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

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

∈ decision-making under uncertainty

Applications:

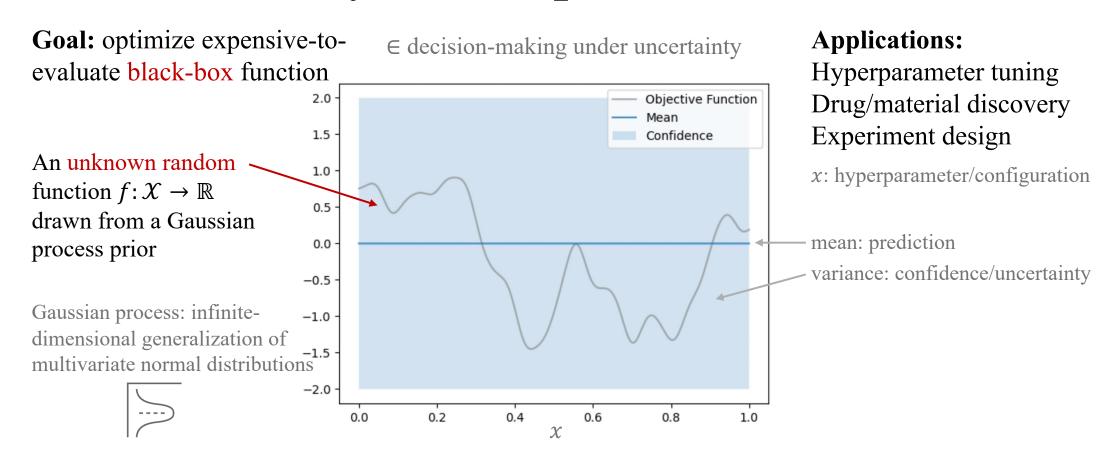
Hyperparameter tuning
Drug/material discovery
Experiment design

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

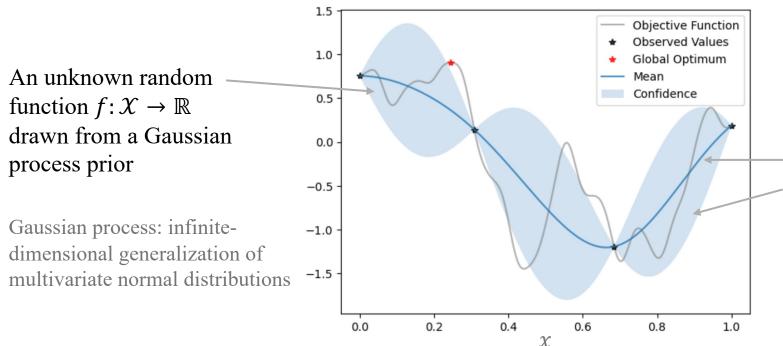
∈ decision-making under uncertainty

Applications:

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



Applications:

Hyperparameter tuning Drug/material discovery Experiment design

x: hyperparameter/configuration

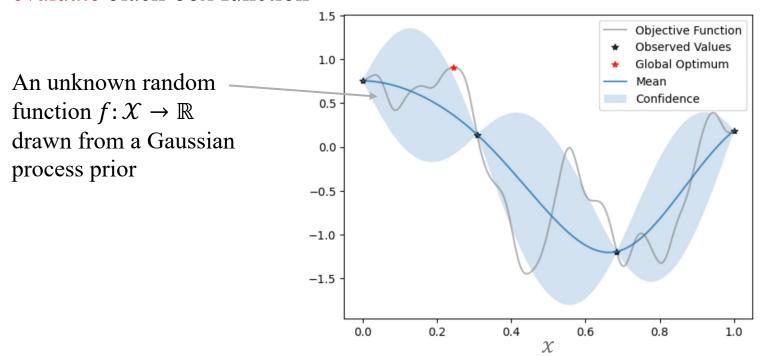
mean: prediction

variance: confidence/uncertainty

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

Decision: evaluate a set of points

Goal: optimize expensive-toevaluate black-box function



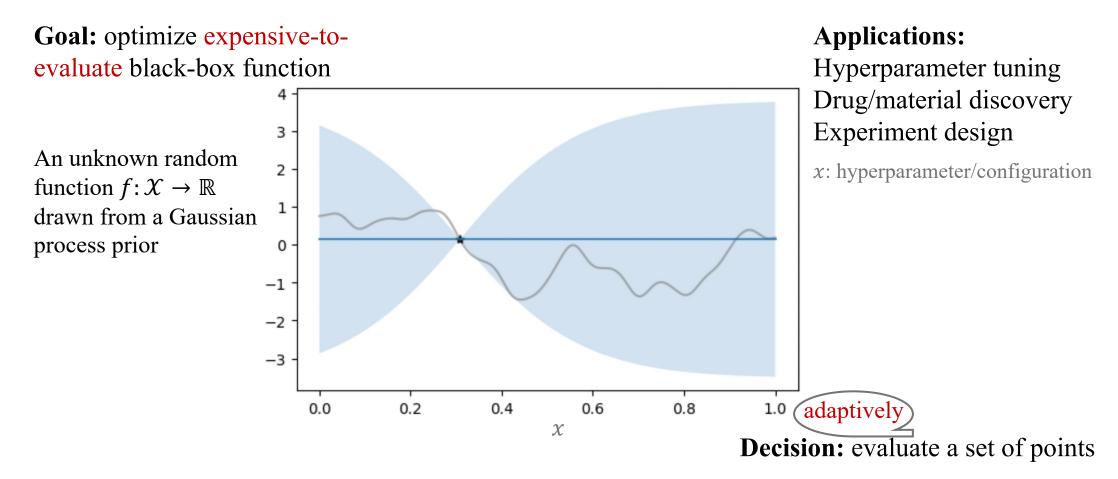
Applications:

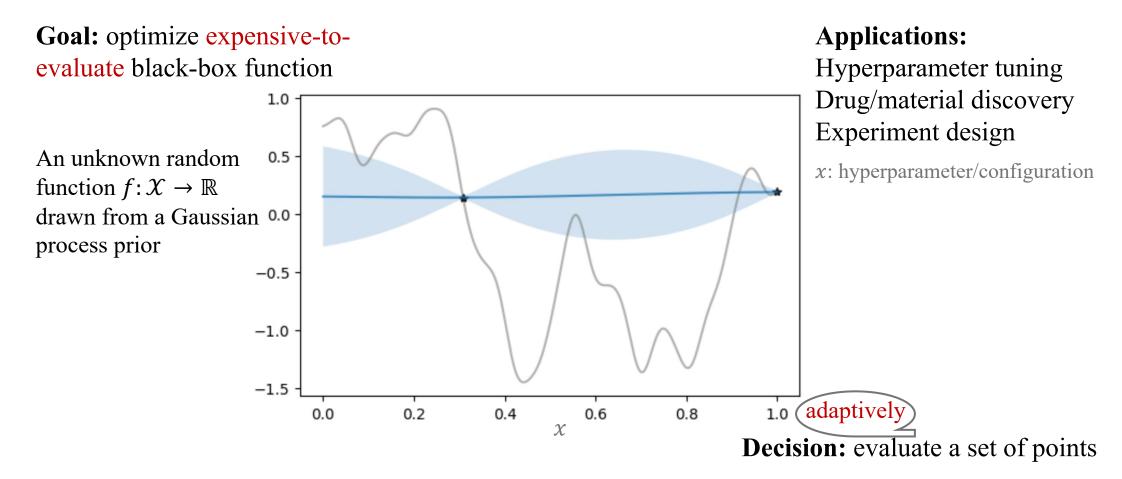
Hyperparameter tuning Drug/material discovery Experiment design

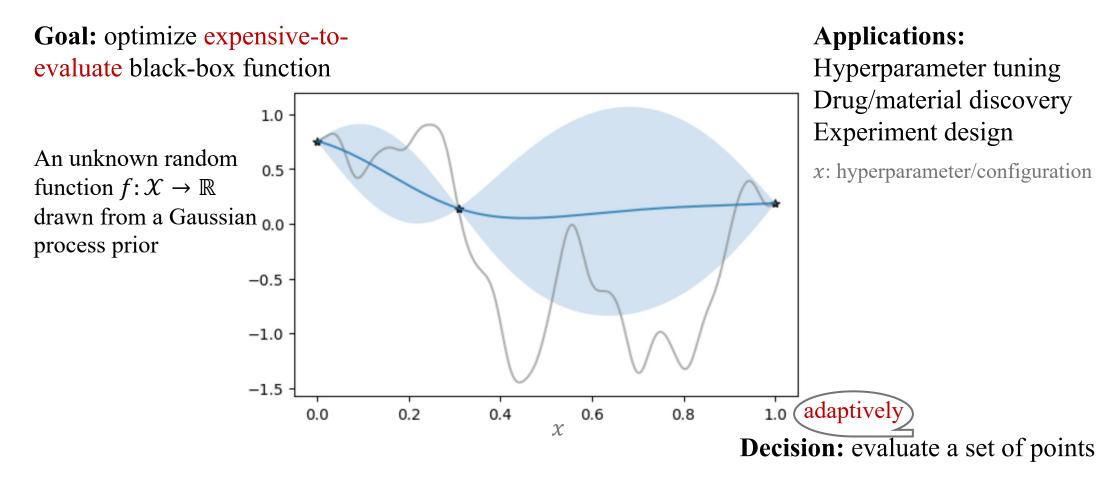
x: hyperparameter/configuration

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

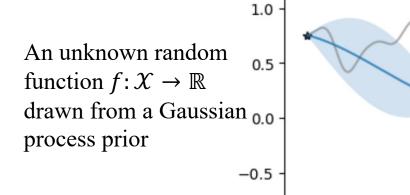
Decision: evaluate a set of points







Goal: optimize expensive-toevaluate black-box function



-1.0

-1.5

0.0

0.2

0.4

0.6

0.8



Hyperparameter tuning Drug/material discovery Experiment design

x: hyperparameter/configuration

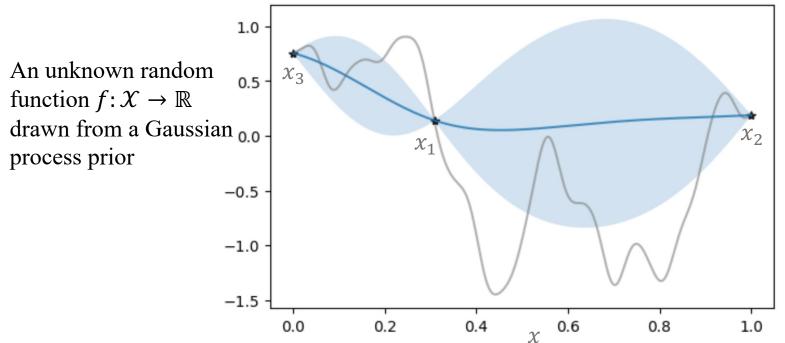
Decision: adaptively evaluate a set of points

