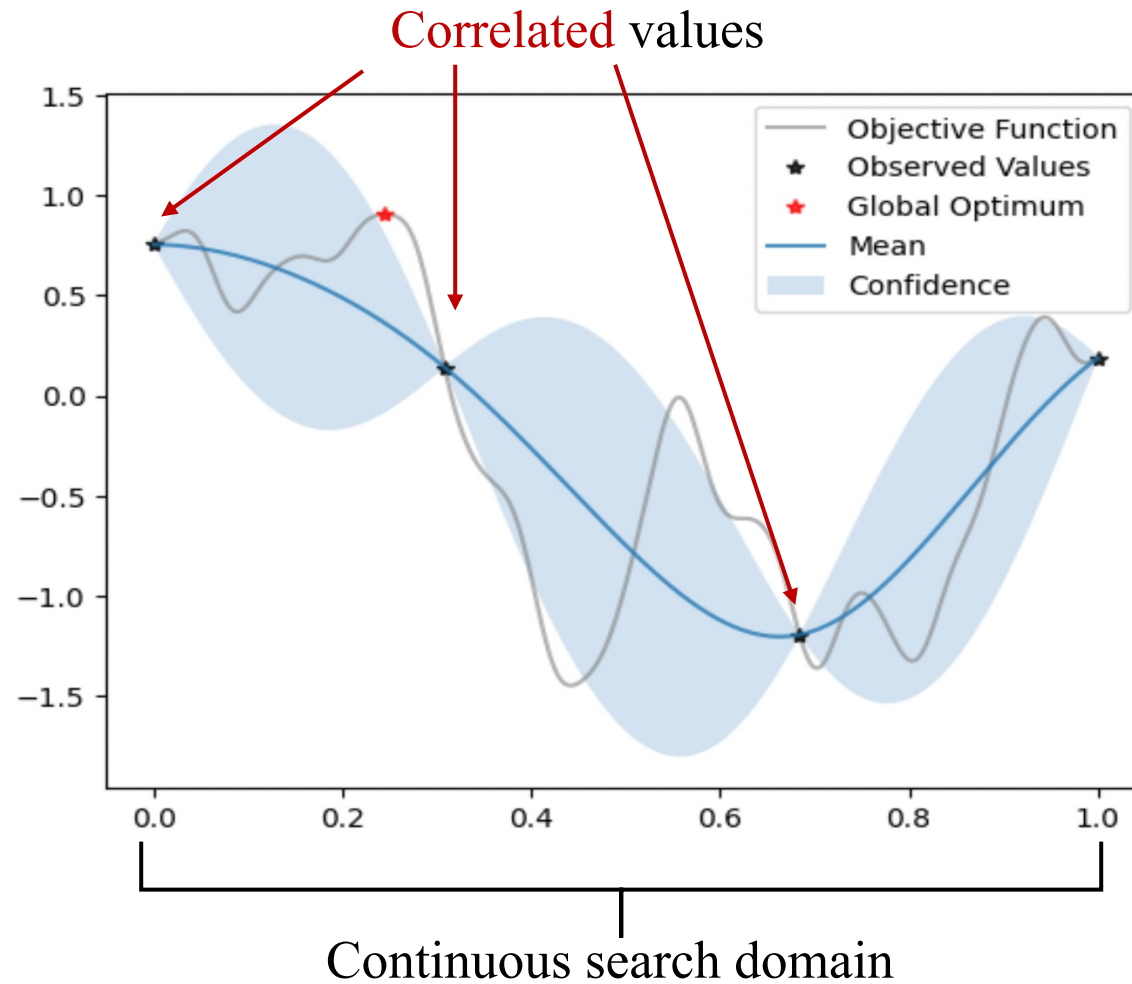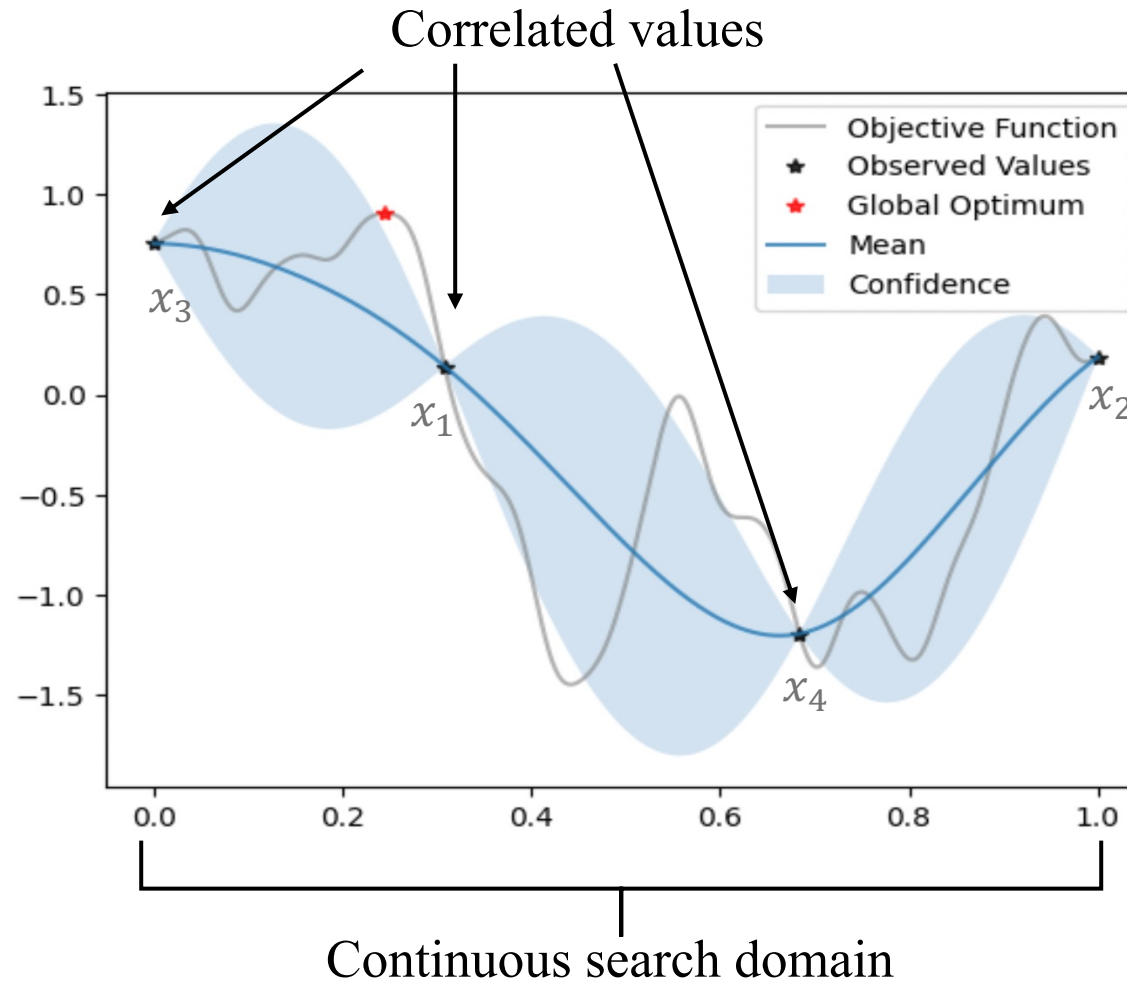
Continuous search domain

Why is it hard?

Why is it hard?

Hard budget constraint

Correlated values

$t = 1$

$t = 2$

$t = 3$

$t = 4$

$\vdots$

$t = T$

Continuous search domain

Why is it hard?

Hard budget constraint

$t = 1$

$t = 2$

$t = 3$

$t = 4$

$\vdots$

$t = T$

Correlated values

Evaluation costs handling

uniform   heterogeneous

Continuous search domain

Why is it hard?

Hard budget constraint

$t = 1$

$t = 2$

$t = 3$

$t = 4$

$\vdots$

$t = T$

Correlated values

Evaluation costs handling

uniform   heterogeneous

Continuous search domain
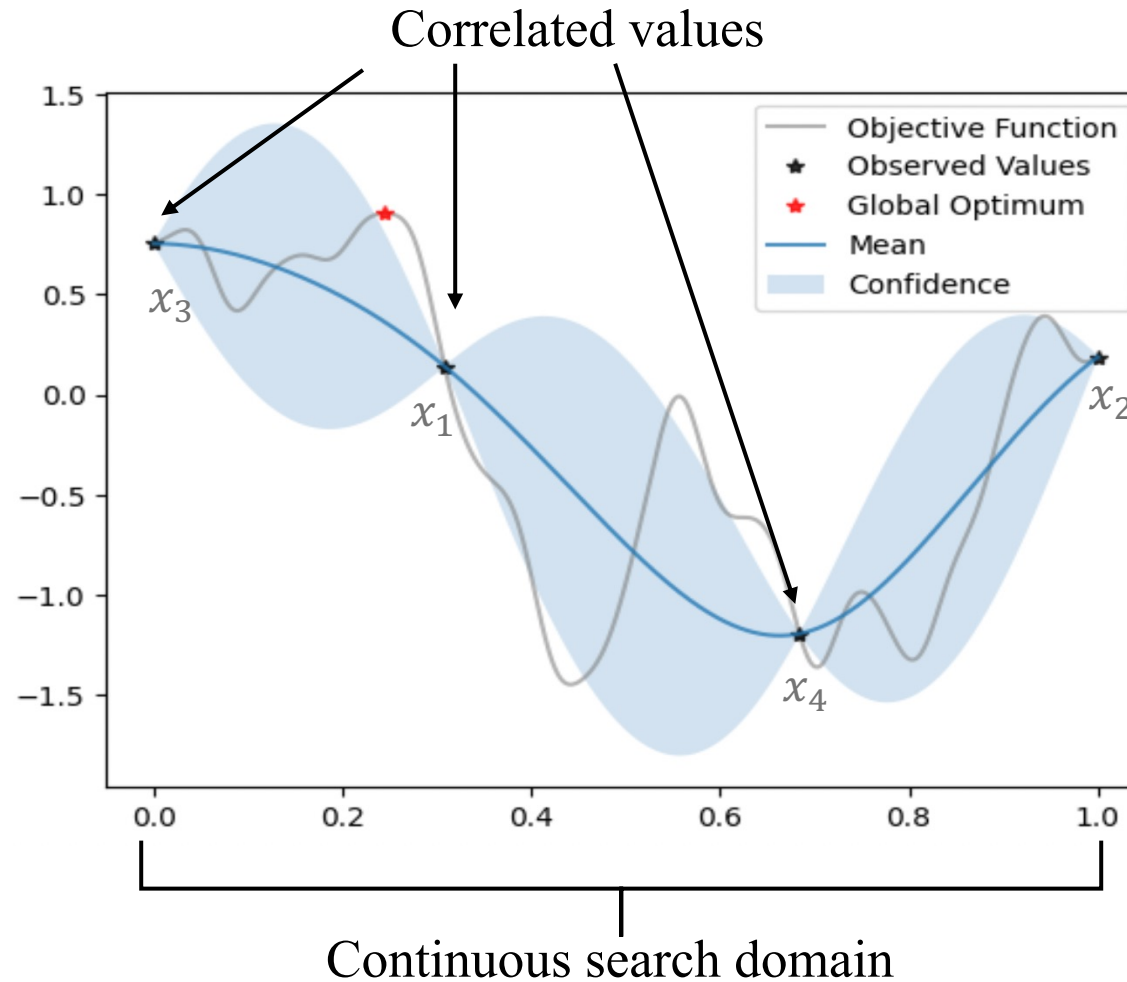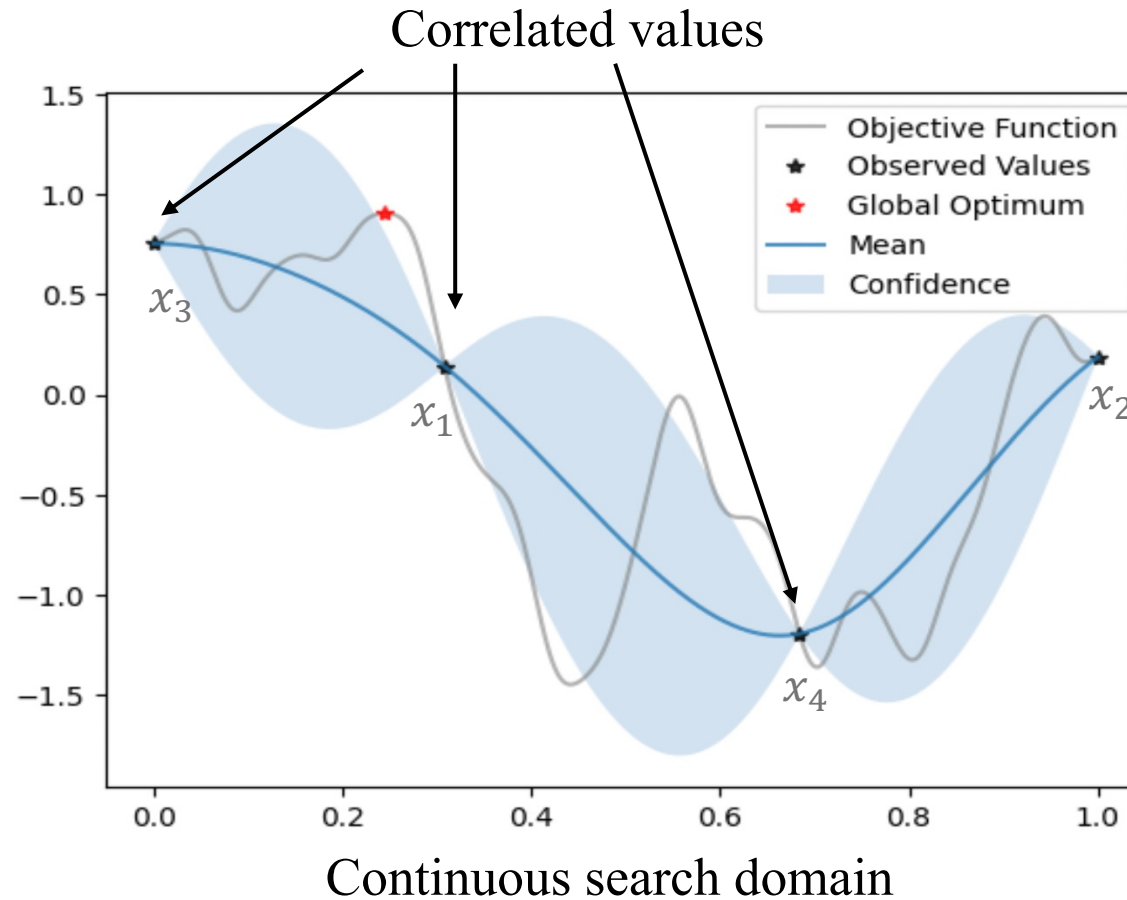
$\Rightarrow$ Optimal policy unknown!

