Gittins Indices for Bayesian Optimization: Insights from Pandora's Box

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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

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∈ decision-making under uncertainty

Applications:
Hyperparameter tuning
Drug discovery
Control design

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∈ decision-making under uncertainty

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Bayesian Optimization

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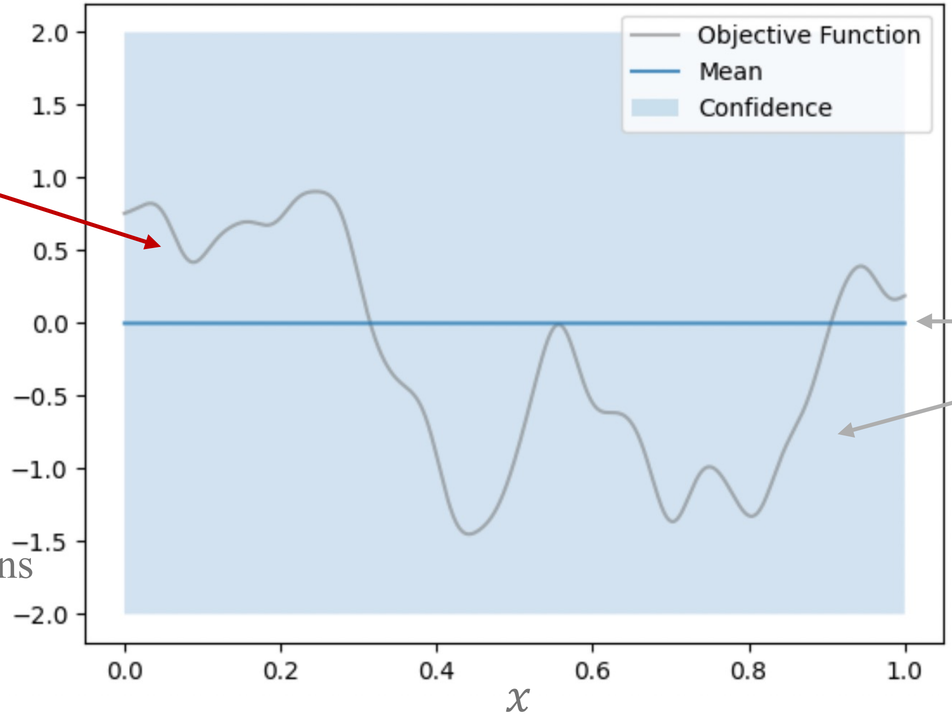
An unknown random function $f: \mathcal{X} \to \mathbb{R}$ drawn from a Gaussian process prior



Gaussian process: infinite-dimensional generalization of multivariate normal distributions

Applications:
Hyperparameter tuning
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Control design

x: hyperparameter/configuration

mean: prediction

variance: confidence/uncertainty

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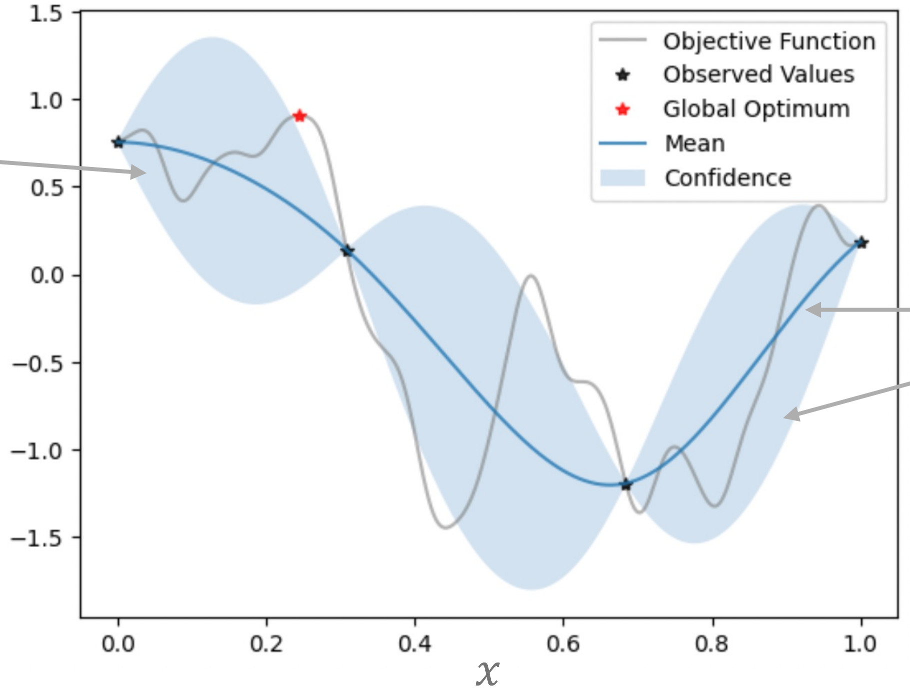