1.0

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

T: time budget

Goal: optimize expensive-toevaluate black-box function



Applications:

Hyperparameter tuning Drug/material discovery Experiment design

x: hyperparameter/configuration

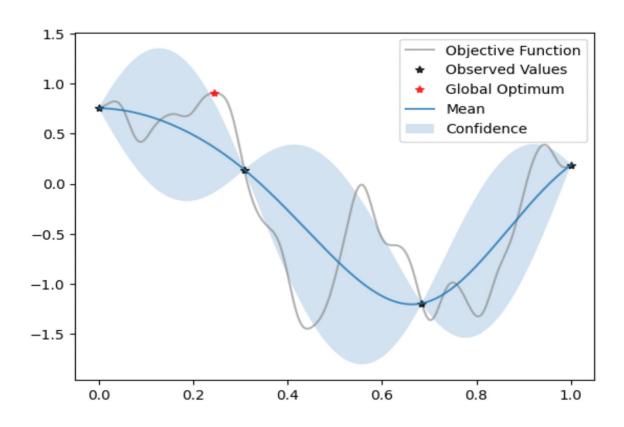
Objective: optimize best observed value at time *T*

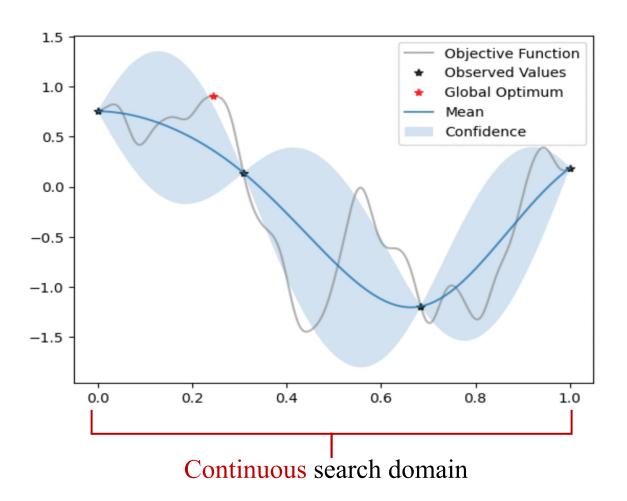
$$\sup_{\text{policy}} \mathbb{E} \max_{t=1,2,\dots,T} f(x_t)$$

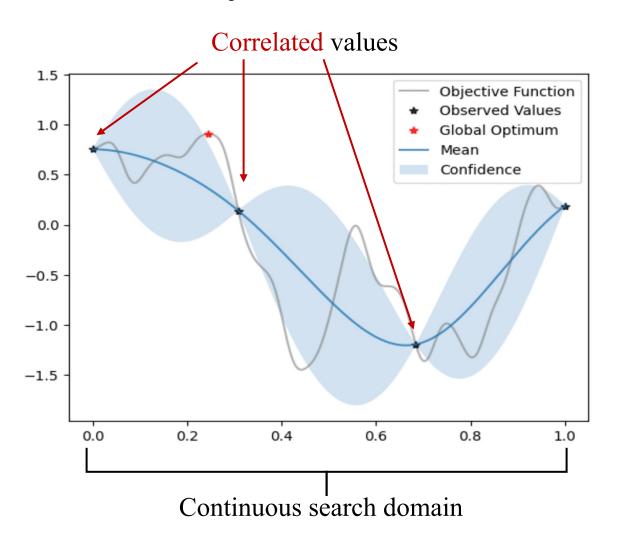
Decision: adaptively evaluate a set of points

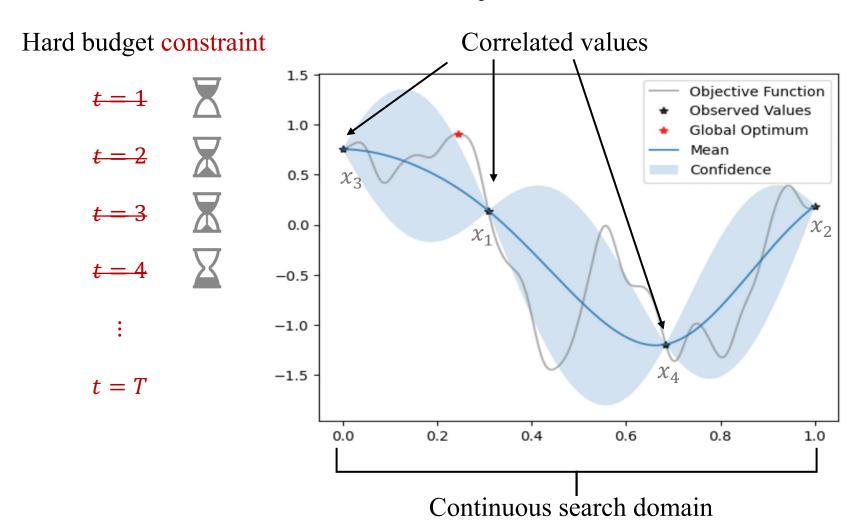
$$x_1, x_2, \dots, x_T \in \mathcal{X}$$