Why is it hard?

Hard budget constraint

$t = 1$ ⌛

$t = 2$ ⌛

$t = 3$ ⌛

$t = 4$ ⌛

⋮

$t = T$

Correlated values

Continuous search domain

Evaluation costs handling

⚖ 🛢
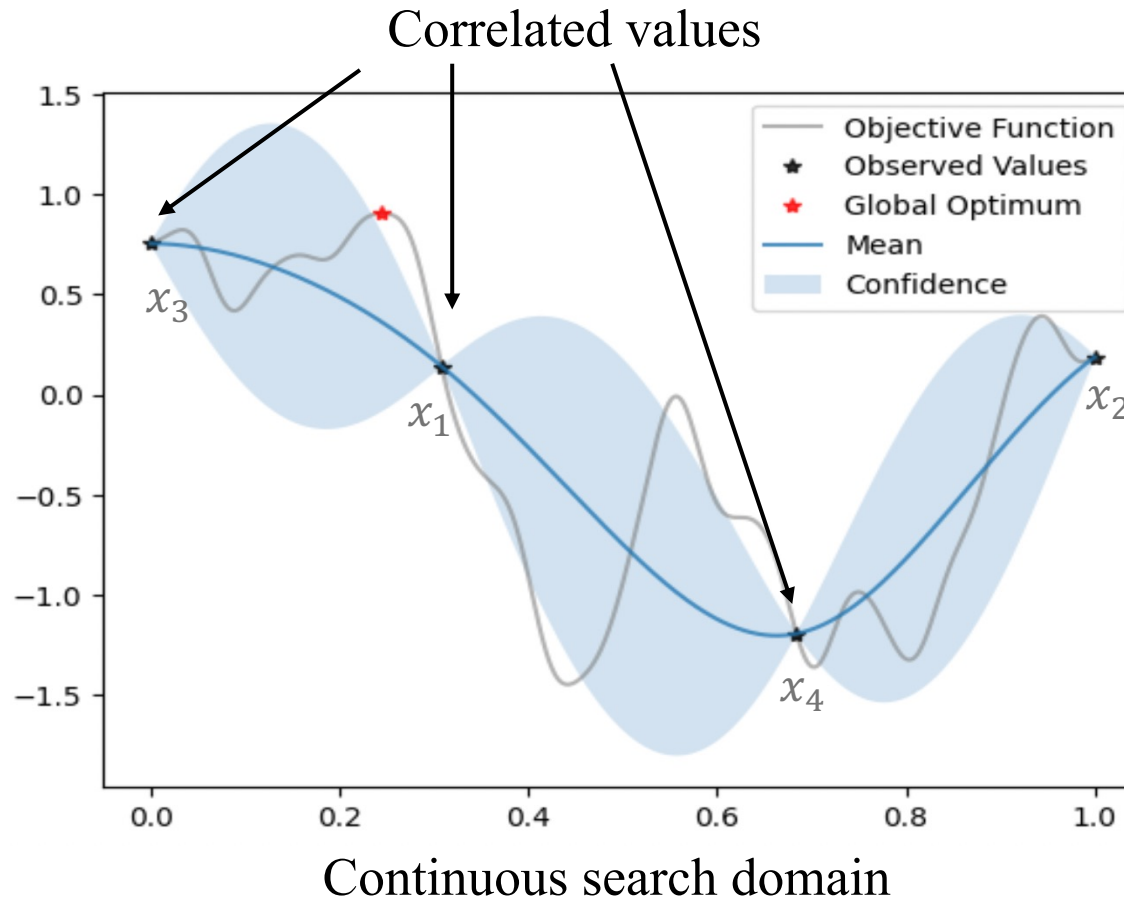
uniform   heterogeneous

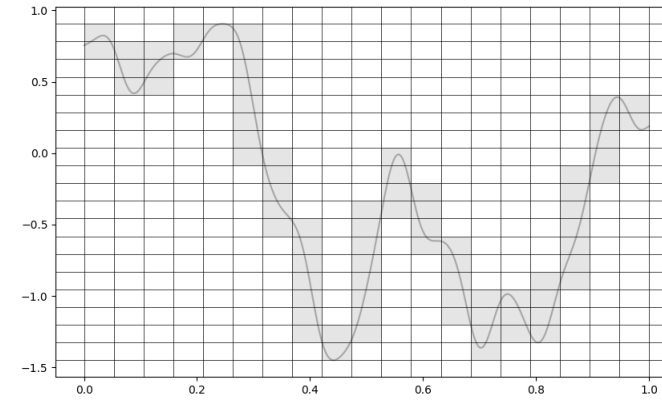Can we convert it to a solvable problem?
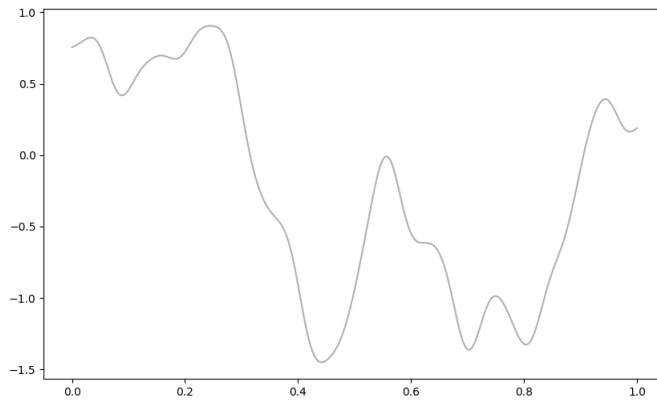
Bayesian Optimization
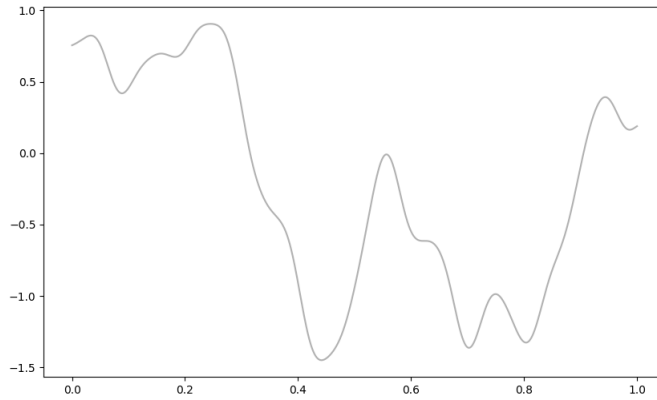
Continuous