Applications:
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x: hyperparameter/configuration

mean: prediction

variance: confidence/uncertainty

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

Decision: evaluate a set of points

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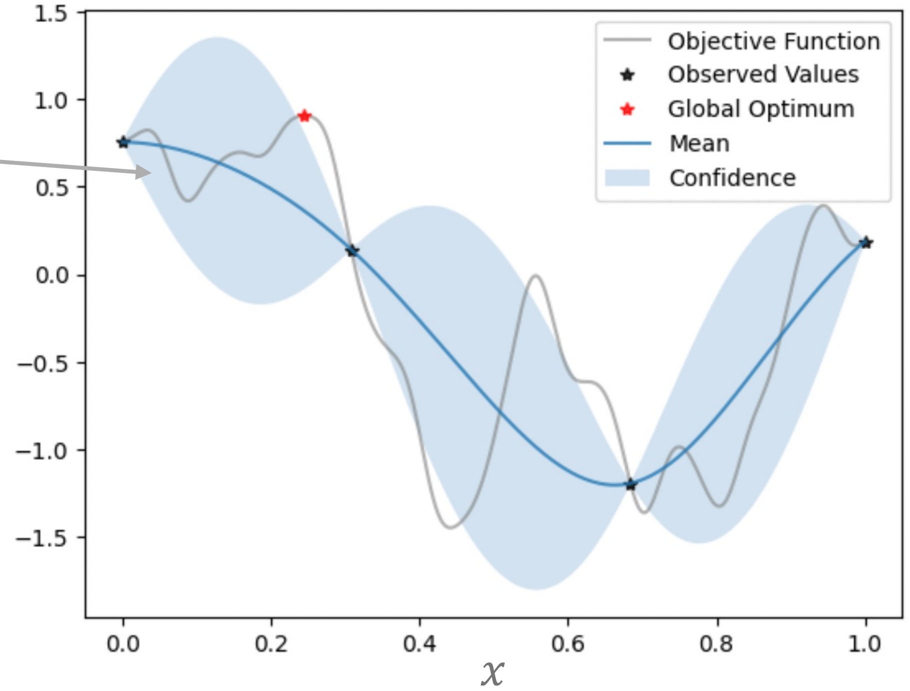

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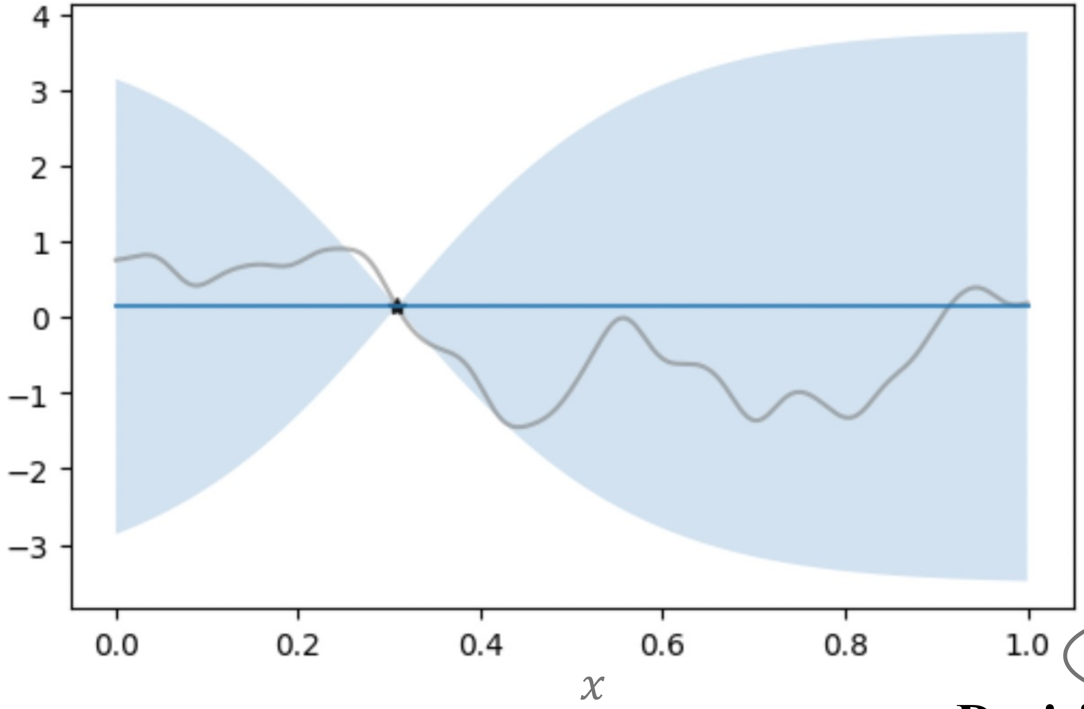

Applications:
Hyperparameter tuning
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x: hyperparameter/configuration

adaptively

Decision: evaluate a set of points

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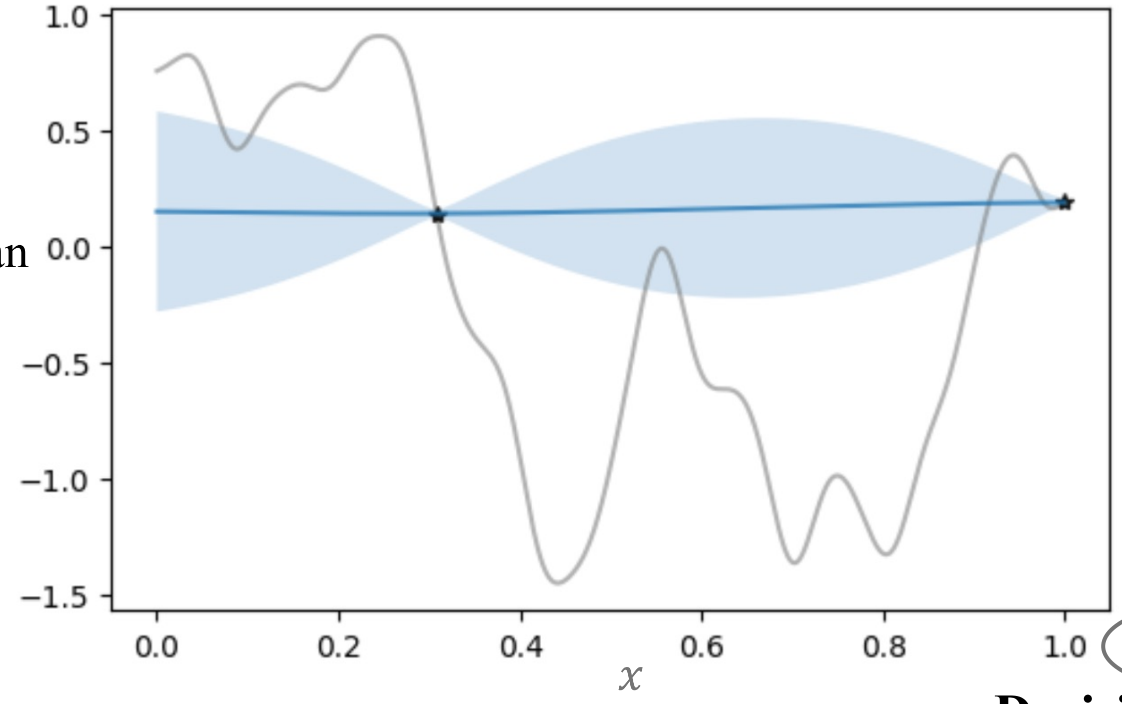