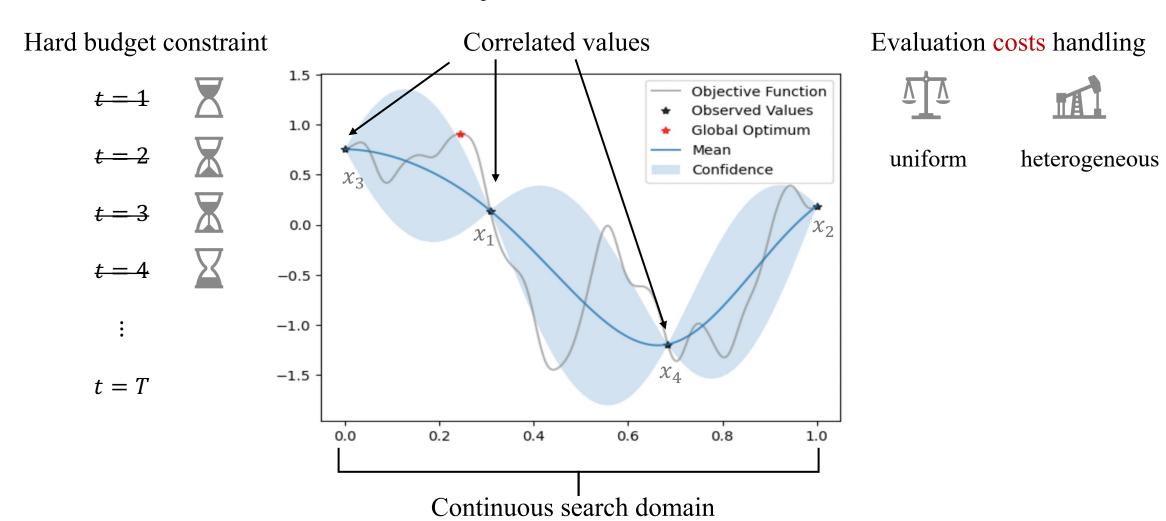
T: time budget

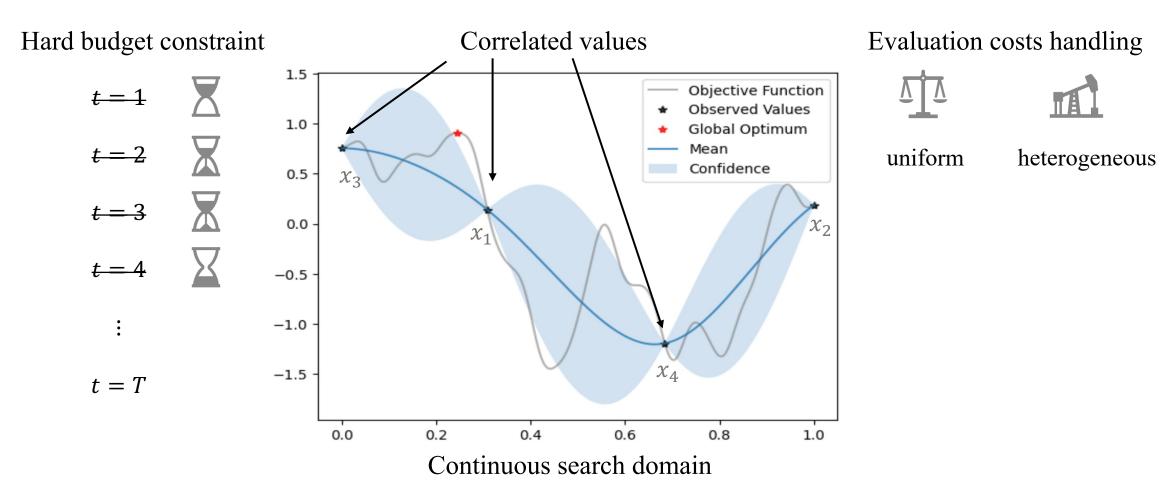




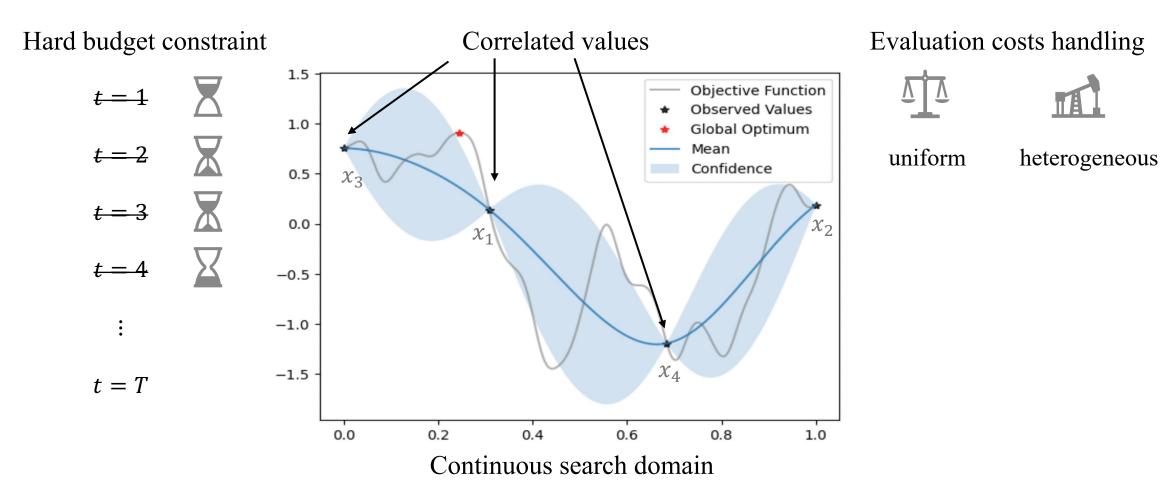




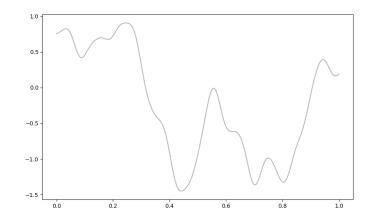




⇒ Optimal policy unknown!



Can we convert it to a solvable problem?

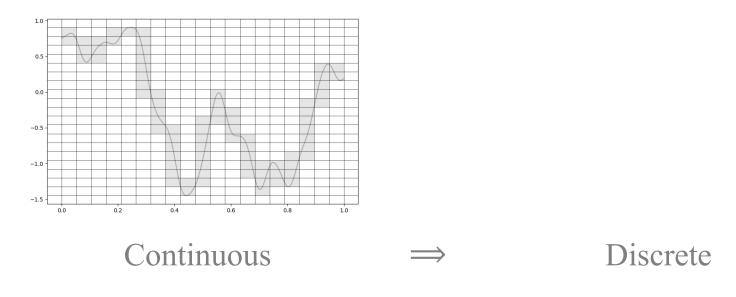


Continuous

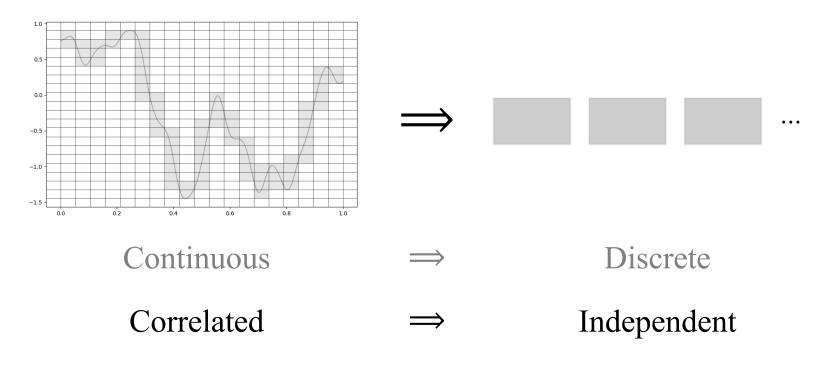
Correlated



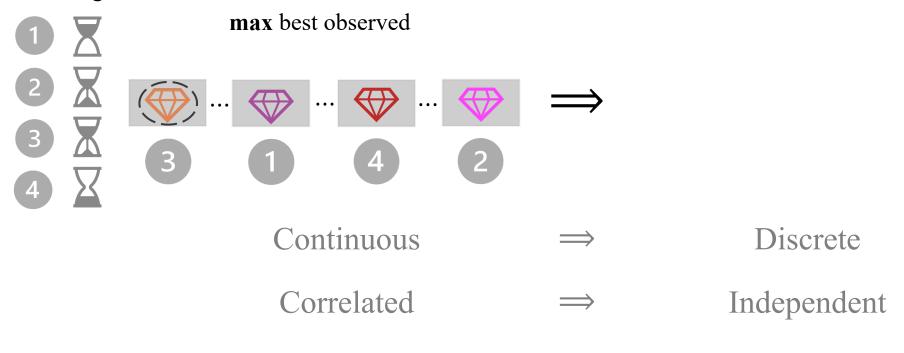
Correlated

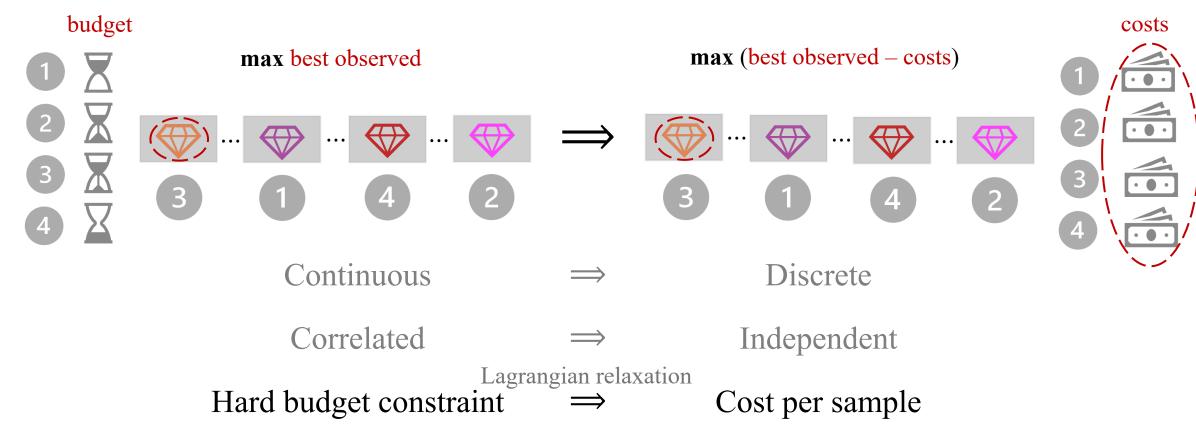


Correlated



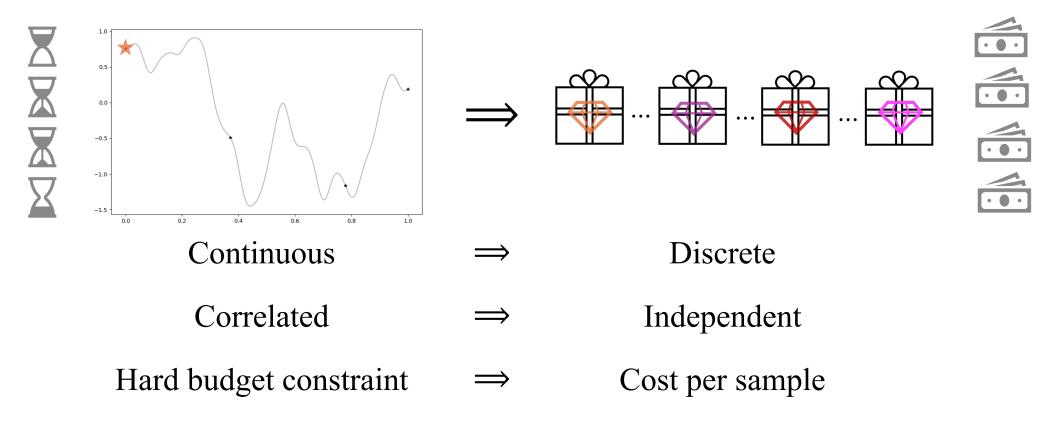
budget



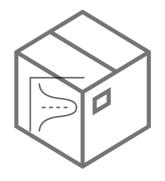


Bayesian Optimization ⇒ Pandora's Box

[Weitzman'79]