Correlated

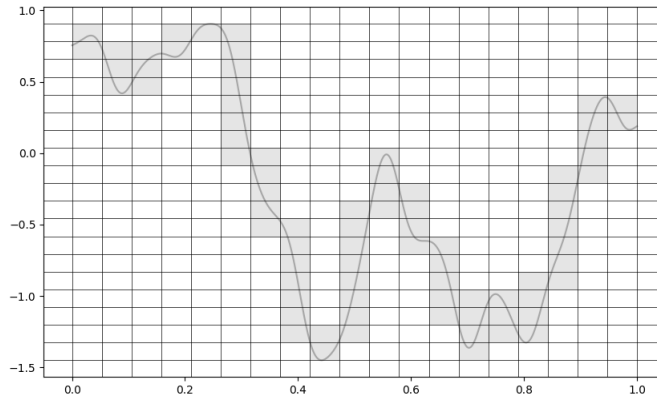Hard budget constraint

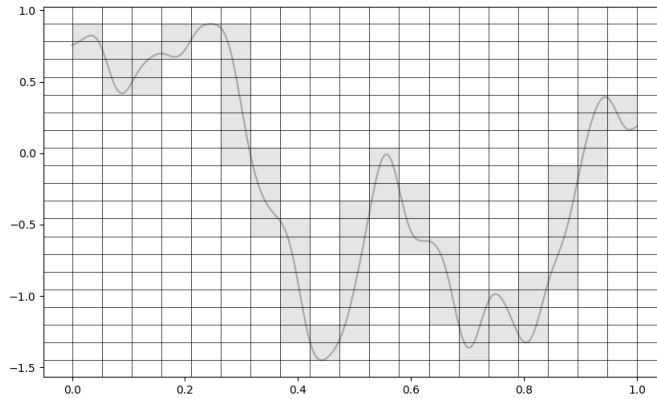# Bayesian Optimization

Continuous $\implies$ Discrete

Correlated

Hard budget constraint
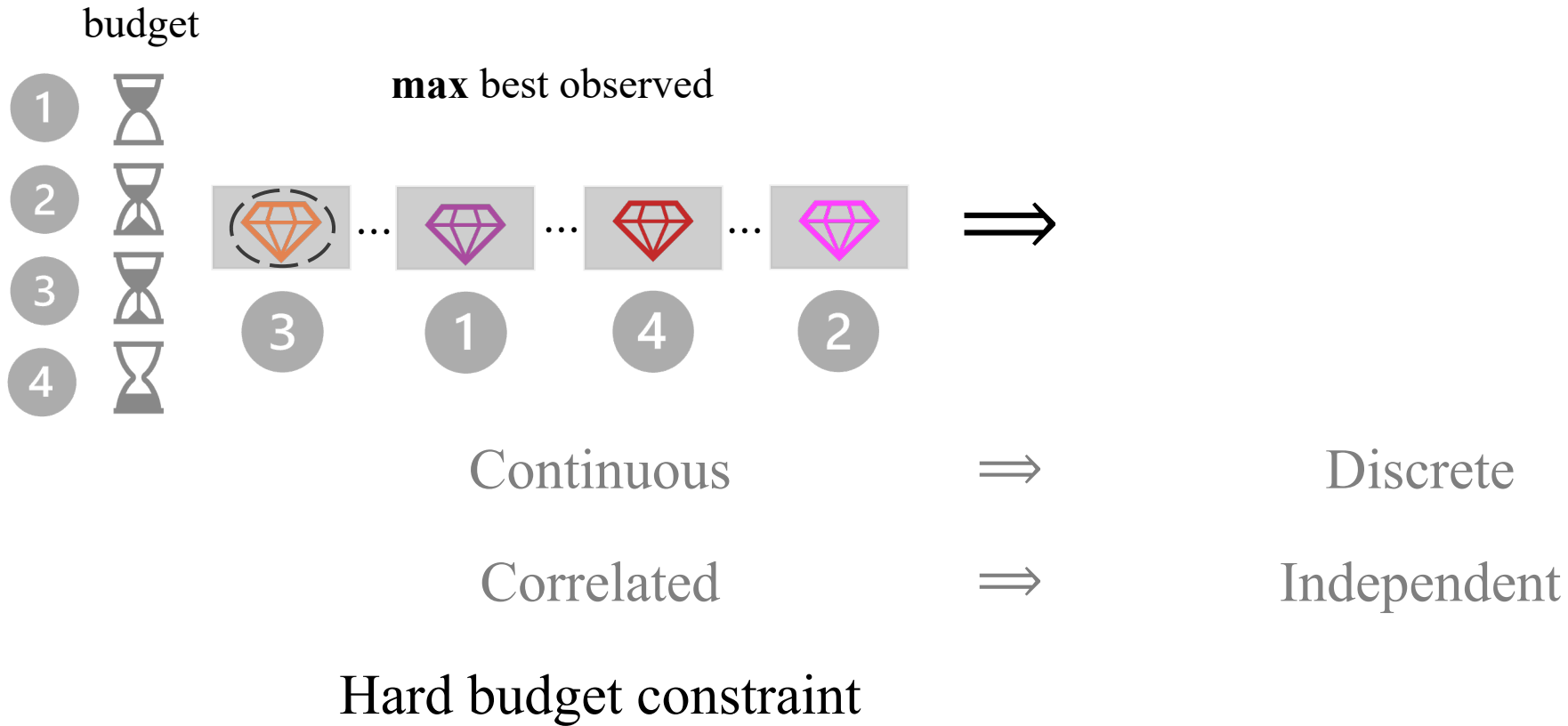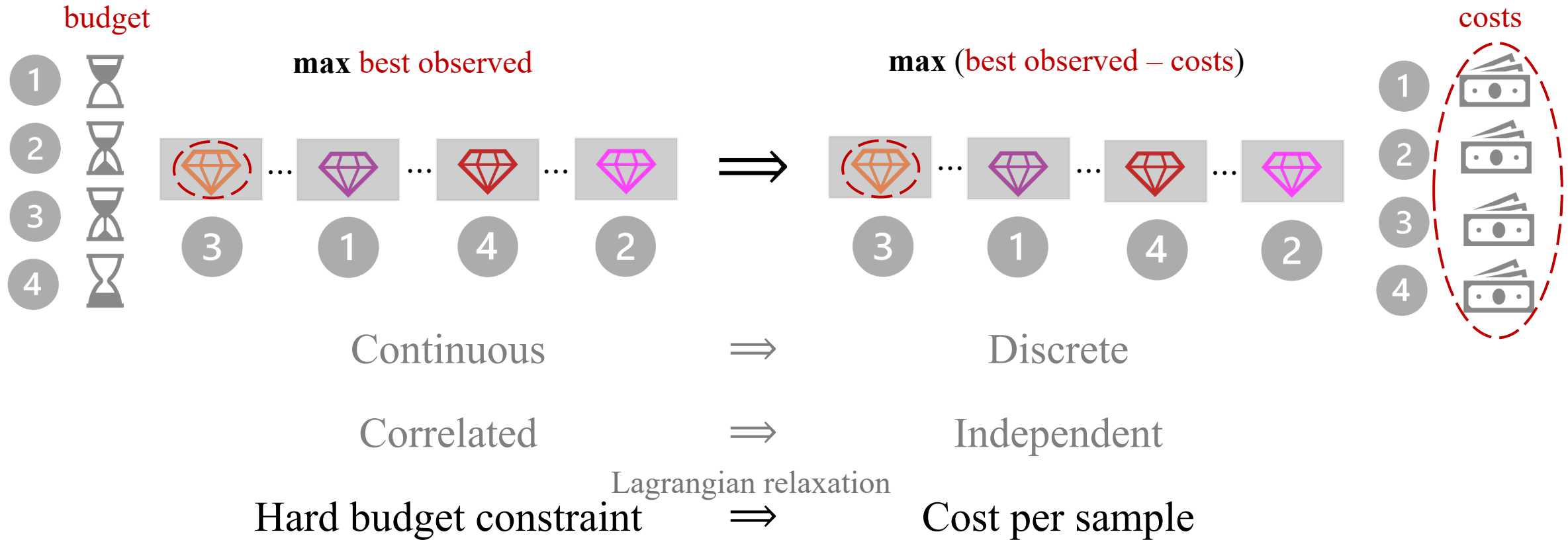
Bayesian Optimization

Continuous $\implies$ Discrete

Correlated

Hard budget constraint

Bayesian Optimization

Continuous $\implies$ Discrete

Correlated $\implies$ Independent

Hard budget constraint

Bayesian Optimization

budget

max best observed

Continuous $\implies$ Discrete

Correlated $\implies$ Independent

Hard budget constraint

Bayesian Optimization

budget

max best observed

max (best observed – costs)

costs

Continuous $\Longrightarrow$ Discrete

Correlated $\Longrightarrow$ Independent

Lagrangian relaxation

Hard budget constraint $\Longrightarrow$ Cost per sample

Bayesian Optimization $\implies$ Pandora's Box

[Weitzman'79]
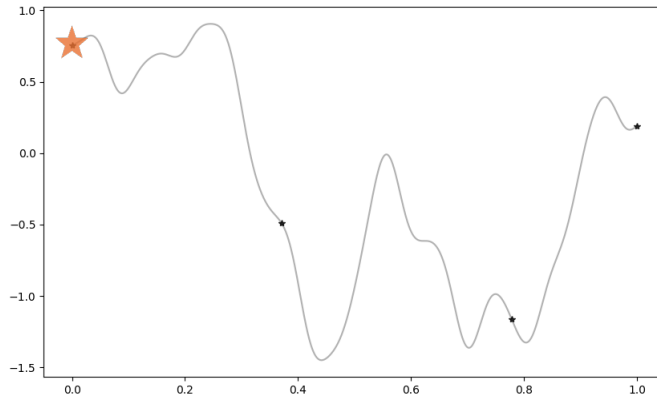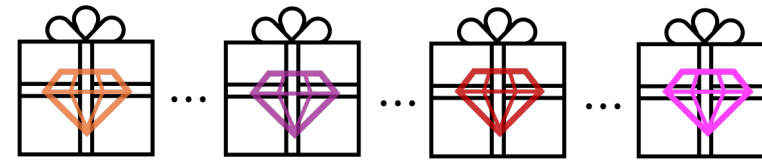
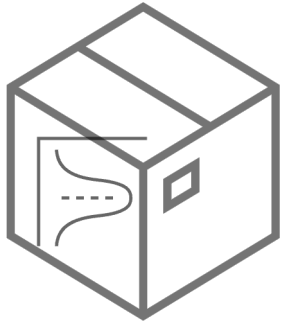| Continuous | $\implies$ | Discrete |
| Correlated | $\implies$ | Independent |
| Hard budget constraint | $\implies$ | Cost per sample |

Pandora's Box

$t = 0$
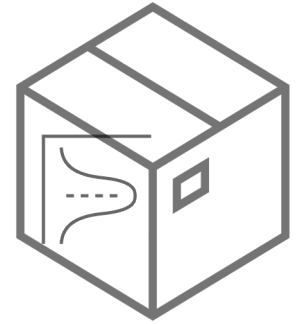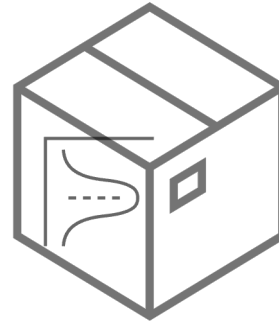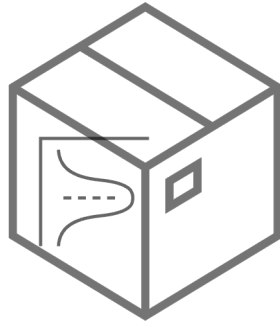
Objective: maximize net utility   **Decision:** adaptively evaluate a random number of boxes

Pandora's Box

$t = 1$

$f(x_1)$

$c(x_1)$

Objective: maximize net utility   **Decision:** adaptively evaluate a random number of boxes

Pandora's Box

$t = 2$
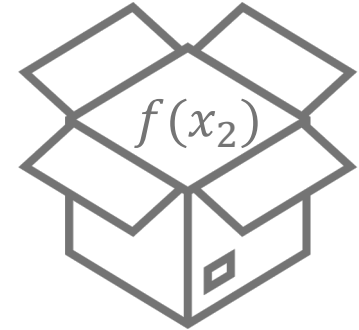
$f(x_1)$

$c(x_1)$

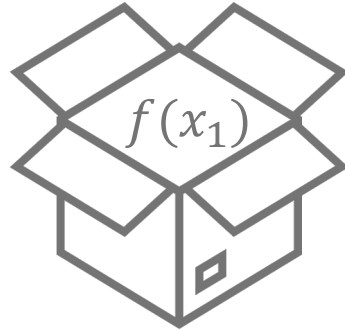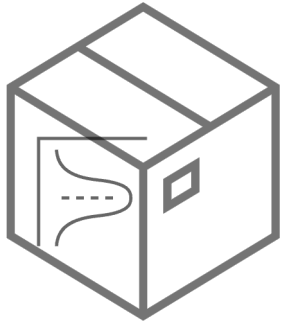$f(x_2)$

$c(x_2)$

Objective: maximize net utility   **Decision:** adaptively evaluate a random number of boxes

Pandora's Box

$t = 3$

$f(x_3)$ $f(x_1)$ $f(x_2)$

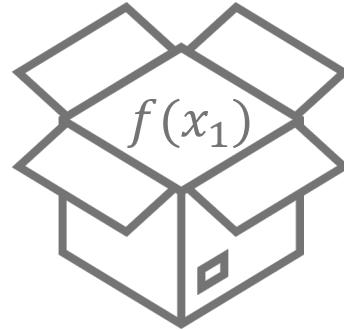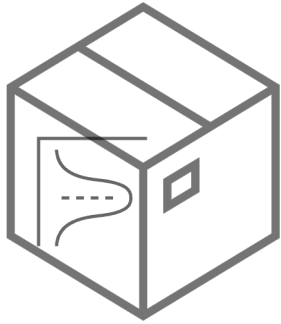$c(x_3)$ $c(x_1)$ $c(x_2)$

Objective: maximize net utility   **Decision:** adaptively evaluate a random number of boxes

Pandora's Box

$t = 3$

$f(x_3)$

$f(x_1)$

$f(x_2)$
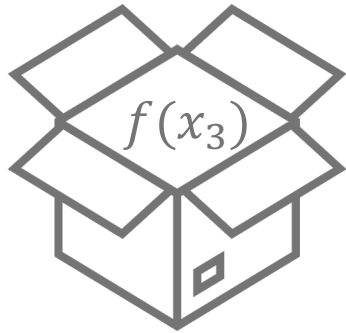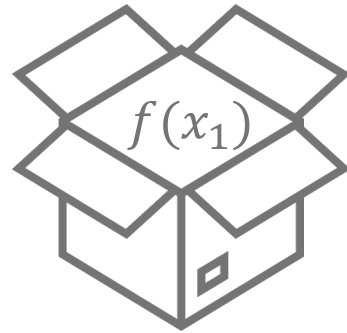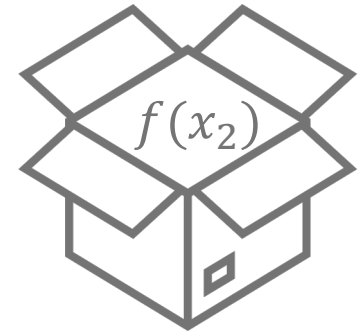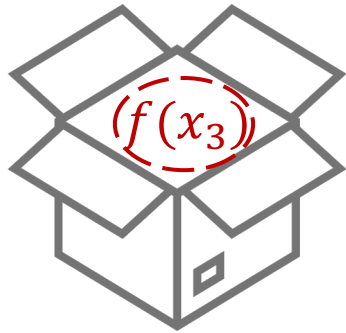
$c(x_3)$ $c(x_1)$ $c(x_2)$
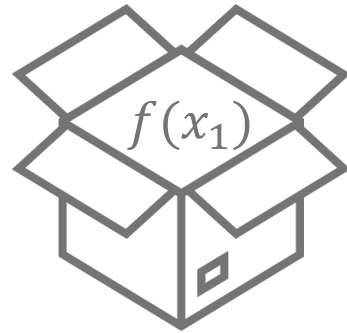
Objective: maximize net utility

Decision: adaptively evaluate a random number of boxes

max (best observed value − total costs)