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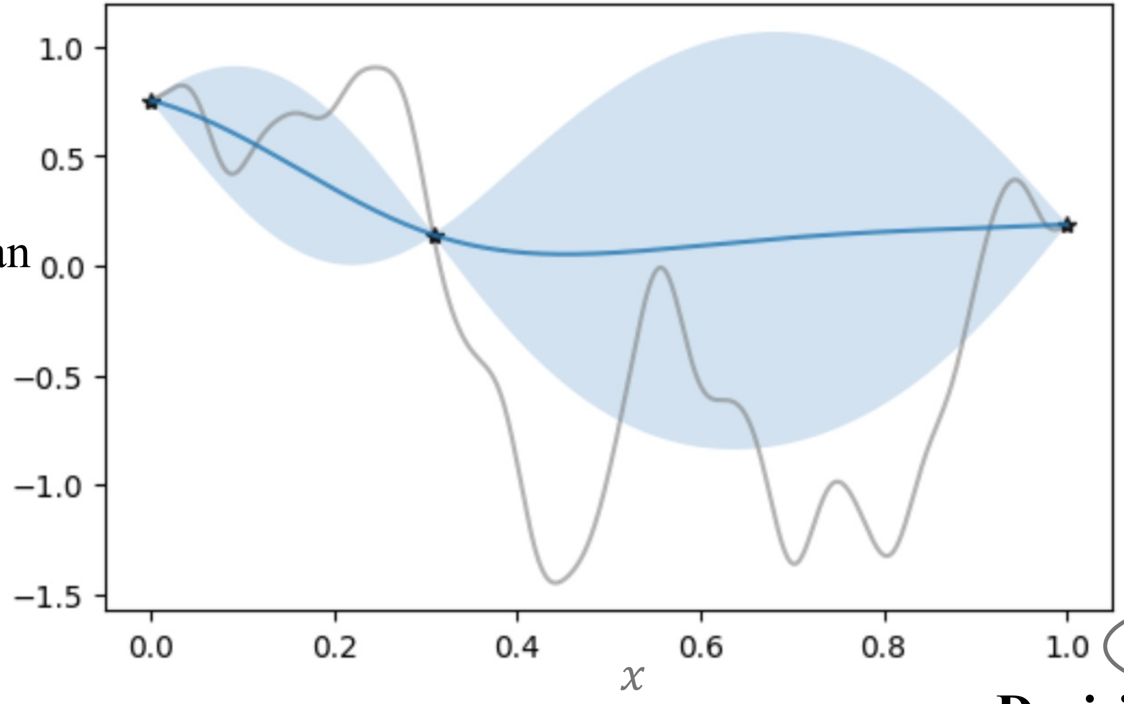

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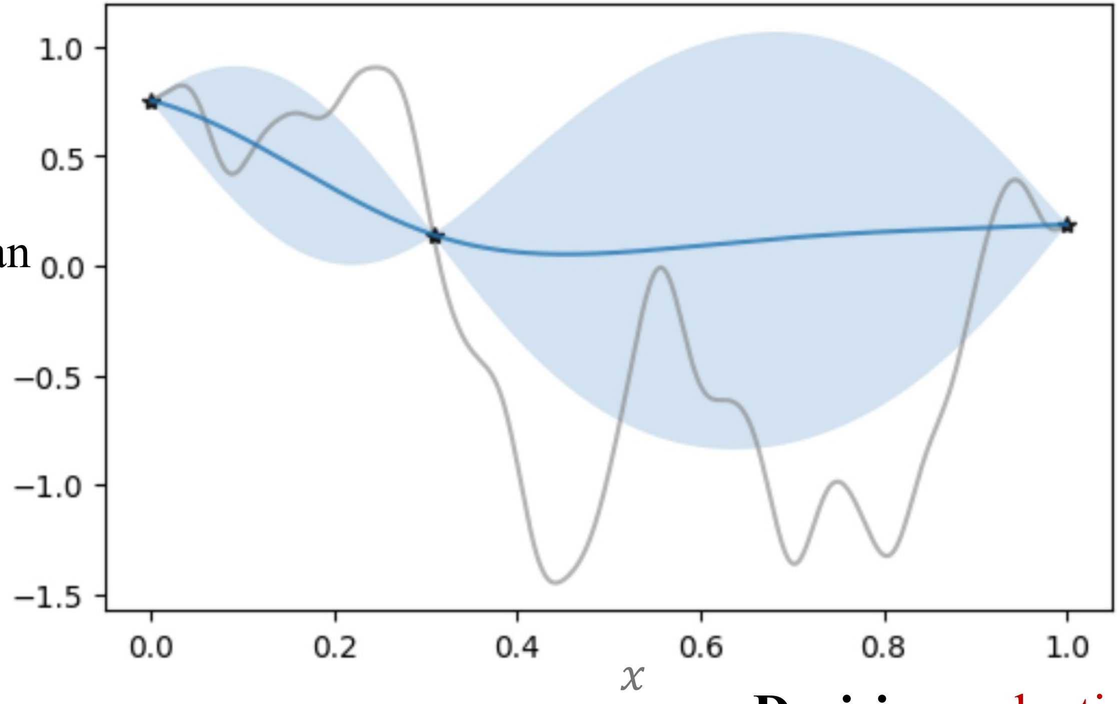