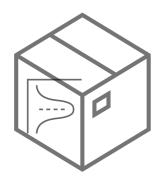


t = 0





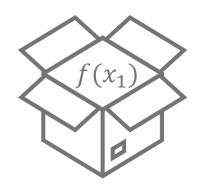




Objective: maximize net utility

t = 1







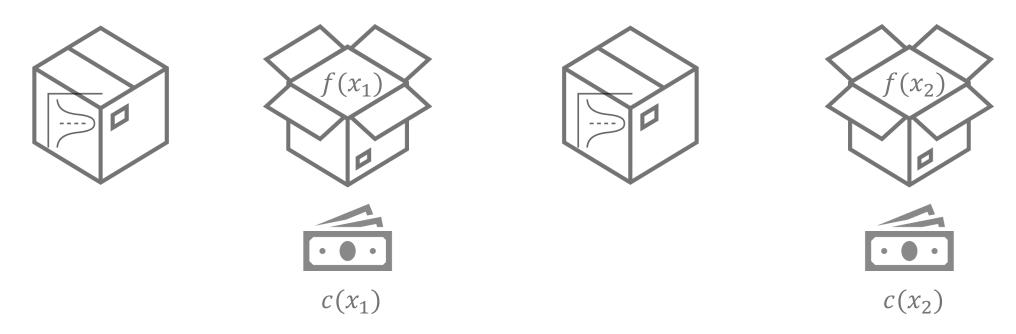




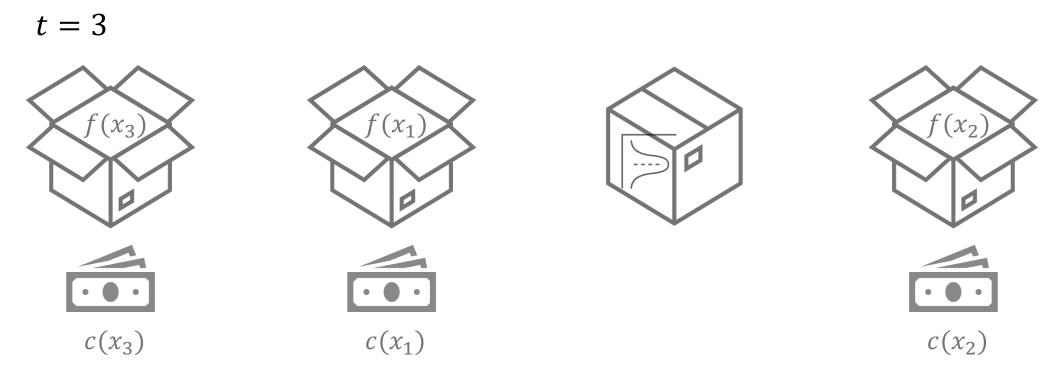
 $c(x_1)$

Objective: maximize net utility

t = 2

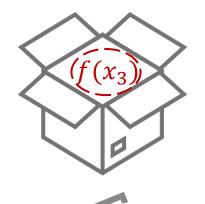


Objective: maximize net utility



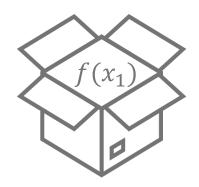
Objective: maximize net utility

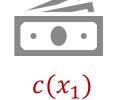




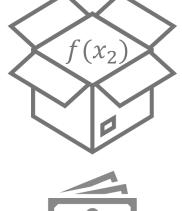














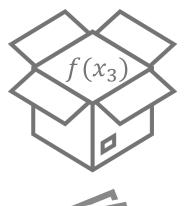
 $c(x_2)$

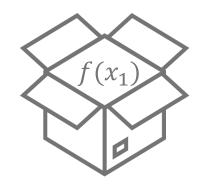
Objective: maximize net utility

Decision: adaptively evaluate a random number of boxes

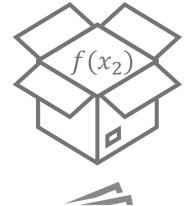
max (best observed value – total costs)

$$t = 3$$









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



$$c(x_2)$$

Objective: maximize net utility

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

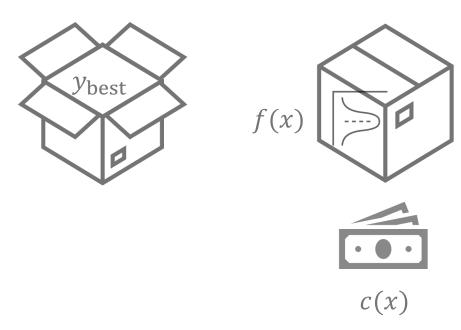
Decision: adaptively evaluate a random number of boxes

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

 \mathcal{X} : discrete

T: random stopping time

Naïve Greedy policy



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

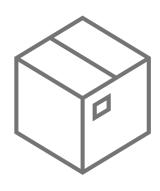
Stopping rule: $\text{EI}_f(x; y_{\text{best}}) \le c(x), \forall x \in \mathcal{X}$

expected improvement - cost

expected improvement \leq cost

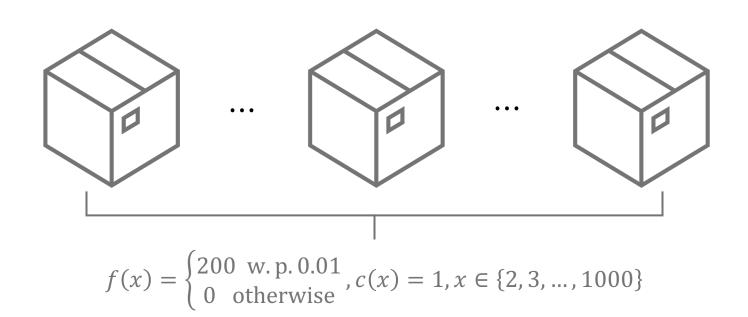
 y_{best} : current best observed value

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

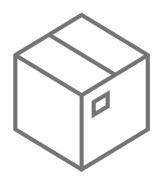


$$f(1) = 200 \text{ w. p. } 1$$

 $c(1) = 198$

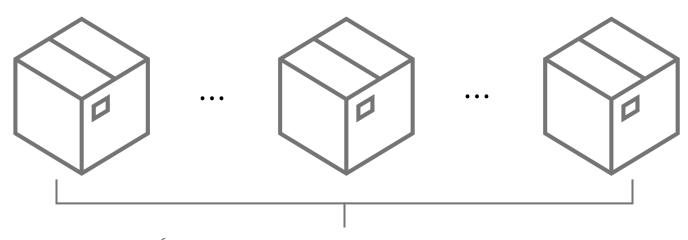


t = 0 $y_{\text{best}} = 0$



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

 $c(1) = 198$
 $EI_f(1; 0) - c(1)$
 $= 200 - 198 = 2$



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

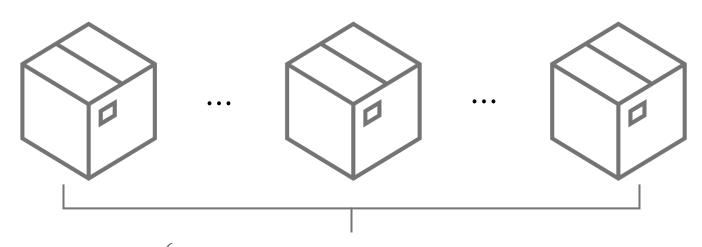
Inspection rule: $\operatorname{argmax}_{x} \left(\operatorname{El}_{f}(x; y_{\operatorname{best}}) - c(x) \right)$ **Stopping rule:** $\operatorname{El}_{f}(x; y_{\operatorname{best}}) \leq c(x), \forall x \in \mathcal{X}$ $\operatorname{El}_{f}(x; y) = \mathbb{E}[(f(x) - y)^{+}]$

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



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

 $c(1) = 198$



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

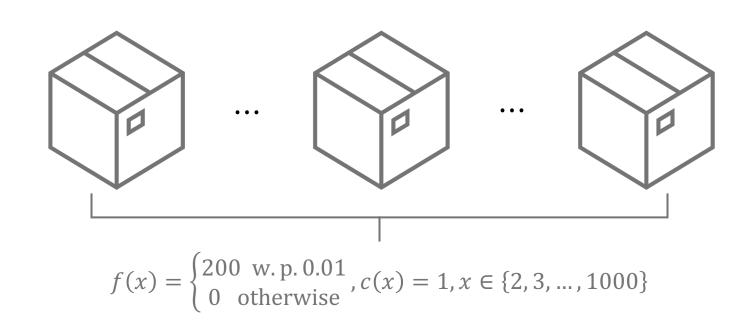
Inspection rule: $\operatorname{argmax}_{x} \left(\operatorname{El}_{f}(x; y_{\operatorname{best}}) - c(x) \right)$ **Stopping rule:** $\operatorname{El}_{f}(x; y_{\operatorname{best}}) \leq c(x), \forall x \in \mathcal{X}$ $\operatorname{El}_{f}(x; y) = \mathbb{E}[(f(x) - y)^{+}]$

$$t = 1$$



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

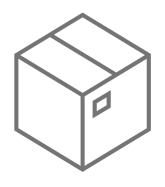
 $c(1) = 198$



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

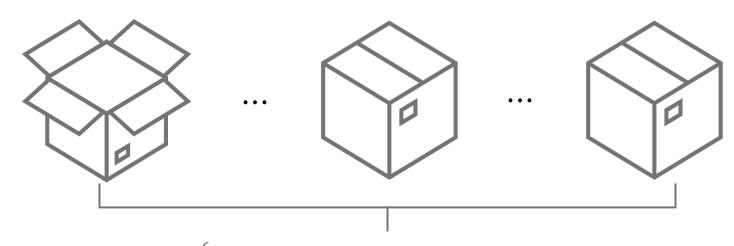
Naïve Greedy policy can fail [Singla'18]

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



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

 $c(1) = 198$



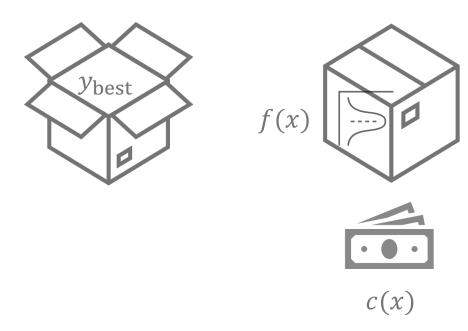
$$f(x) = \begin{cases} 200 \text{ w. p. } 0.01\\ 0 \text{ otherwise} \end{cases}, c(x) = 1, x \in \{2, 3, ..., 1000\}$$