Pandora's Box

$t = 3$

$f(x_3)$ $f(x_1)$ $f(x_2)$

$c(x_3)$ $c(x_1)$ $c(x_2)$
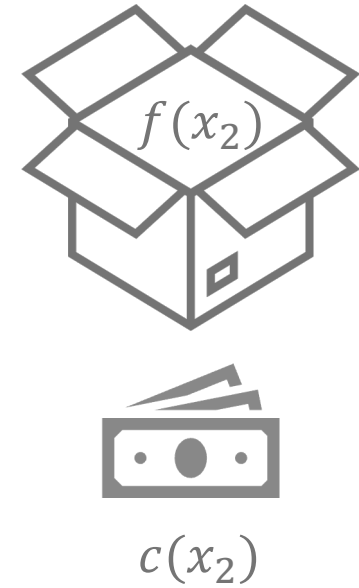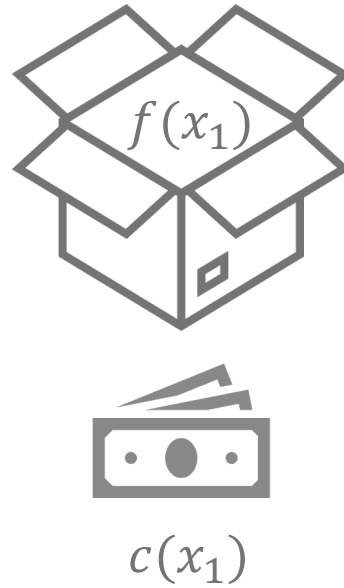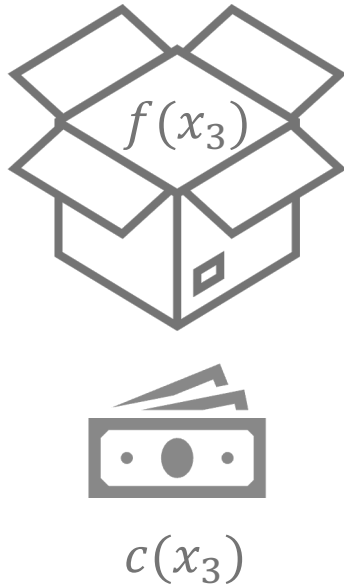
Objective: maximize net utility

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

Decision: adaptively evaluate a random number of boxes

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

$\mathcal{X}$: discrete

T: random stopping time

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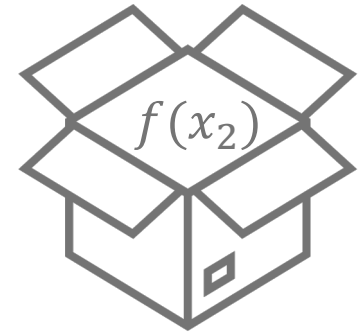
Naïve Greedy policy

y_{best}

$f(x)$

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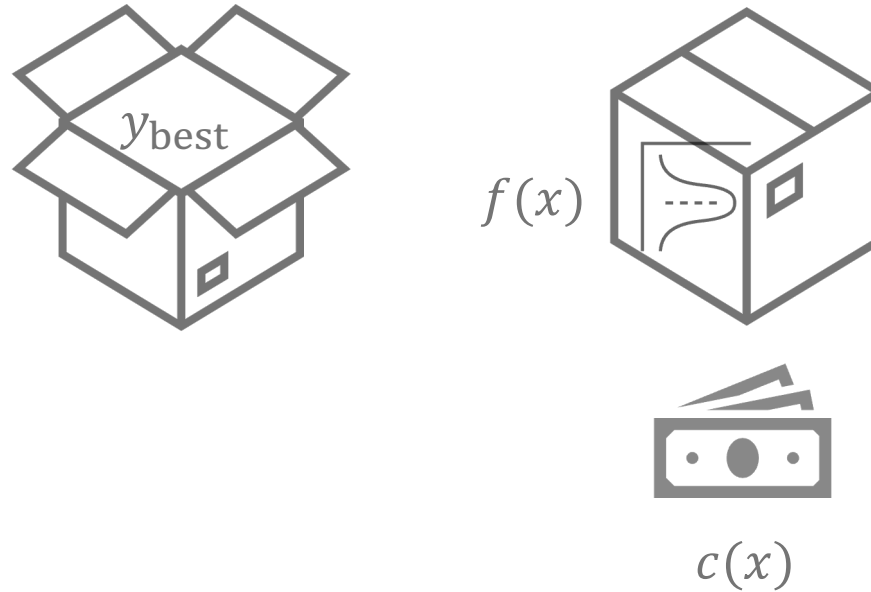
Inspection rule: $\text{argmax}_x \left(\text{EI}_f(x; y_{\text{best}}) - c(x) \right)$ **Stopping rule:** $\text{EI}_f(x; y_{\text{best}}) \leq c(x), \forall x \in \mathcal{X}$

expected improvement - cost   expected improvement $\leq$ cost

y_{best}: current best observed value

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

Naïve Greedy policy can fail [Singla'18]
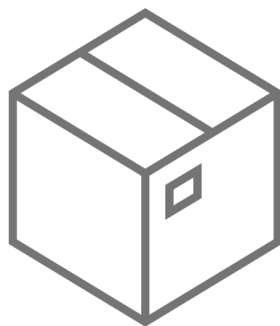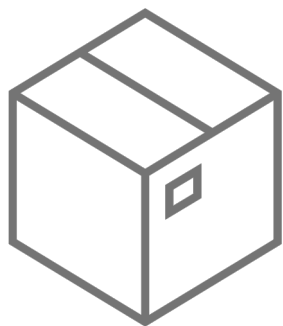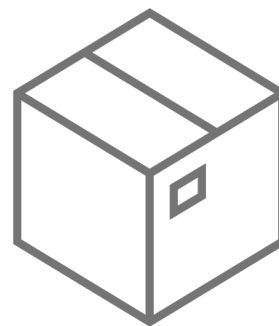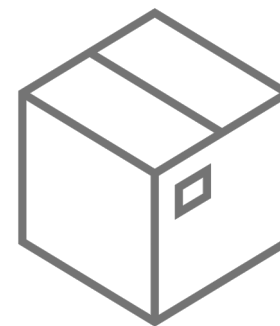
$f(1) = 200 \text{ w. p. } 1$

$c(1) = 198$

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

Naïve Greedy policy can fail [Singla'18]

$t = 0$ $y_{\text{best}} = 0$
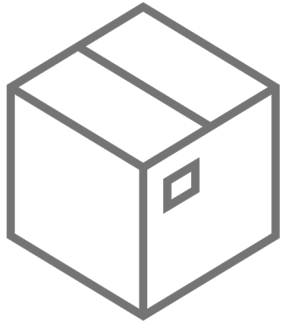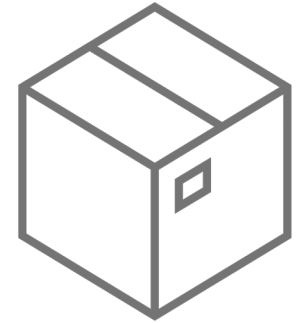
$f(1) = 200 \text{ w. p. } 1$

$c(1) = 198$

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

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

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

Inspection rule: $\text{argmax}_x \left(\text{EI}_f(x; y_{\text{best}}) - c(x) \right)$ **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]

$t = 1$

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

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

$c(1) = 198$

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

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

Inspection rule: $\text{argmax}_x \left(\text{EI}_f(x; y_{\text{best}}) - c(x) \right)$ **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]

$t = 1$

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

$c(1) = 198$

$f(x) = \begin{cases} 200 & \text{w. p. } 0.01 \\ 0 & \text{otherwise} \end{cases}, c(x) = 1, x \in \{2, 3, \ldots, 1000\}$
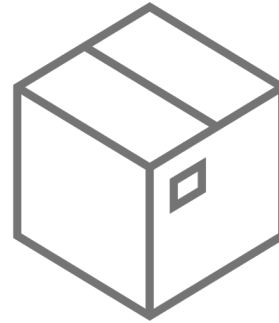
Inspection rule: $\text{argmax}_x \left(\text{EI}_f(x; y_{\text{best}}) - c(x) \right)$ **Stopping rule:** $\text{EI}_f(x; y_{\text{best}}) \leq c(x), \forall x \in \mathcal{X}$

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

Naïve Greedy policy can fail [Singla'18]

$t \approx 100$

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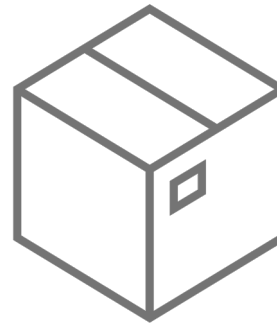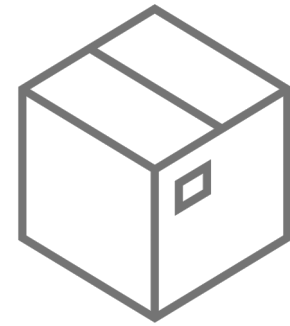
$f(1) = 200 \text{ w.p. } 1$

$c(1) = 198$

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

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

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

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

Optimal policy: Gittins policy

Gittins policy

y_{best}

$f(x)$

$c(x)$

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

solution to expected improvement = cost   Gittins index $\leq$ current best

y_{best}: current best observed value

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

Optimal policy: Gittins policy

Gittins policy

y_best

$\alpha^*(x)$

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

solution to expected improvement = cost   Gittins index $\le$ current best

y_best: current best observed value

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

Optimal policy: Gittins policy

$t = 0$

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

$c(1) = 198$

$200 - ? = 198$
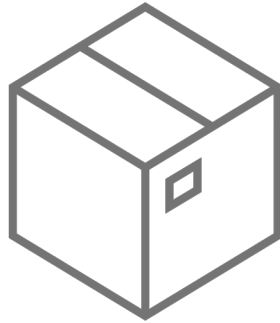
$f(x) = \begin{cases} 200 & \text{w. p. } 0.01 \\ 0 & \text{otherwise} \end{cases}, c(x) = 1, x \in \{2, 3, \dots, 1000\}$
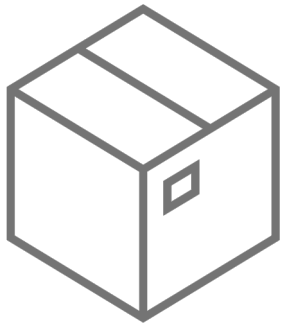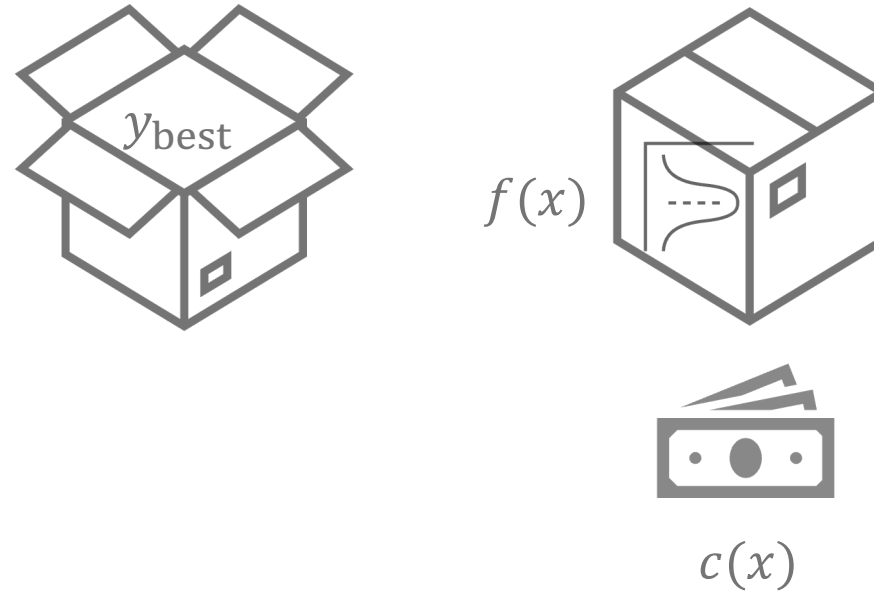
$(200 - ?) * 0.01 = 1$

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

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

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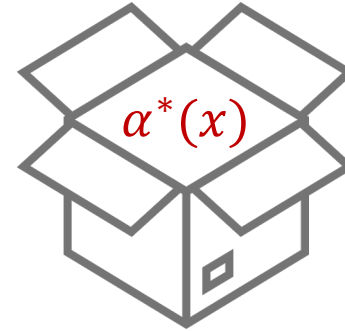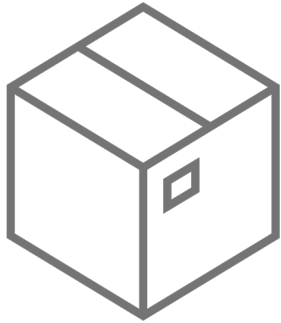
$$\text{EI}_f(x; y) = \mathbb{E}[(f(x) - y)^+]$$