Applications:
Hyperparameter tuning
Drug discovery
Control design

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

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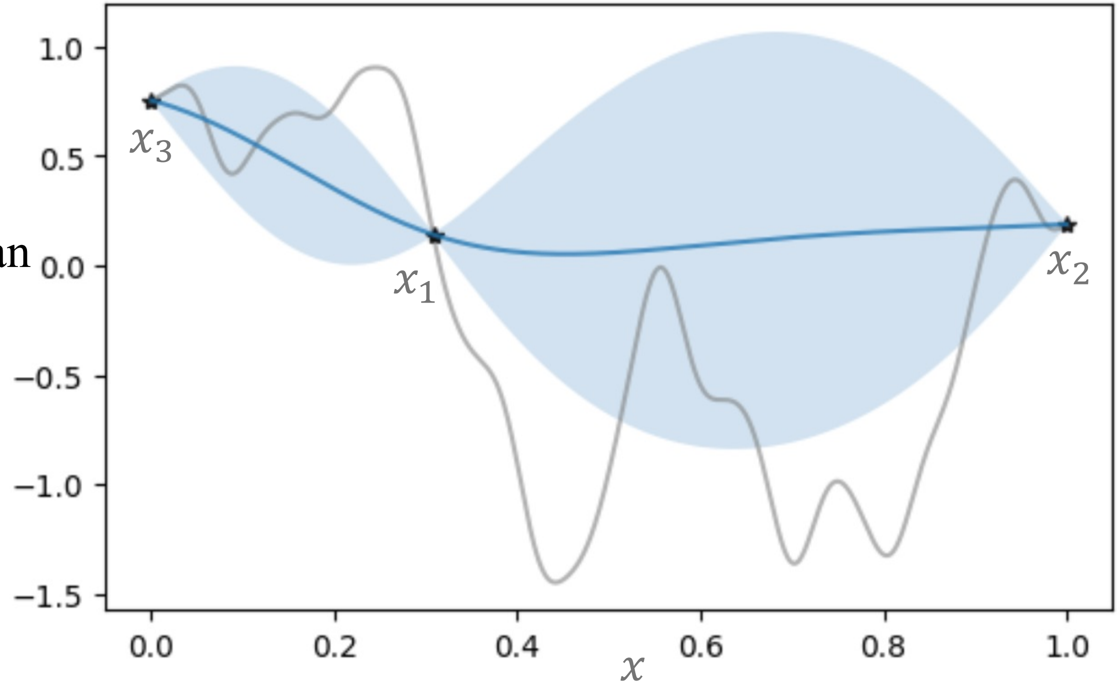


Applications:
Hyperparameter tuning
Drug discovery
Control design

x: hyperparameter/configuration

Objective: optimize best observed value at time T

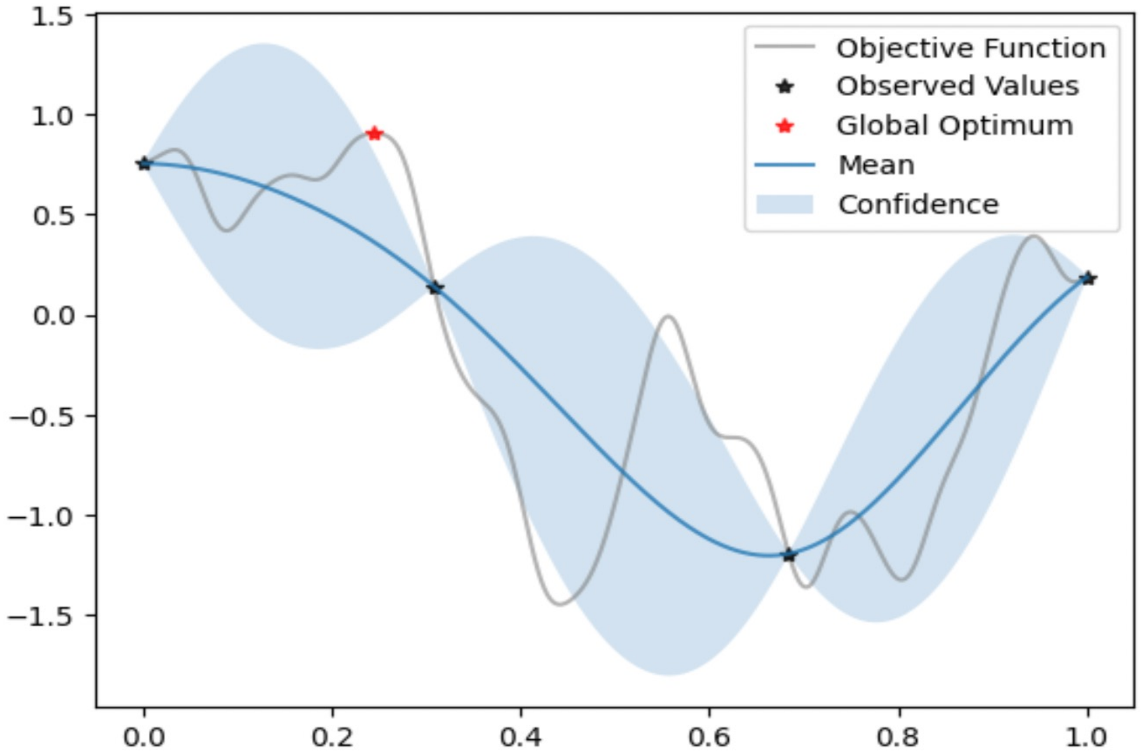
$$\sup_{\text{policy}} \mathbb{E} \max_{t=1,2,\ldots,T} f(x_t)$$

Decision: adaptively evaluate a set of points

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

T: time budget

Why is it hard?