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

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

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

Gittins policy



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

solution to expected improvement = cost

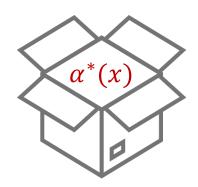
Gittins index \leq current best

 y_{best} : current best observed value

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

Gittins policy





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

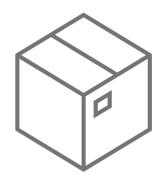
solution to expected improvement = cost

Gittins index \leq current best

 y_{best} : current best observed value

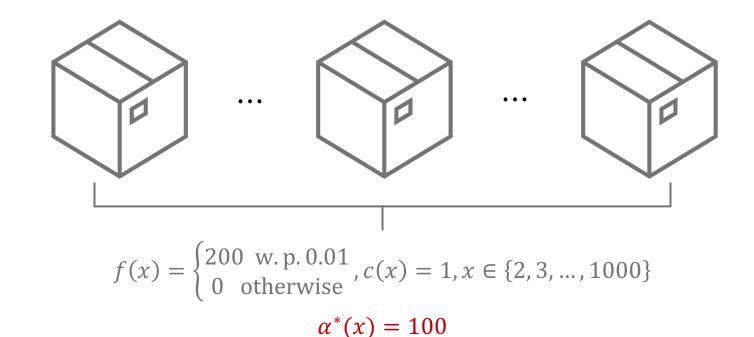
$$EI_f(x; y) = \mathbb{E}[(f(x) - y)^+]$$

$$t = 0$$



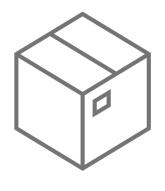
$$f(1) = 200 \text{ w. p. 1}$$

 $c(1) = 198$
 $\alpha^*(1) = 2$



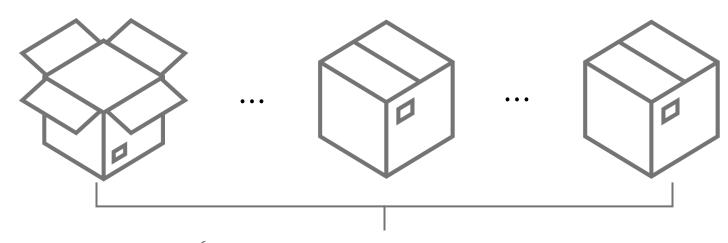
Inspection rule:
$$\alpha^*(x)$$
 s.t. $\text{El}_f(x; \alpha^*(x)) = c(x)$ Stopping rule: $\alpha^*(x) \leq y_{\text{best}}, \forall x \in \mathcal{X}$ $\text{El}_f(x; y) = \mathbb{E}[(f(x) - y)^+]$

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



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

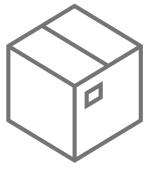
 $c(1) = 198$
 $\alpha^*(1) = 2$



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

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

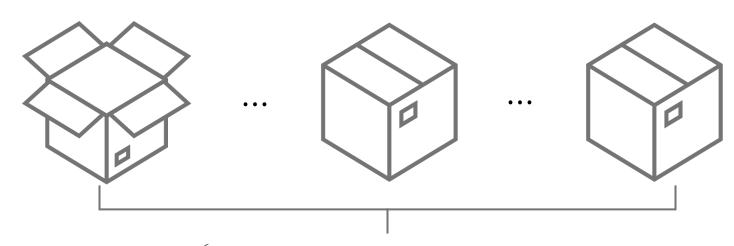
 $t \approx 100$ $y_{\text{best}} = 200$



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

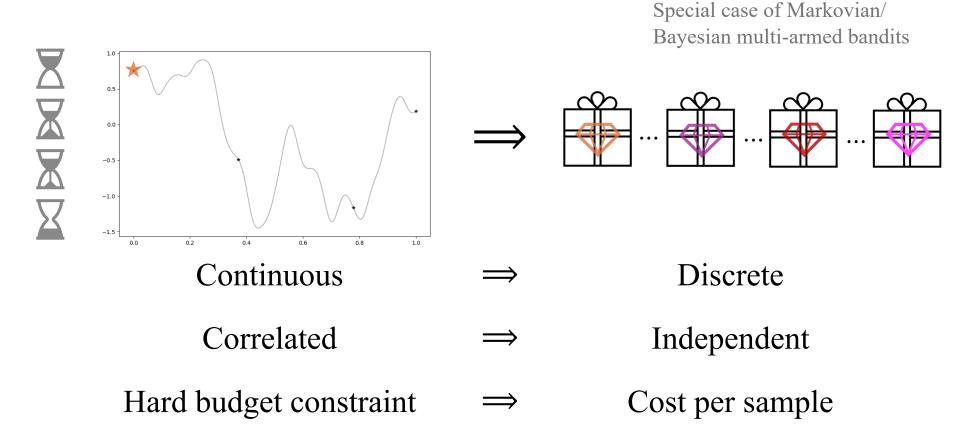
 $c(1) = 198$

 $\alpha^*(1) = 2$

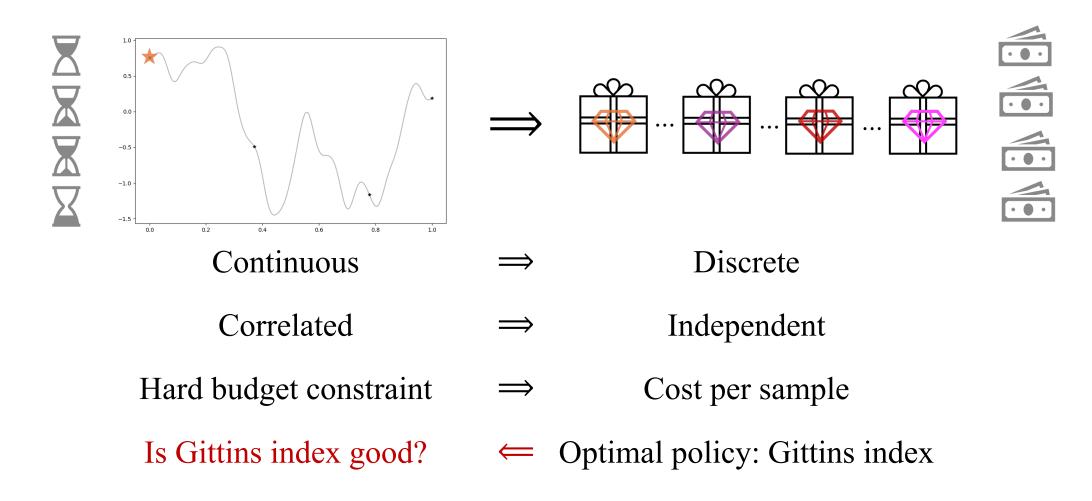


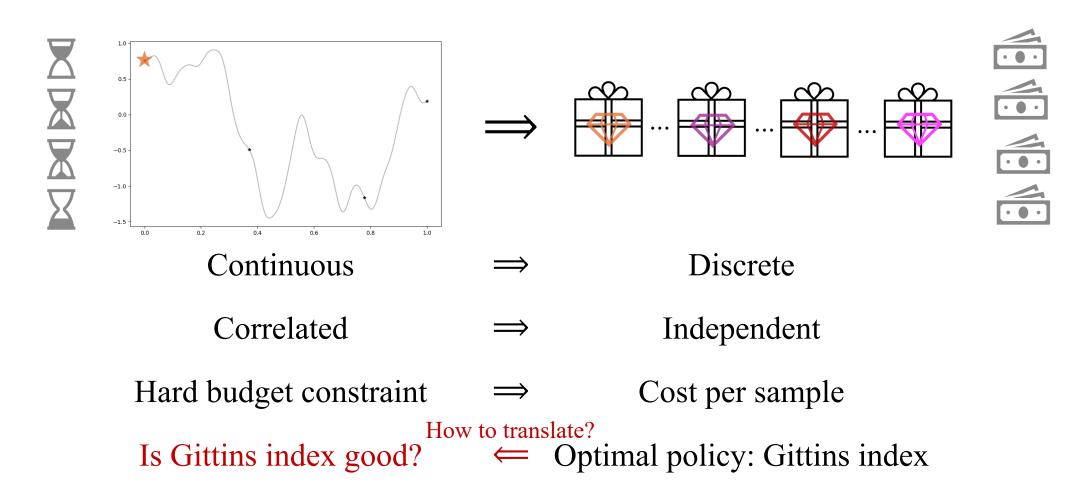
$$f(x) = \begin{cases} 200 \text{ w. p. } 0.01 \\ 0 \text{ otherwise} \end{cases}, c(x) = 1, x \in \{2, 3, ..., 1000\}$$
$$\alpha^*(x) = 100$$