Optimal policy: Gittins policy

$t = 1$

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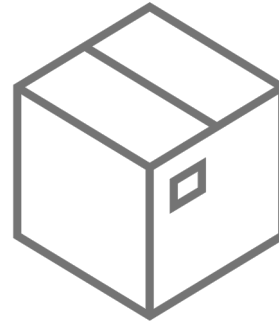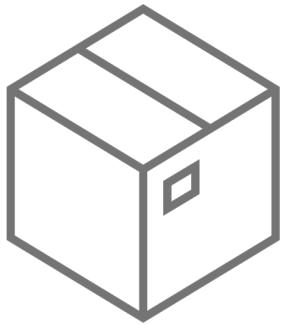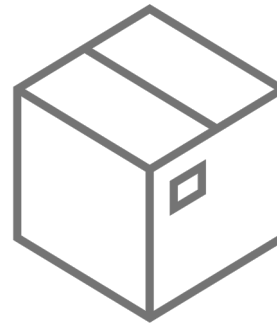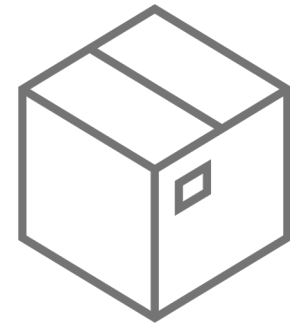

$f(1) = 200 \text{ w. p. } 1$

$c(1) = 198$

$\alpha^*(1) = 2$

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

$\alpha^*(x) = 100$

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

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

Optimal policy: Gittins policy

$t \approx 100$

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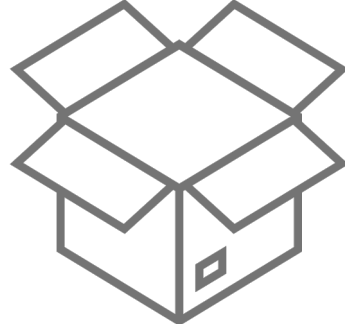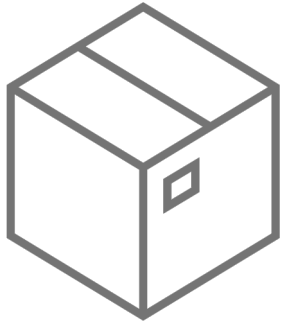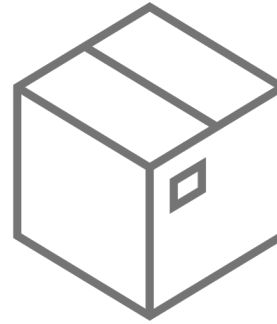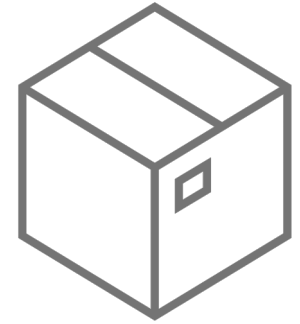
$f(1) = 200 \text{ w. p. } 1$

$c(1) = 198$

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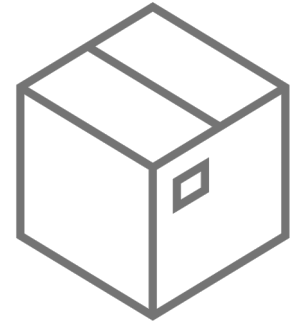
$f(x) = \begin{cases} 200 & \text{w. p. } 0.01 \\ 0 & \text{otherwise} \end{cases}, c(x) = 1, x \in \{2, 3, \dots, 1000\}$
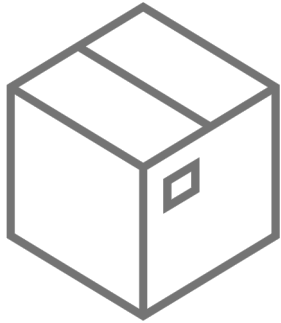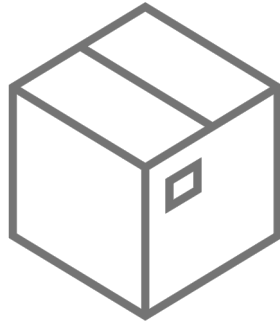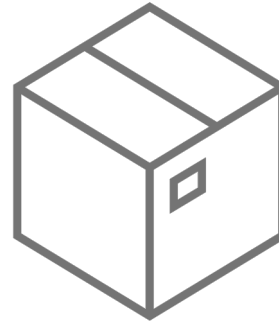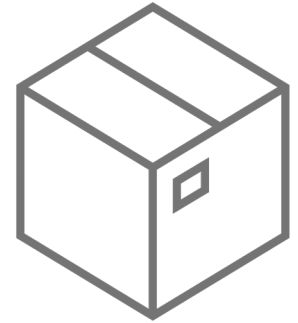
$\alpha^*(x) = 100$

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

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

Bayesian Optimization ⟹ Pandora's Box

Special case of Markovian/
Bayesian multi-armed bandits
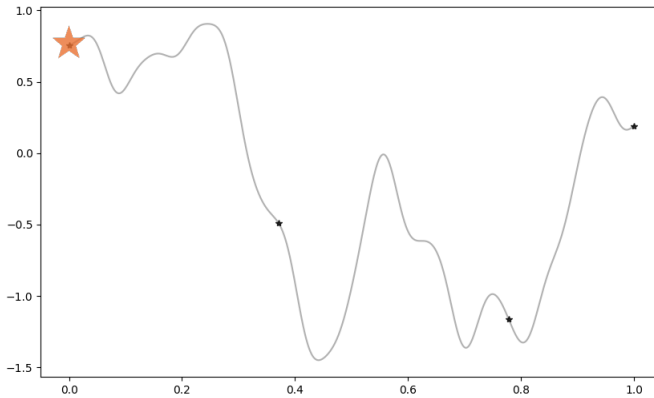
Continuous ⟹ Discrete

Correlated ⟹ Independent
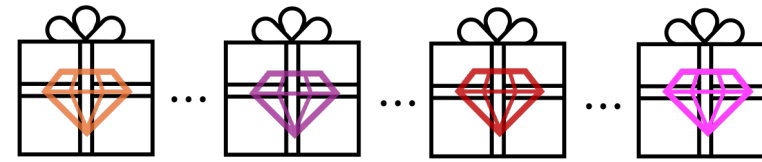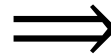
Hard budget constraint ⟹ Cost per sample

Optimal policy: Gittins index [Weitzman'79]

Bayesian Optimization $\Longrightarrow$ Pandora's Box
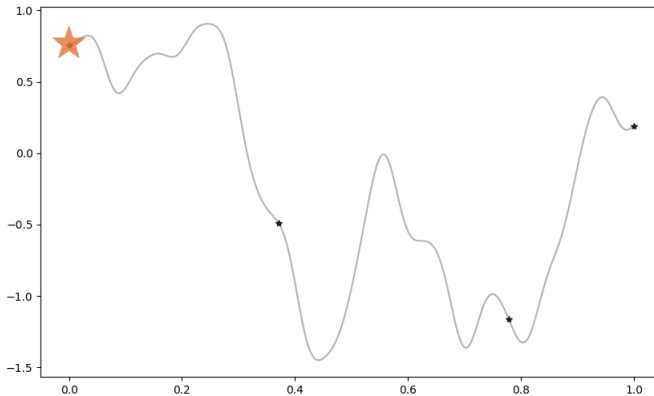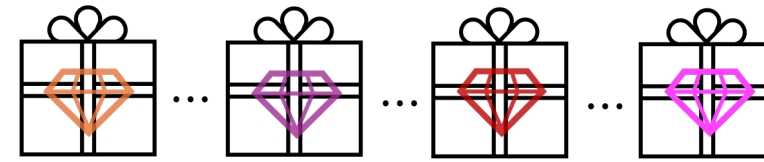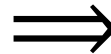
Continuous	$\Longrightarrow$	Discrete
Correlated	$\Longrightarrow$	Independent
Hard budget constraint	$\Longrightarrow$	Cost per sample
Is Gittins index good?	$\Longleftarrow$	Optimal policy: Gittins index

Bayesian Optimization $\implies$ Pandora's Box

Continuous	$\implies$	Discrete
Correlated	$\implies$	Independent
Hard budget constraint	$\implies$	Cost per sample

How to translate?

Is Gittins index good? $\impliedby$ Optimal policy: Gittins index

Bayesian Optimization $\Longrightarrow$ Pandora's Box

Continuous	$\Longrightarrow$	Discrete
Correlated	$\Longrightarrow$	Independent
Hard budget constraint	$\Longrightarrow$	Cost per sample

How to translate?

Is Gittins index good? $\Longleftarrow$ Optimal policy: Gittins index

Our contributions!

How to translate?

budget

Pandora's box

costs

max best observed
s.t. budget constraint

max (best observed – costs)
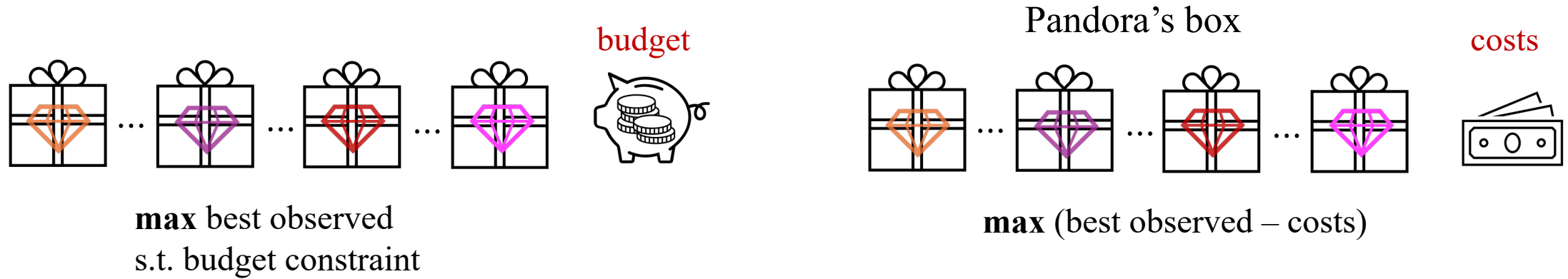
Expected budget constraint $\iff$ Cost per sample

Optimal policy? $\Longleftarrow$ Optimal policy: Gittins index

Expected budget constraint ⟺ Cost per sample

budget

max best observed
s.t. budget constraint

Pandora's box

scaled costs

max (best observed $– \lambda_B^*$ costs))

λ_B^*: budget-dependent scaling factor

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

Expected budget constraint $\iff$ Cost per sample

budget

Pandora's box

scaled costs

max best observed
s.t. budget constraint

max (best observed $- \lambda_B^*$ costs))

λ_B^*: budget-dependent scaling factor

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

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

Expected budget constraint ⟺ Cost per sample

Constrained

budget

Unconstrained

costs

$$\mathop{\textbf{sup}}_{\text{policy}} \; \mathbb{E} \max_{t=1,2,\ldots,T} f(x_t)$$

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

Lagrangian relaxation

⟺

$$\mathop{\textbf{sup}}_{\text{policy}} \mathop{\textbf{inf}}_{\lambda \geq 0} \; \mathbb{E}\left(\max_{t=1,2,\ldots,T} f(x_t) + \lambda \left(B - \mathbb{E} \sum_{t=1}^{T} c(x_t) \right) \right)$$

λ: Lagrange multiplier

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

Extension to [Aminian, Manshadi, Niazadeh]

Expected budget constraint ⟺ Cost per sample

Constrained

budget

Unconstrained

costs

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

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

Lagrangian relaxation

⟺

$$\underset{\text{policy}}{\textbf{sup}}\ \underset{\lambda\ge 0}{\textbf{inf}}\ \mathbb{E}\left(\max_{t=1,2,\ldots,T} f(x_t) + \lambda\left(B - \mathbb{E}\sum_{t=1}^{T} c(x_t)\right)\right)$$

Lagrange multiplier theorem

⟺

$$\underset{\lambda\ge 0}{\textbf{inf}}\ \underset{\text{policy}}{\textbf{sup}}\ \mathbb{E}\left(\max_{t=1,2,\ldots,T} f(x_t) + \lambda\left(B - \mathbb{E}\sum_{t=1}^{T} c(x_t)\right)\right)$$

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

Extension to [Aminian, Manshadi, Niazadeh]