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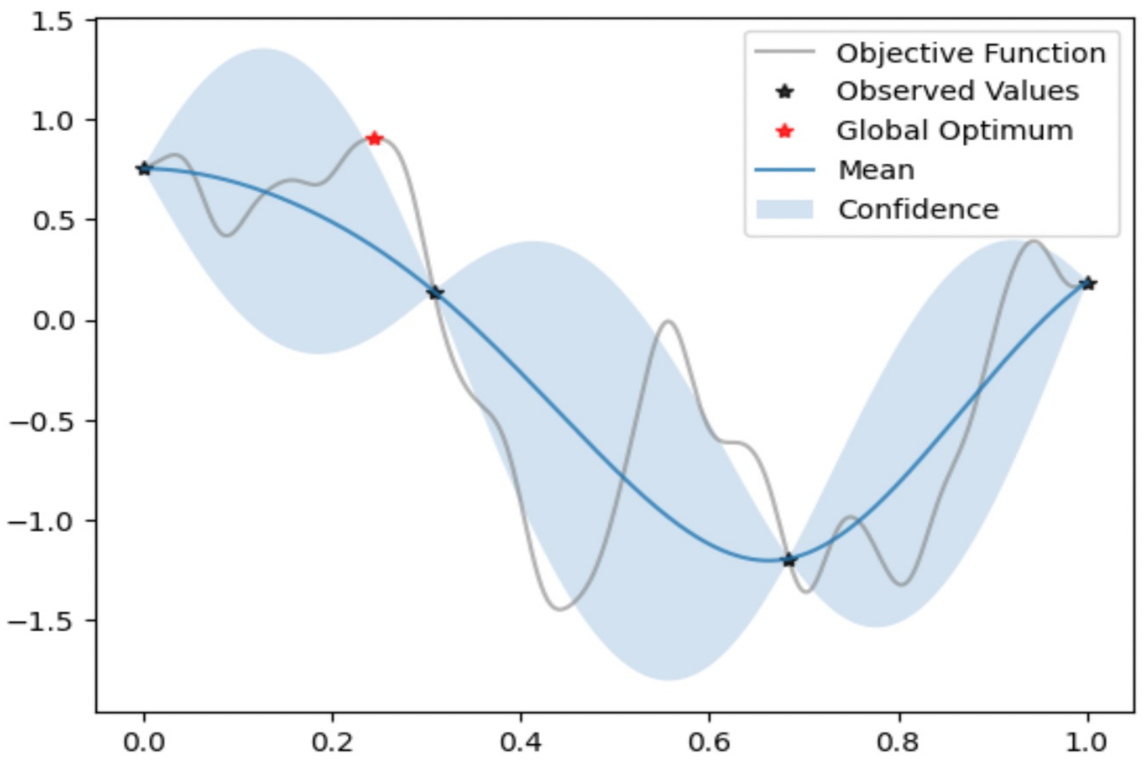
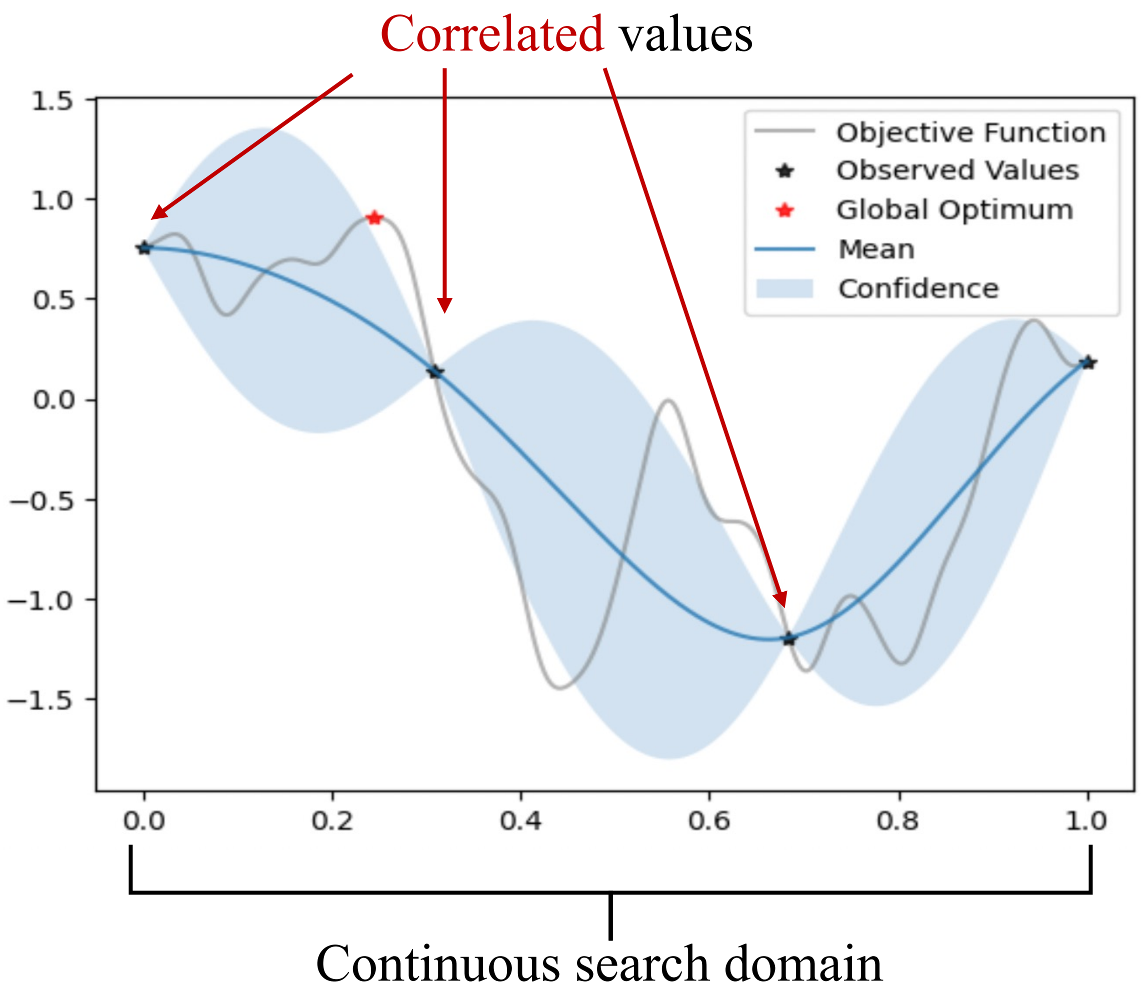