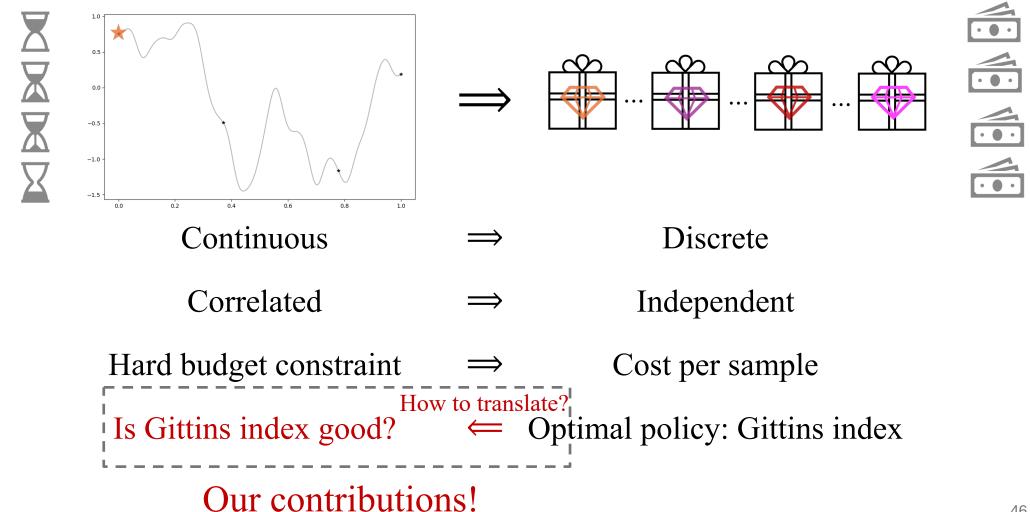
Inspection rule: $\alpha^*(x)$ s.t. $\text{EI}_f(x; \alpha^*(x)) = c(x)$ Stopping rule: $\alpha^*(x) \leq y_{\text{best}}, \forall x \in \mathcal{X}$ Expected utility: $\mathbb{E}[\text{Gittins}] = 200 - 100 * 1 = 100$

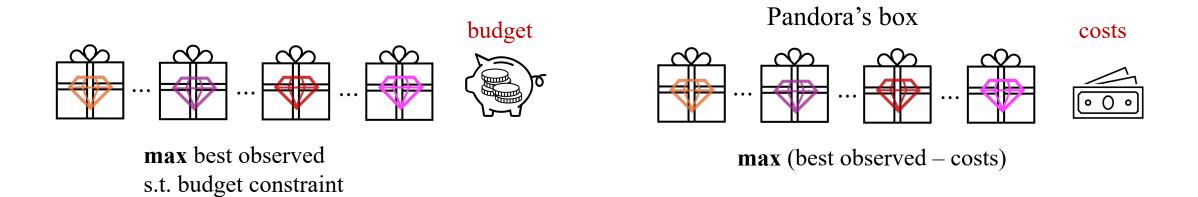


Optimal policy: Gittins index [Weitzman'79]



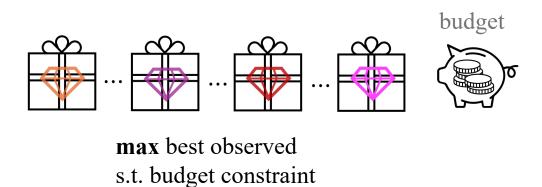


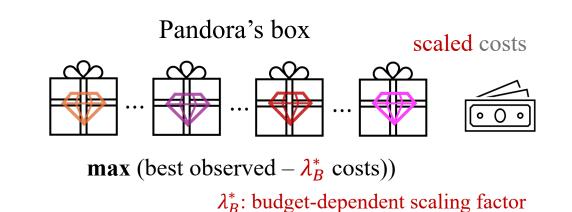




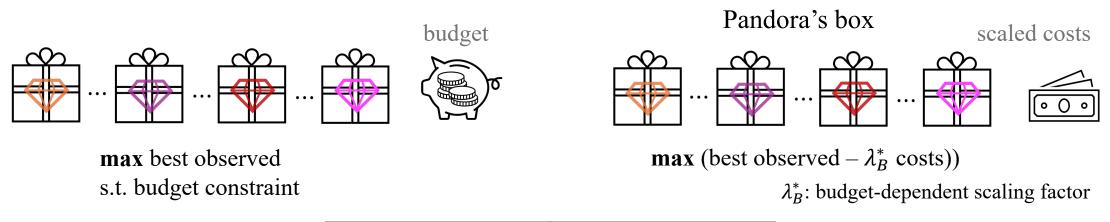
Expected budget constraint \Leftrightarrow Cost per sample

Optimal policy? \Leftarrow Optimal policy: Gittins index



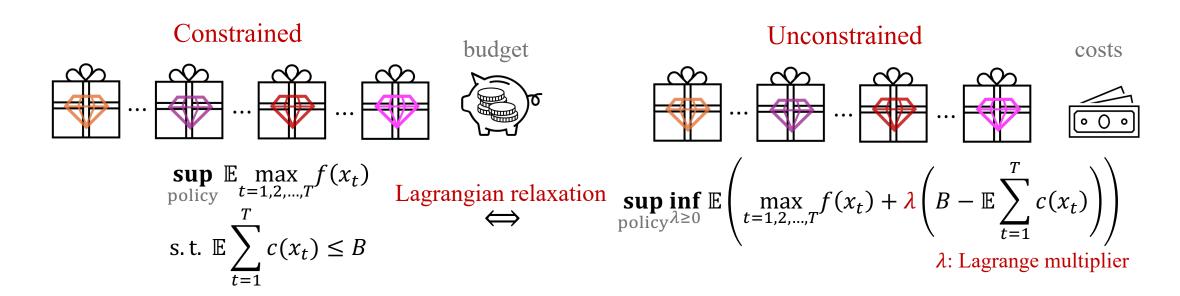


Optimal policy: Gittins solution to \leftarrow Optimal policy: Gittins index Pandora's box with scaled costs



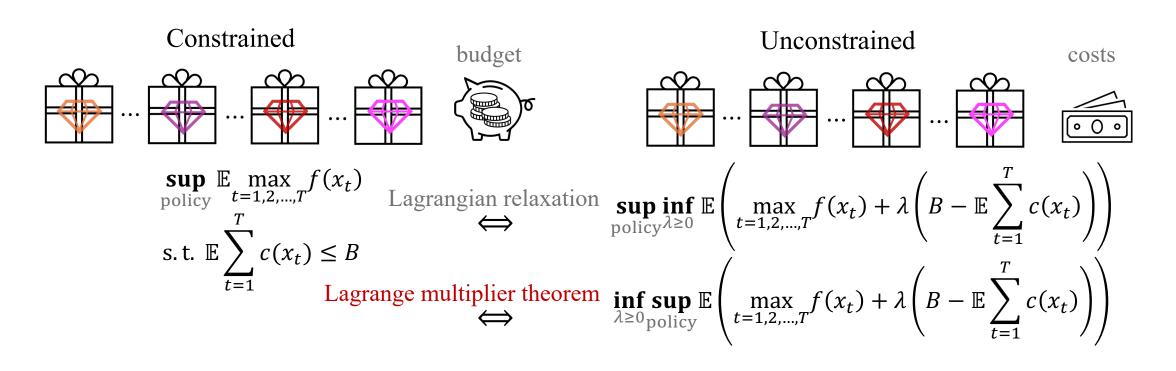
Reward distribution	Reference
finite support	[Aminian et al.'24]
general support	our work

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



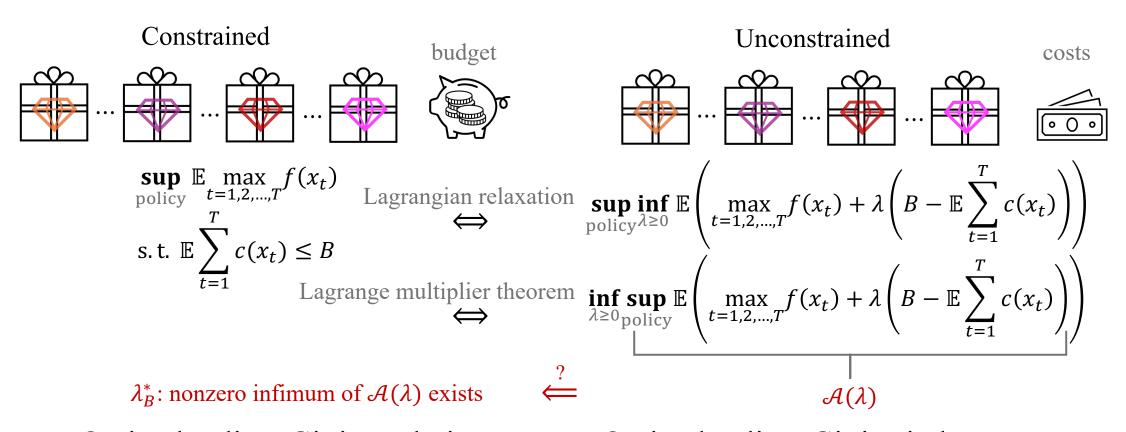
Optimal policy: Gittins solution to ← Optimal policy: Gittins index Pandora's box with scaled costs

Extension to [Aminian et al.'24]



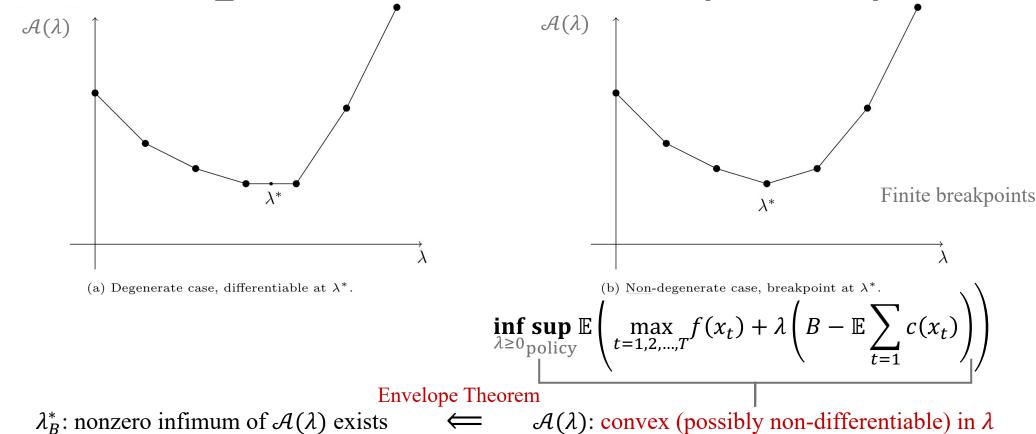
Optimal policy: Gittins solution to ← Optimal policy: Gittins index Pandora's box with scaled costs