52

Expected budget constraint ⟺ Cost per sample

Constrained

Unconstrained

budget

costs

$$\underset{\text{policy}}{\sup} \; \mathbb{E} \; \underset{t=1,2,\dots,T}{\max} f(x_t)$$

Lagrangian relaxation

$$\underset{\text{policy}}{\sup} \underset{\lambda \geq 0}{\inf} \; \mathbb{E} \left(\underset{t=1,2,\dots,T}{\max} f(x_t) + \lambda \left(B - \mathbb{E} \sum_{t=1}^{T} c(x_t) \right) \right)$$

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

⟺

Lagrange multiplier theorem

$$\underset{\lambda \geq 0}{\inf} \underset{\text{policy}}{\sup} \; \mathbb{E} \left(\underset{t=1,2,\dots,T}{\max} f(x_t) + \lambda \left(B - \mathbb{E} \sum_{t=1}^{T} c(x_t) \right) \right)$$

⟺

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

$\mathcal{A}(\lambda)$

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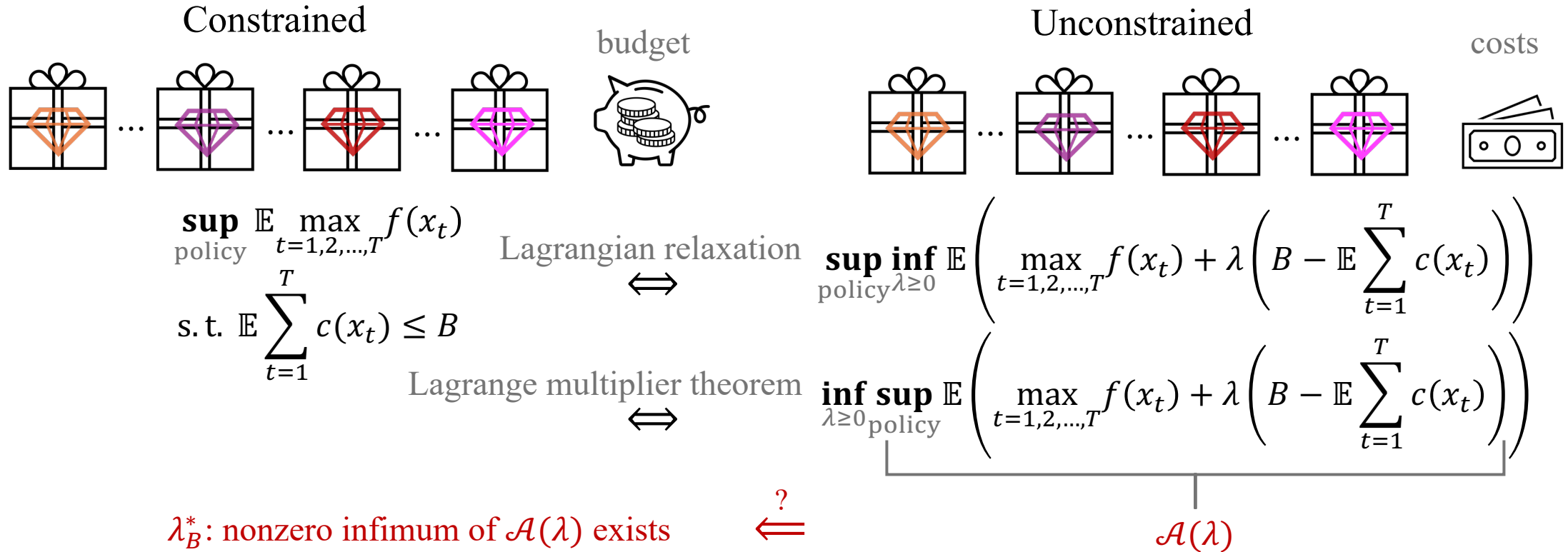Pandora's box with scaled costs

Extension to [Aminian, Manshadi, Niazadeh]

53

Expected budget constraint ⟺ Cost per sample

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

Finite breakpoints

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

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

Envelope Theorem

λ_B^*: nonzero infimum of $\mathcal{A}(\lambda)$ exists $\Longleftarrow$ $\mathcal{A}(\lambda)$: convex (possibly non-differentiable) in λ

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

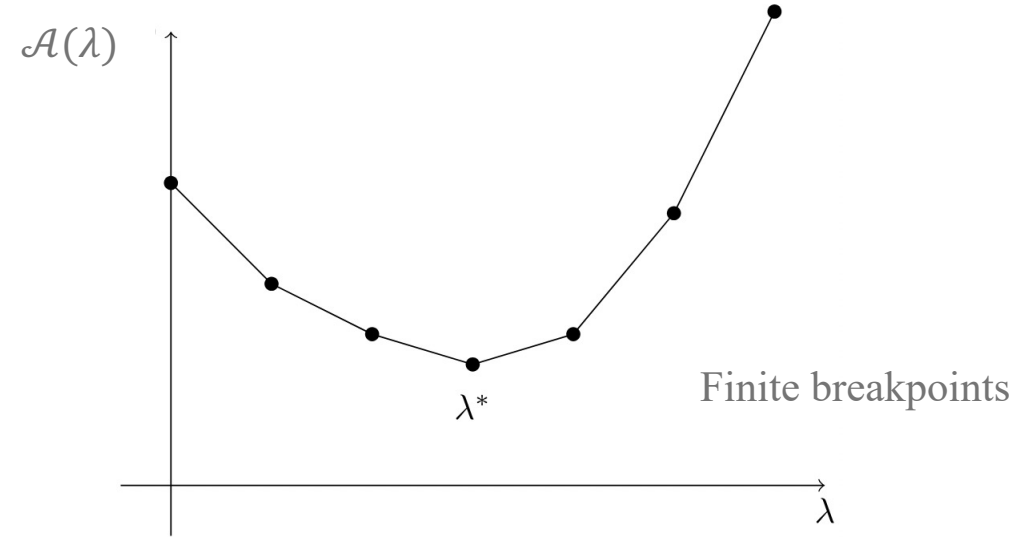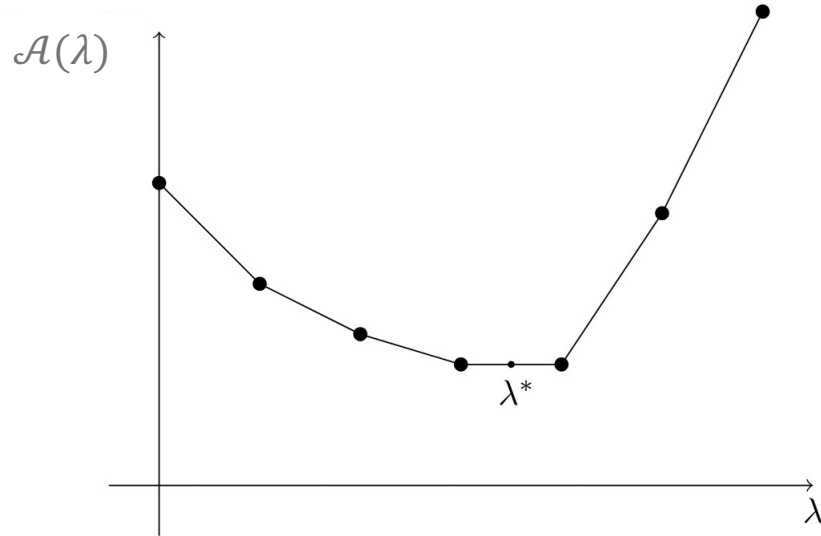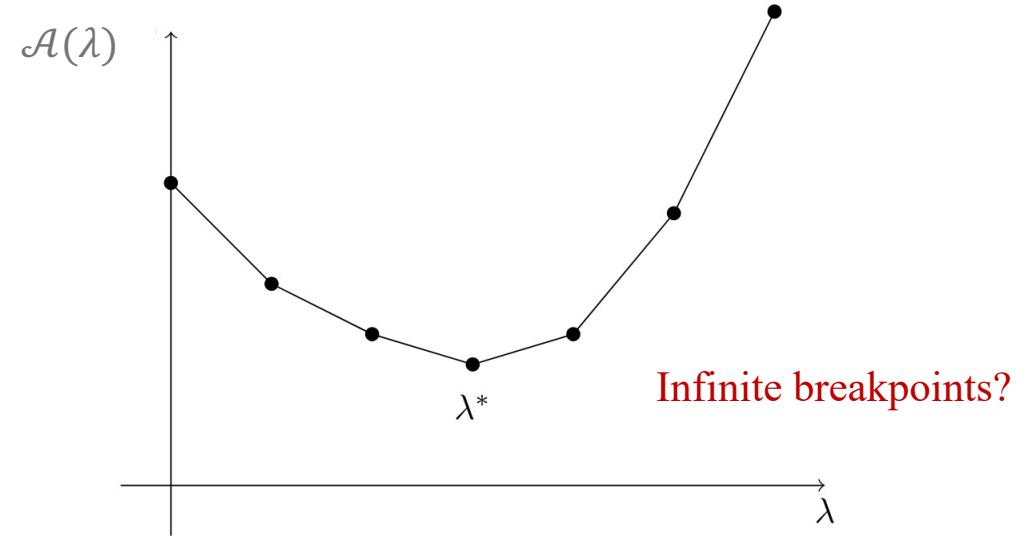Extension to [Aminian, Manshadi, Niazadeh]

Figure from [Aminian, Manshadi, Niazadeh]

Expected budget constraint ⟺ Cost per sample

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

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

Infinite breakpoints?

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

λ_B^*: nonzero infimum of $\mathcal{A}(\lambda)$ exists $\impliedby$ $\mathcal{A}(\lambda)$: convex (possibly non-differentiable) in λ

Optimal policy: Gittins solution to $\impliedby$ Optimal policy: Gittins index
Pandora's box with scaled costs
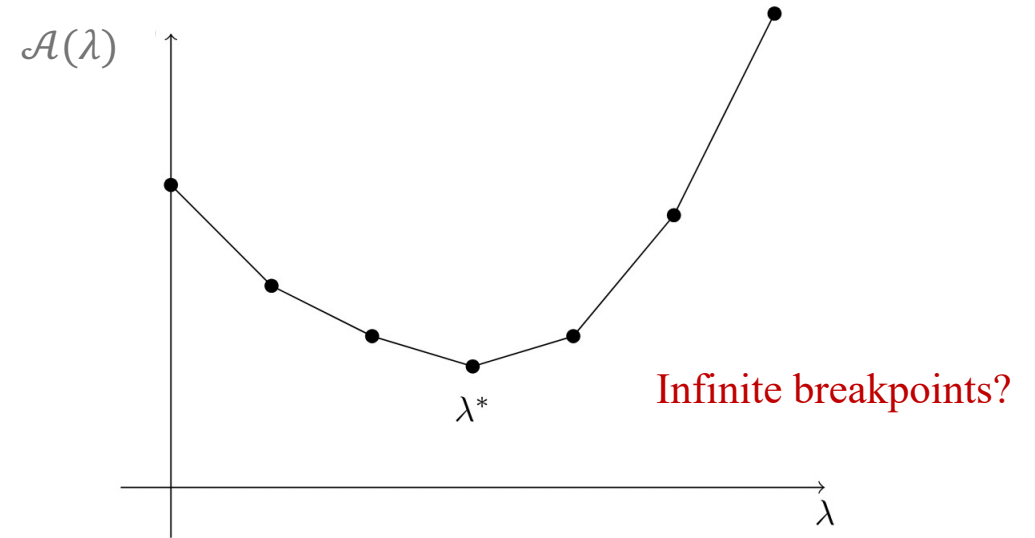
Extension to [Aminian, Manshadi, Niazadeh]

Figure from [Aminian, Manshadi, Niazadeh]

55

Expected budget constraint ⟺ Cost per sample

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

Infinite breakpoints?