Continuous search domain

Why is it hard?



Why is it hard?

Hard budget constraint

$\cancel{t=1}$

$\cancel{t=2}$

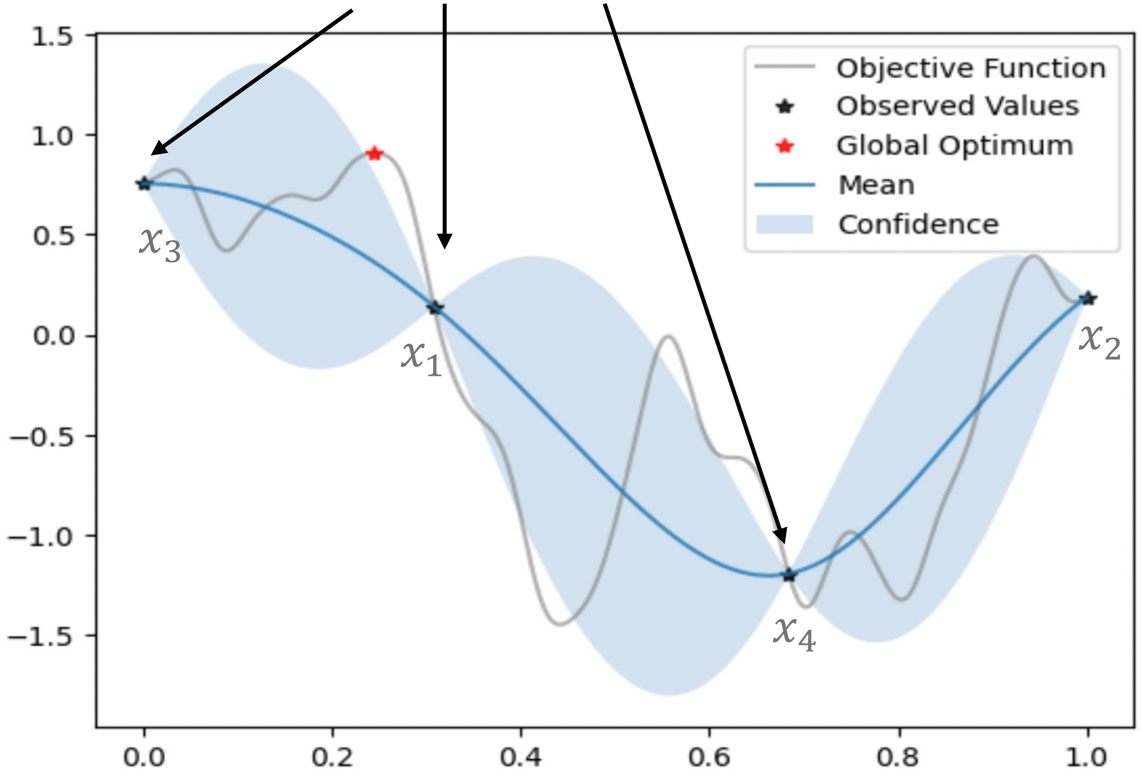
$\cancel{t=3}$

$\cancel{t=4}$

$\vdots$

$t = T$

Correlated values



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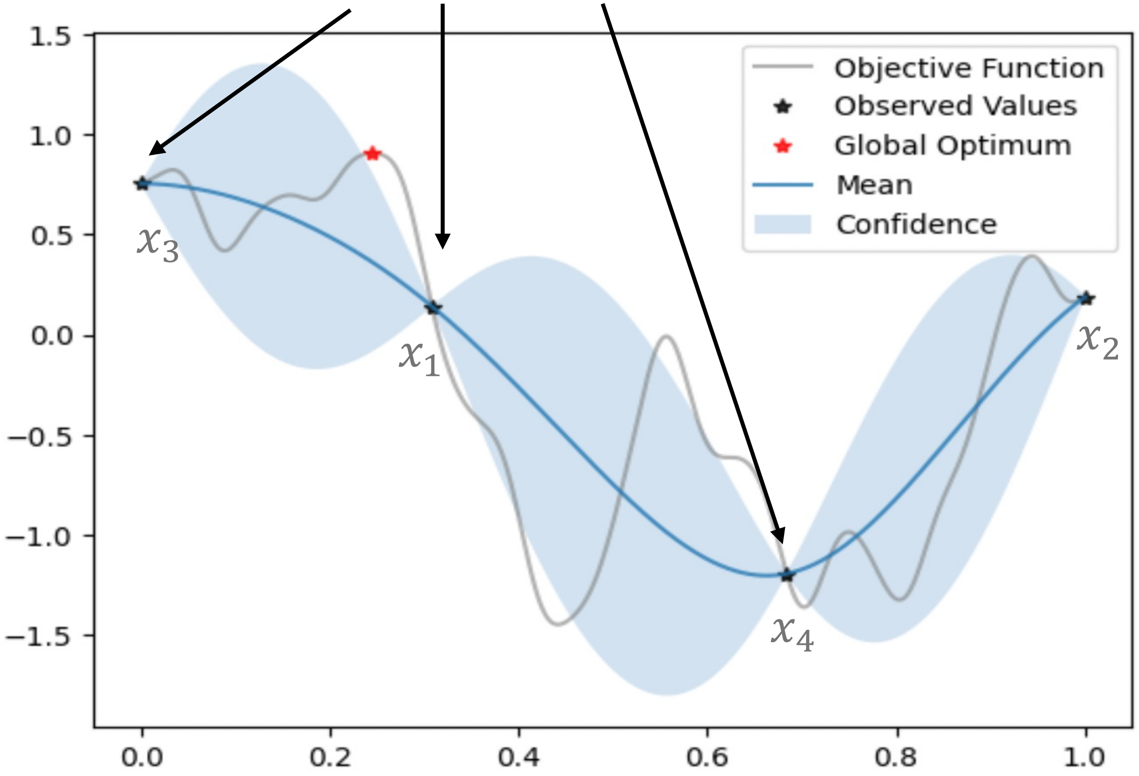


Continuous search domain

Evaluation costs handling

cheap	expensive
risk-seeking	risk-averse