Extension to [Aminian et al.'24]



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

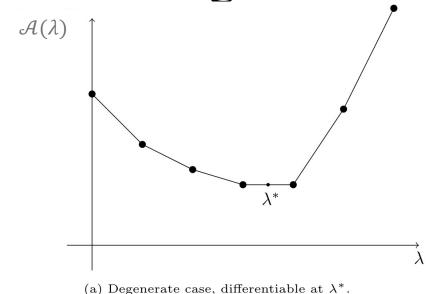
Extension to [Aminian et al.'24]

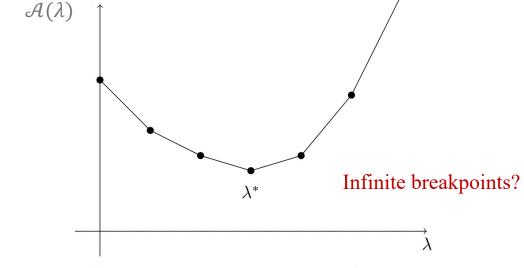


Optimal policy: Gittins solution to \leftarrow Optimal policy: Gittins index Pandora's box with scaled costs

Extension to [Aminian et al.'24]

Figure from [Aminian et al.'24]





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

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

 \Leftarrow

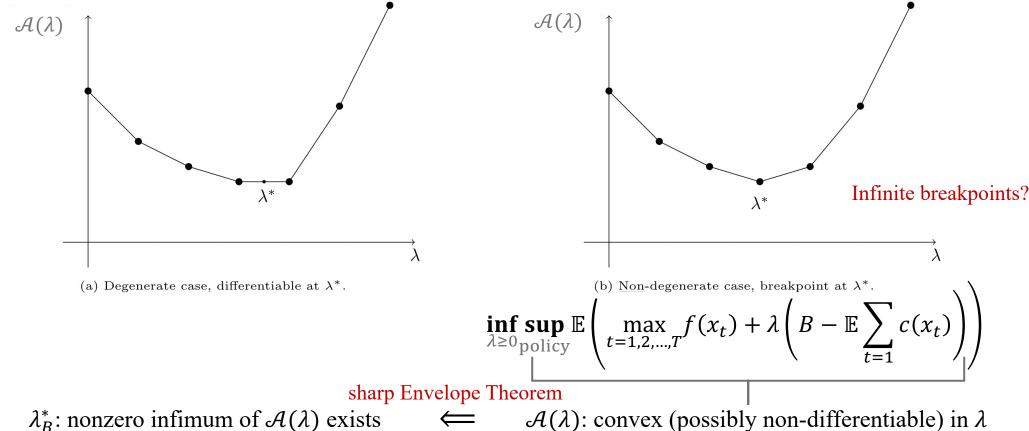
 $\mathcal{A}(\lambda)$: convex (possibly non-differentiable) in λ

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

Extension to [Aminian et al.'24]

Figure from [Aminian et al.'24]

Expected budget constraint ⇔ Cost per sample



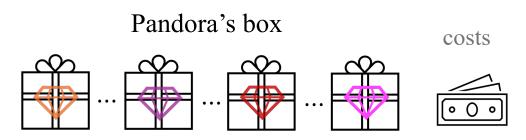
Optimal policy: Gittins solution to \leftarrow Optimal policy: Gittins index Pandora's box with scaled costs

Extension to [Aminian et al.'24]

Figure from [Aminian et al.'24]



max best observed
s.t. budget constraint



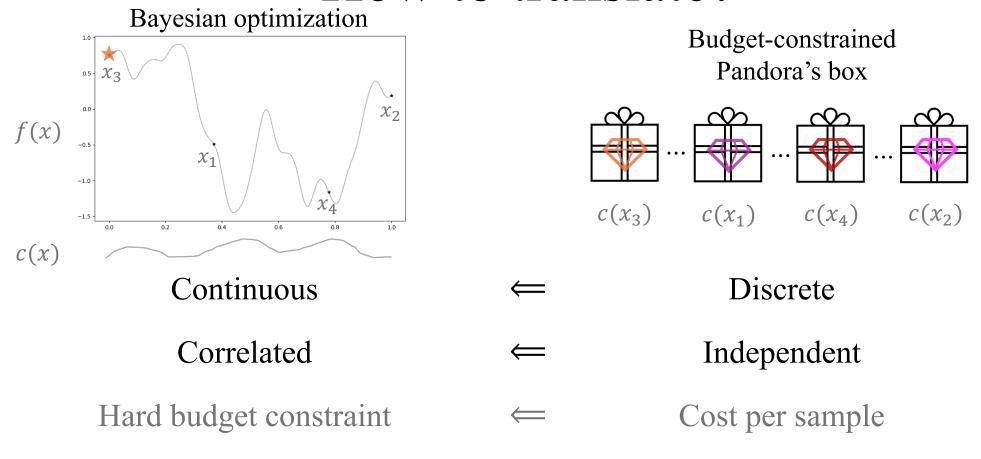
max (best observed – costs)

Hard budget constraint

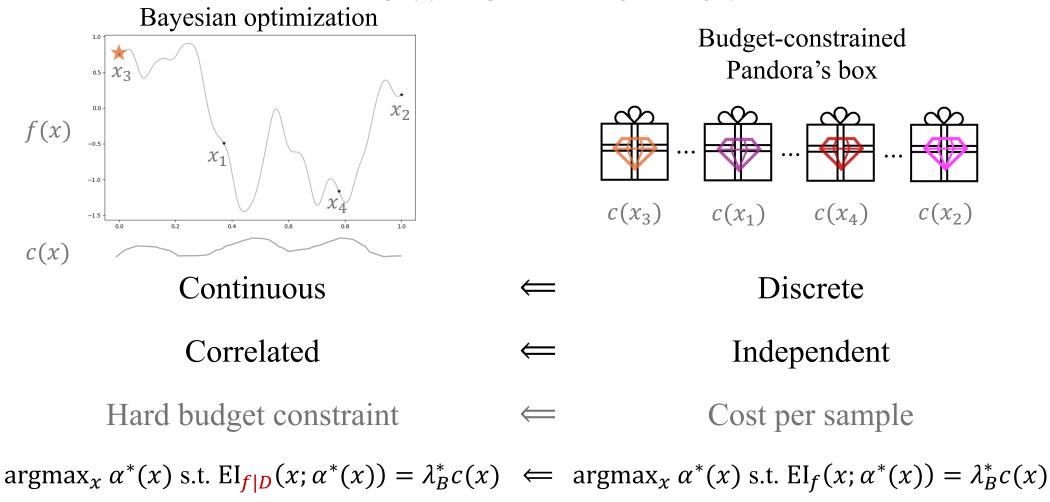
 \Leftarrow

Cost per sample

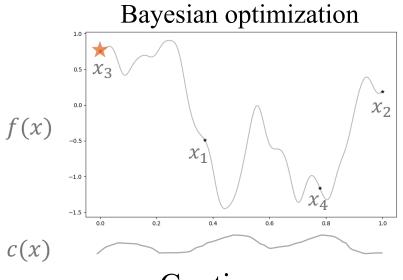
 $\operatorname{argmax}_{x} \alpha^{*}(x) \text{ s.t. } \operatorname{EI}_{f}(x; \alpha^{*}(x)) = \lambda_{B}^{*} c(x) \iff \operatorname{argmax}_{x} \alpha^{*}(x) \text{ s.t. } \operatorname{EI}_{f}(x; \alpha^{*}(x)) = c(x)$



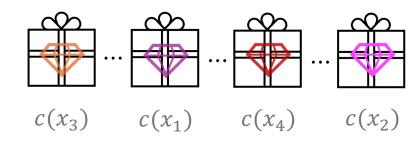
How to incorporate Gaussian process? ← Optimal policy: Gittins solution to Pandora's box with scaled costs