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

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

sharp Envelope Theorem

λ_B^*: nonzero infimum of $\mathcal{A}(\lambda)$ exists $\quad \Longleftarrow \quad$ $\mathcal{A}(\lambda)$: convex (possibly non-differentiable) in λ

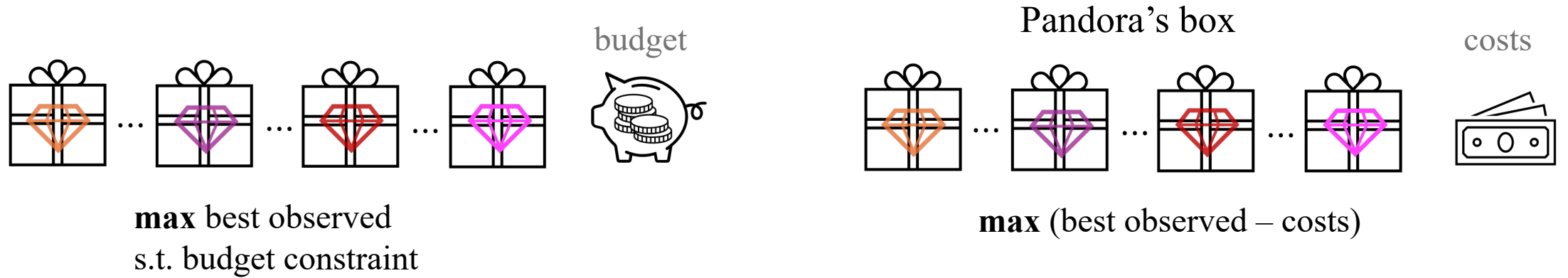Optimal policy: Gittins solution to $\quad \Longleftarrow \quad$ Optimal policy: Gittins index
Pandora's box with scaled costs

Extension to [Aminian, Manshadi, Niazadeh]

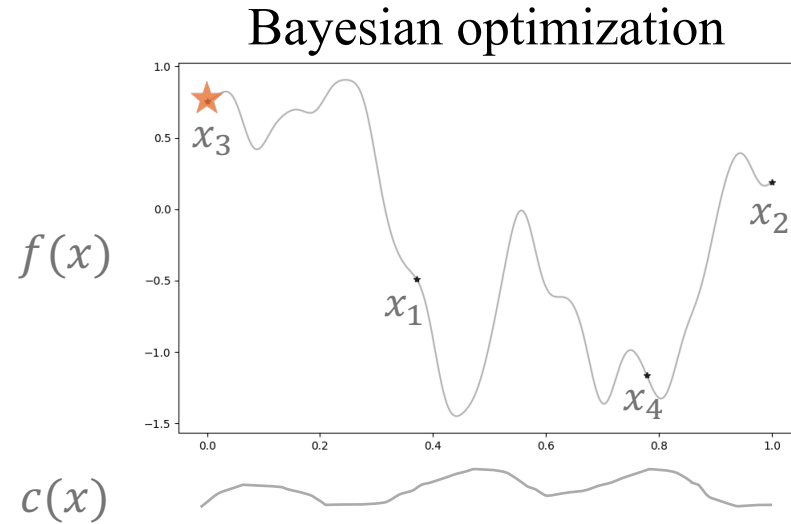Figure from [Aminian, Manshadi, Niazadeh]

How to translate?

budget

Pandora's box

costs

max best observed
s.t. budget constraint

max (best observed – costs)

Hard budget constraint $\quad\Longleftarrow\quad$ Cost per sample

$$\text{argmax}_x\, \alpha^*(x) \text{ s.t. } \text{EI}_f(x; \alpha^*(x)) = \textcolor{red}{\lambda_B^*}\, c(x) \quad\Longleftarrow\quad \text{argmax}_x\, \alpha^*(x) \text{ s.t. } \text{EI}_f(x; \alpha^*(x)) = c(x)$$

How to translate?

Bayesian optimization

Budget-constrained
Pandora's box

$c(x_3)$ $c(x_1)$ $c(x_4)$ $c(x_2)$
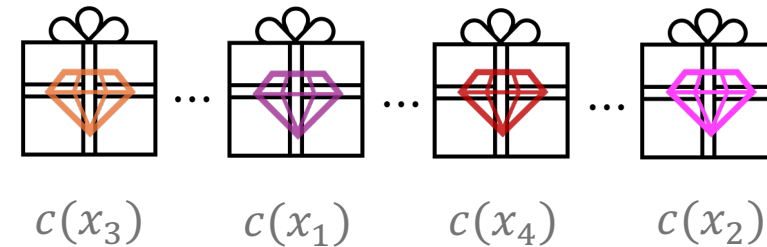
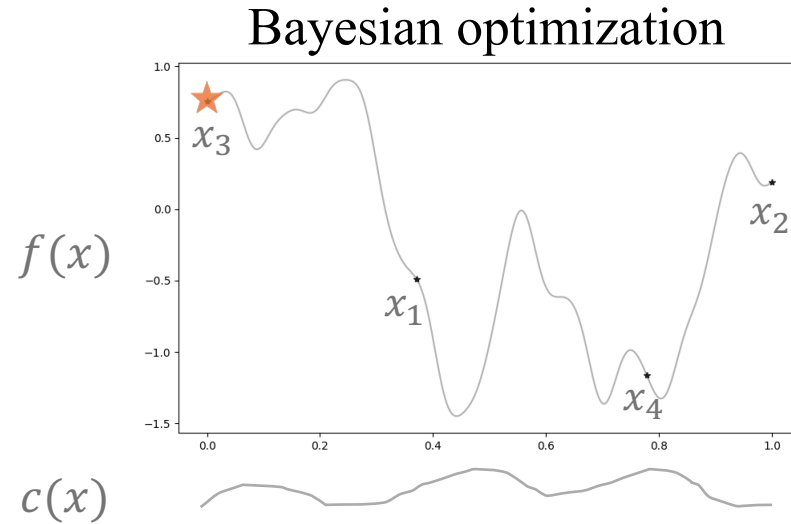| Continuous	$\Longleftarrow$	Discrete
Correlated	$\Longleftarrow$	Independent
Hard budget constraint	$\Longleftarrow$	Cost per sample

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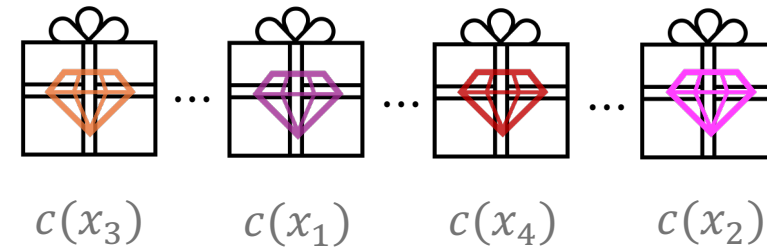Pandora's box with scaled costs

How to translate?

Bayesian optimization

$f(x)$

$c(x)$

Budget-constrained
Pandora's box

$c(x_3)$ $c(x_1)$ $c(x_4)$ $c(x_2)$

Continuous $\Longleftarrow$ Discrete

Correlated $\Longleftarrow$ Independent

Hard budget constraint $\Longleftarrow$ Cost per sample

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

D: observed data

How to translate?

Bayesian optimization

Budget-constrained
Pandora's box

$c(x_3)$ $c(x_1)$ $c(x_4)$ $c(x_2)$

Continuous $\Longleftarrow$ Discrete

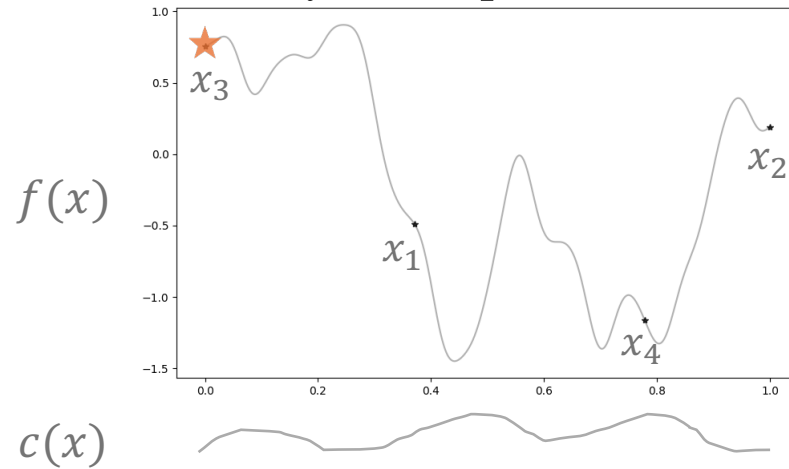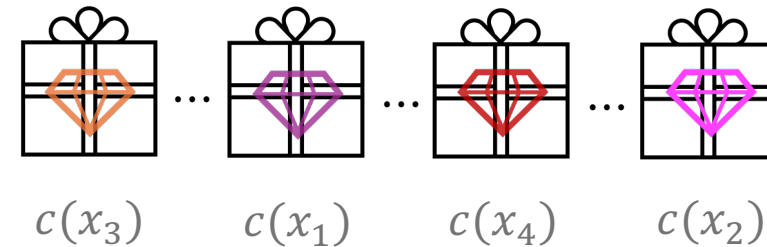Correlated $\Longleftarrow$ Independent

Hard budget constraint $\Longleftarrow$ Cost per sample

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

popular one-step
heuristic: EI policy

How to translate?

Bayesian optimization

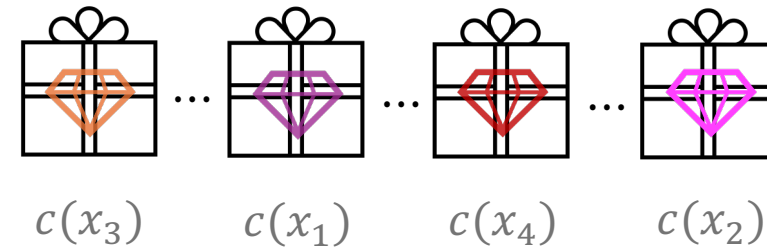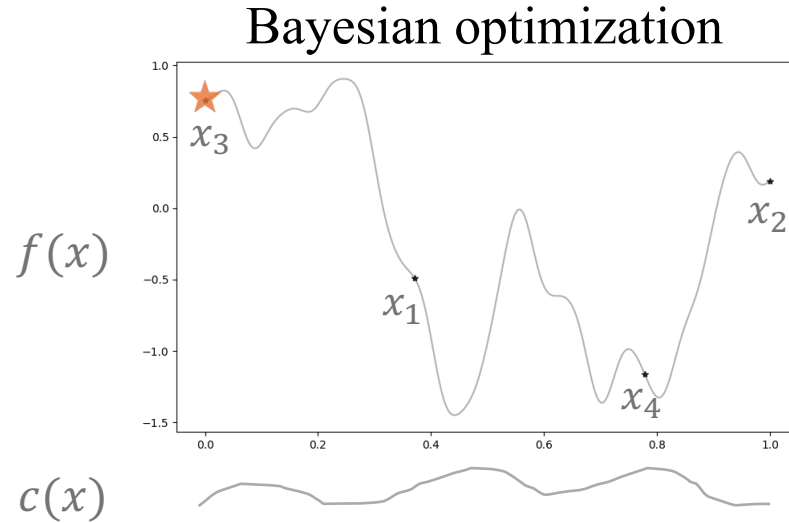Budget-constrained
Pandora's box

$c(x_3)$ $c(x_1)$ $c(x_4)$ $c(x_2)$

Continuous	$\Longleftarrow$	Discrete
Correlated	$\Longleftarrow$	Independent
Hard budget constraint	$\Longleftarrow$	Cost per sample
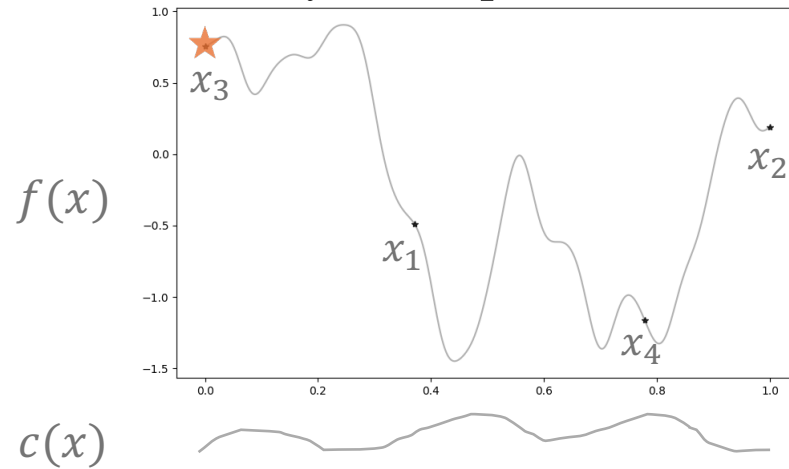
$\text{argmax}_x \, \alpha^*(x) \text{ s.t. } \text{EI}_{f|D}(x; \alpha^*(x)) = \lambda_B^* c(x)$ $\Longleftarrow$ $\text{argmax}_x \, \alpha^*(x) \text{ s.t. } \text{EI}_f(x; \alpha^*(x)) = \lambda_B^* c(x)$

ratio of EI and cost: EIPC policy

How to translate?