exploration	exploitation

Why is it hard?

Hard budget constraint

~~$t = 1$~~

~~$t = 2$~~

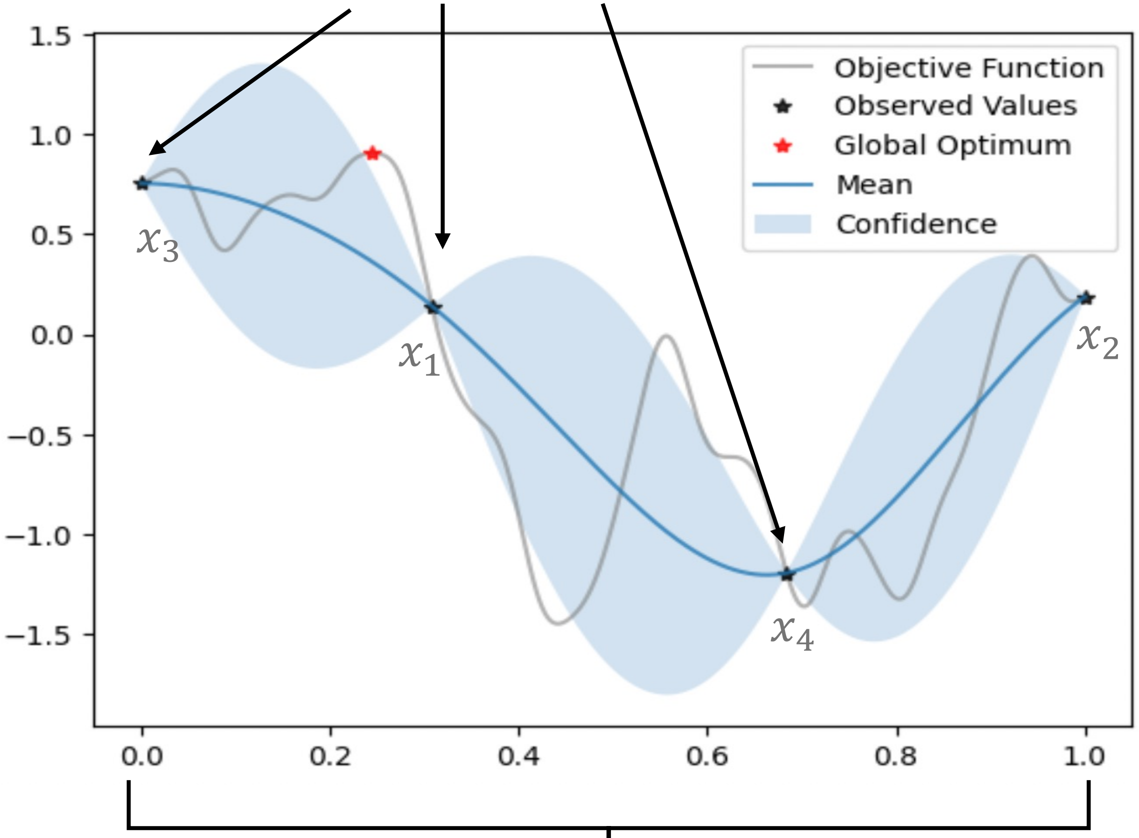
~~$t = 3$~~

~~$t = 4$~~

$\vdots$

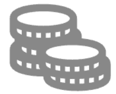
$t = T$

Correlated values



Continuous search domain

Evaluation costs handling



cheap

expensive

risk-seeking

risk-averse

exploration

exploitation

uniform

heterogeneous

Why is it hard?