D: observed data



Budget-constrained Pandora's box



Continuous

 \leftarrow

Discrete

Correlated

 \Leftarrow

Independent

Hard budget constraint

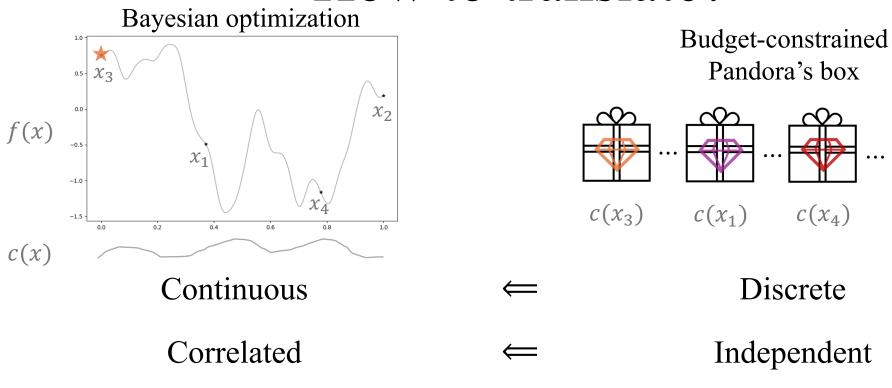
 \leftarrow

Cost per sample

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

popular one-step

heuristic: EI policy



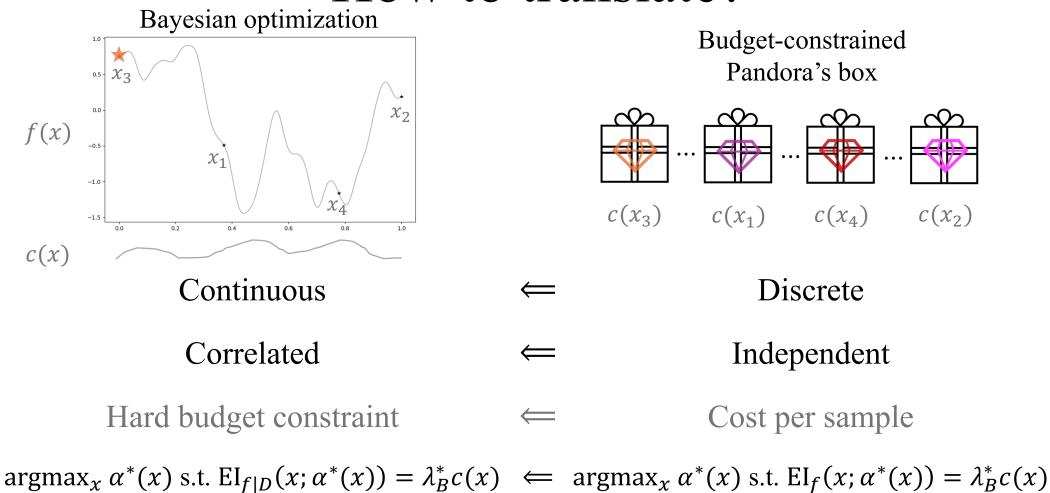
Hard budget constraint

traint \leftarrow Cost per sample

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

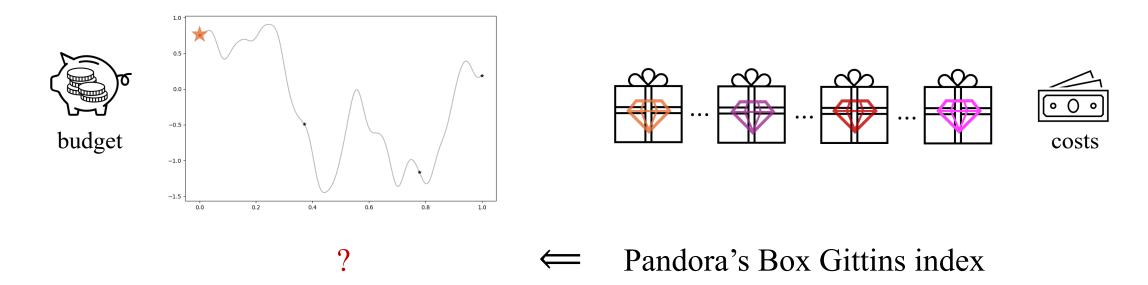
ratio of EI and cost: EIPC policy

 $c(x_2)$



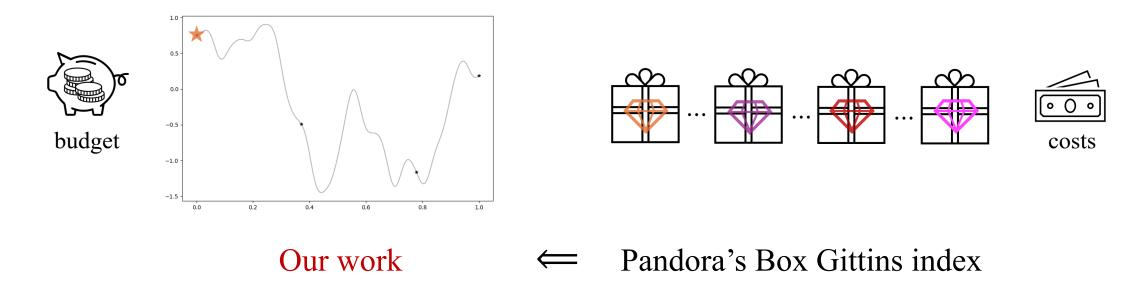
Our Contributions

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



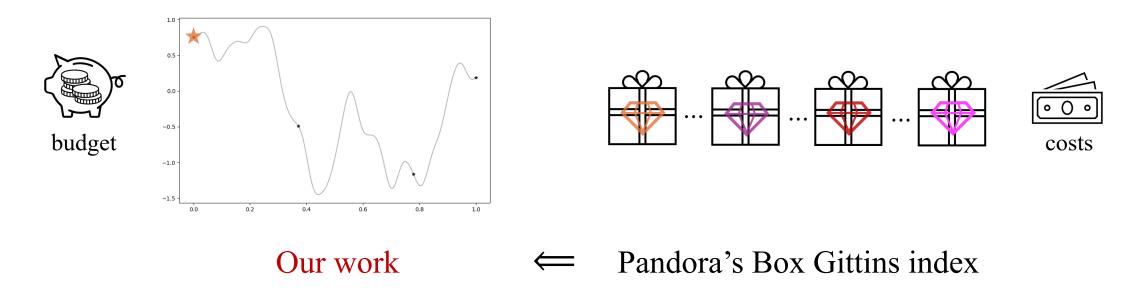
Our Contributions

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

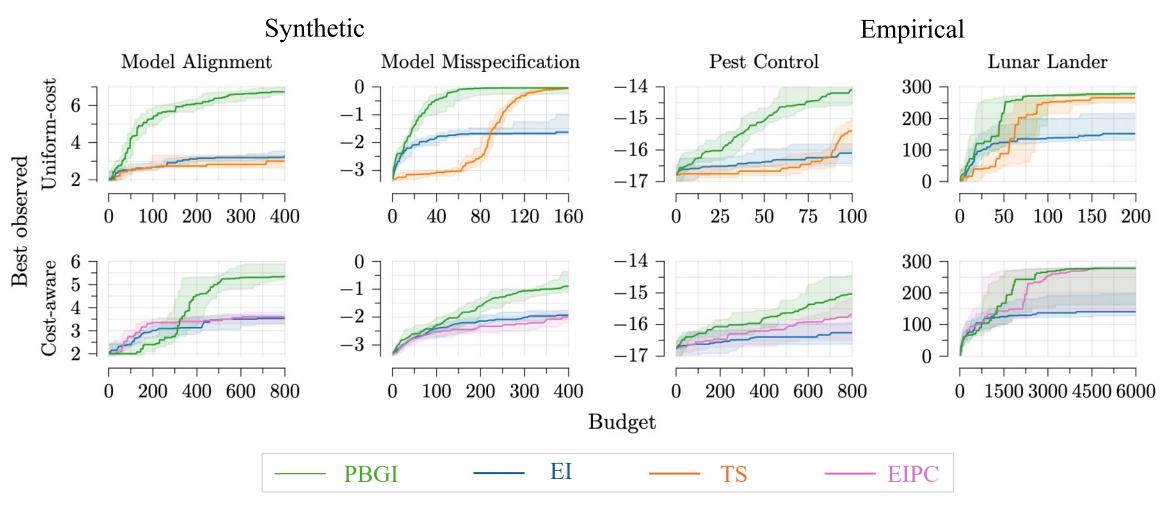


Our Contributions

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

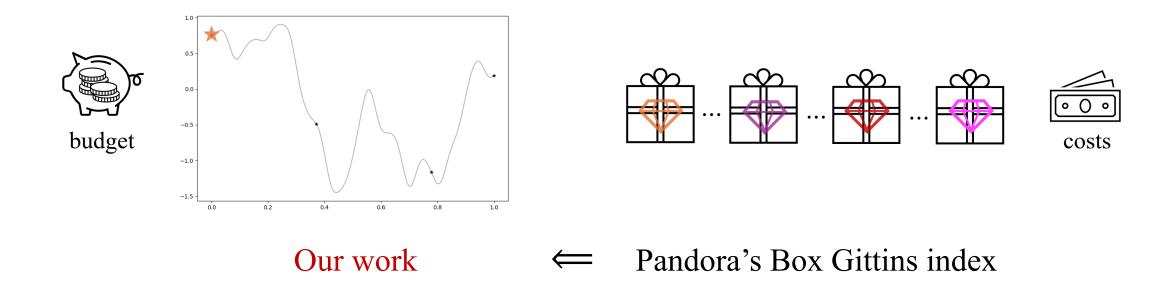


Experiment Results: PBGI vs Baselines



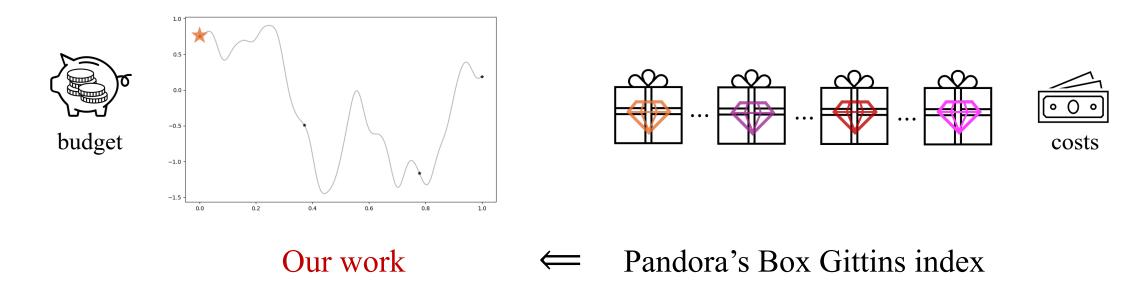
Conclusions

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



Conclusions

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



Conclusions

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