Bayesian optimization

Budget-constrained
Pandora's box

$c(x_3)$ $c(x_1)$ $c(x_4)$ $c(x_2)$

Continuous	$\Longleftarrow$	Discrete
Correlated	$\Longleftarrow$	Independent
Hard budget constraint	$\Longleftarrow$	Cost per sample
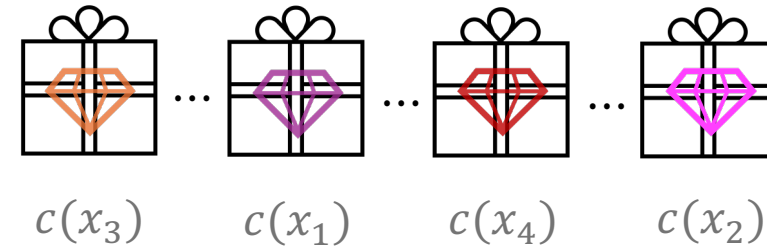
$$\text{argmax}_x\, \alpha^*(x) \text{ s.t. } \text{EI}_{f|D}(x; \alpha^*(x)) = \lambda_B^* c(x) \quad \Longleftarrow \quad \text{argmax}_x\, \alpha^*(x) \text{ s.t. } \text{EI}_f(x; \alpha^*(x)) = \lambda_B^* c(x)$$

EI and EIPC policy can be arbitrarily worse [Astudillo et al.'21]

Our Contributions

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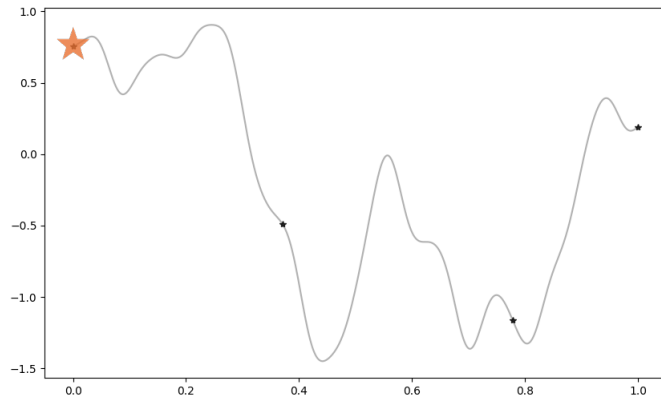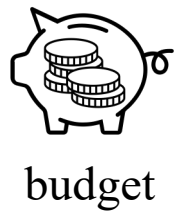
- Is Pandora's Box Gittins index (PBGI) good?
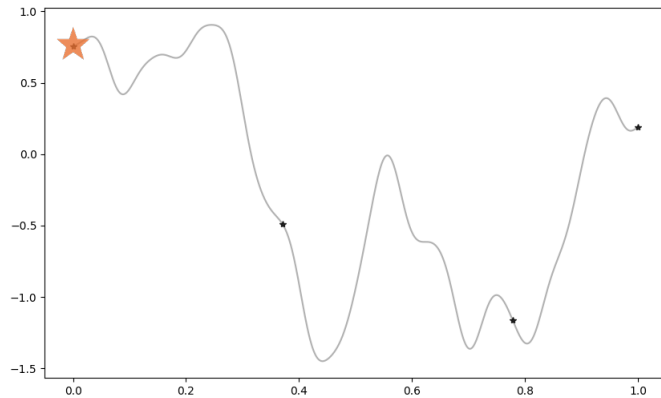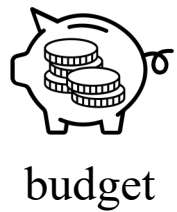
? ⟸ Pandora's Box Gittins index

Our Contributions

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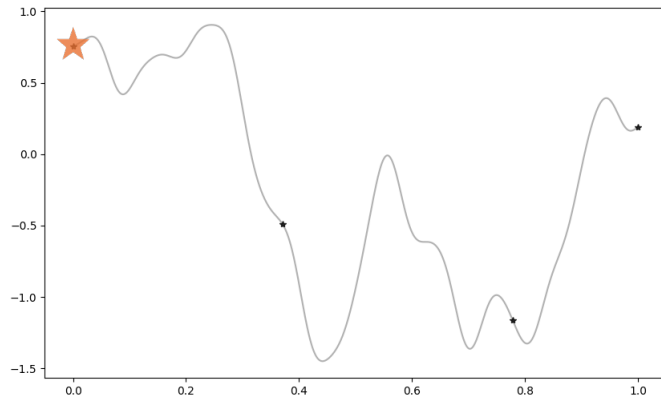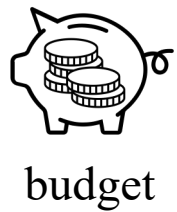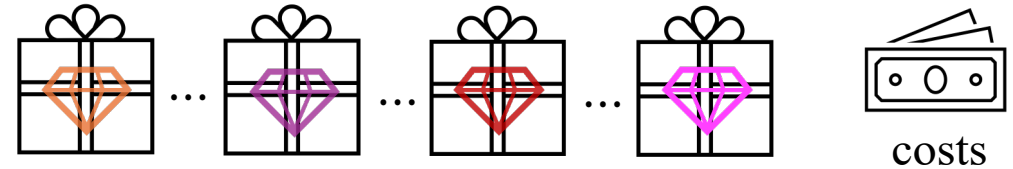- Is Pandora's Box Gittins index (PBGI) good?

Our work   ⟸   Pandora's Box Gittins index

Our Contributions

- Develop PBGI policy for Bayesian optimization

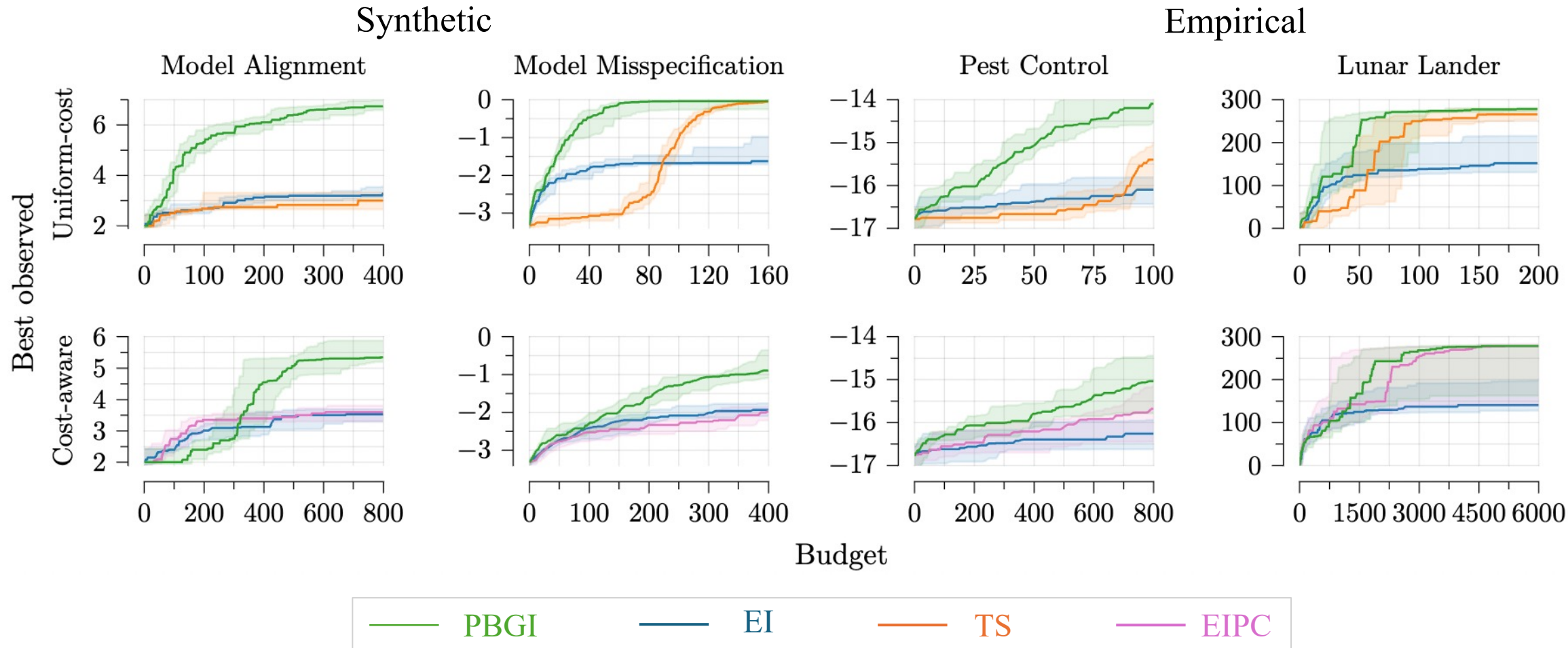- Show performance against baselines on synthetic & empirical experiments

budget

Our work $\impliedby$ Pandora's Box Gittins index

costs

Experiment Results: PBGI vs Baselines
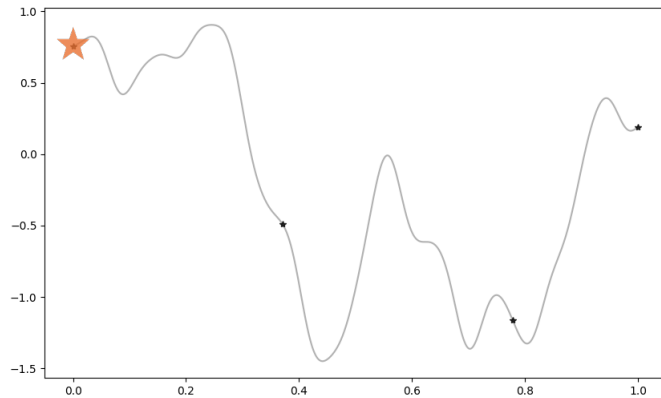

Synthetic

Empirical

EI and EIPC policy can be arbitrarily worse [Astudillo et al.'21]   Check our preprint on arXiv!

Conclusions

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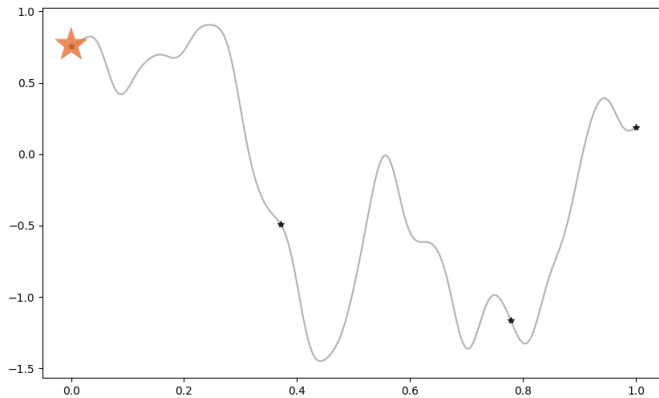

budget

Our work $\Longleftarrow$ Pandora's Box Gittins index

costs

Conclusions

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

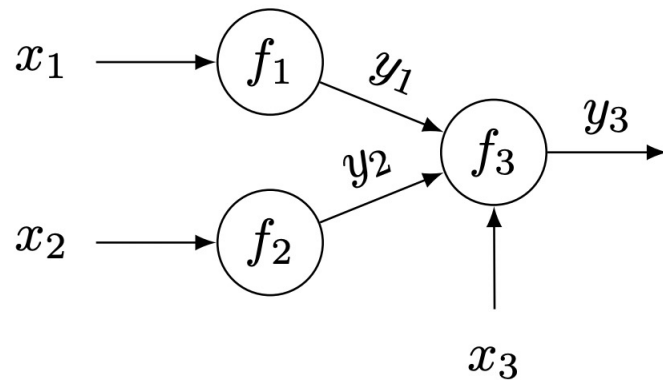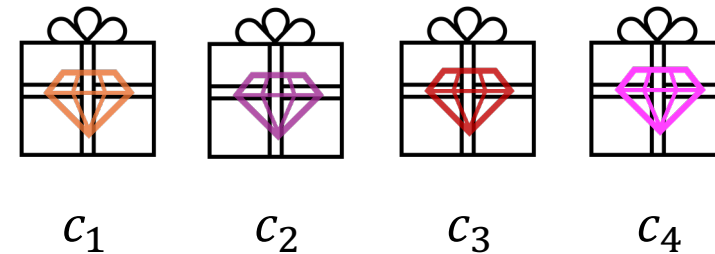Our work $\Longleftarrow$ Pandora's Box Gittins index

Conclusions

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

- Show the effectiveness of PBGI on synthetic & empirical experiments

- Open door for more-complex BO (freeze-thaw, multi-fidelity, function network, etc.) via Gittins variants ("golf" Markovian MAB, optional inspection, etc.)

? $\Longleftarrow$ Pandora's Box Gittins index