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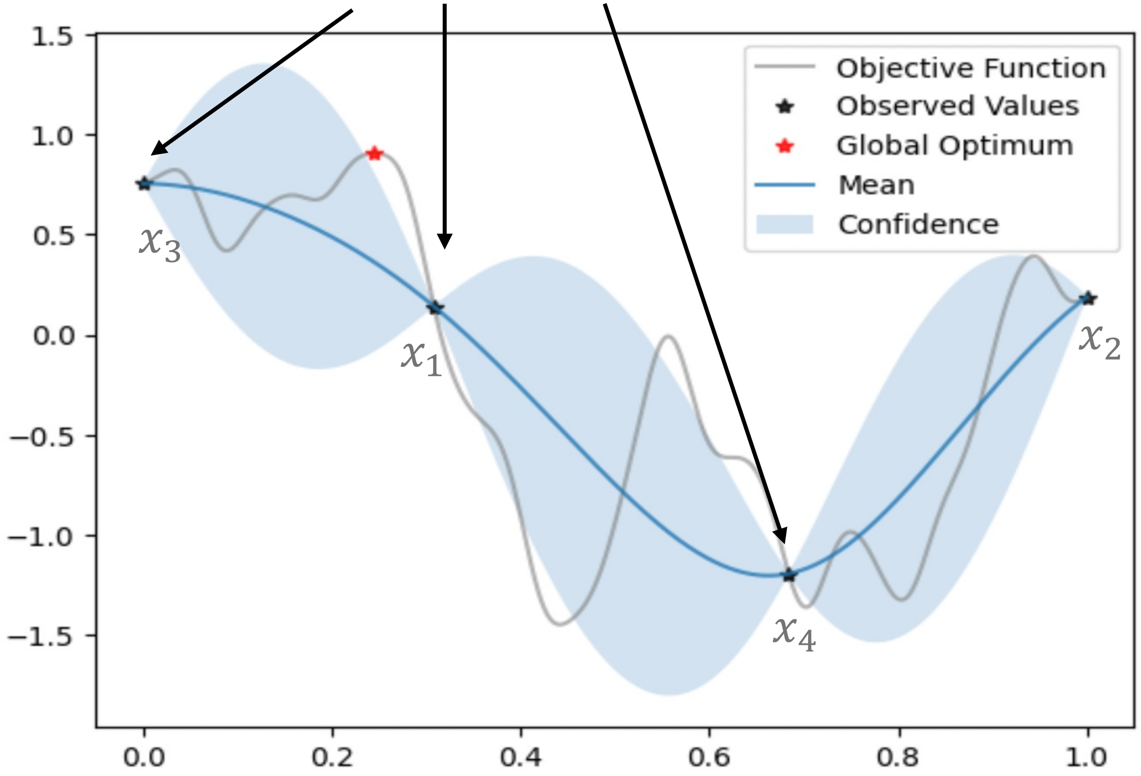
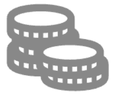
Correlated values



Continuous search domain

Evaluation costs handling



cheap | expensive

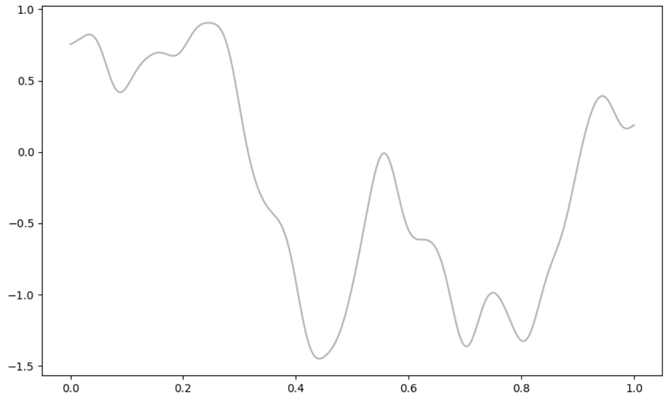
risk-seeking | risk-averse

exploration | exploitation

uniform | heterogeneous

$\Longrightarrow$ Optimal policy unknown!

Bayesian Optimization

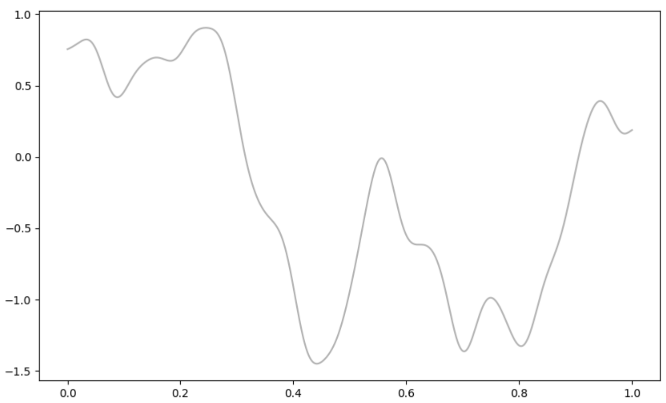


Continuous

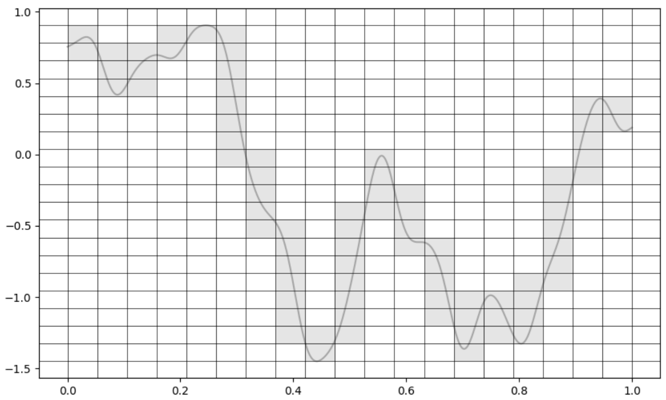
Correlated

Hard budget constraint

Bayesian Optimization



⟹

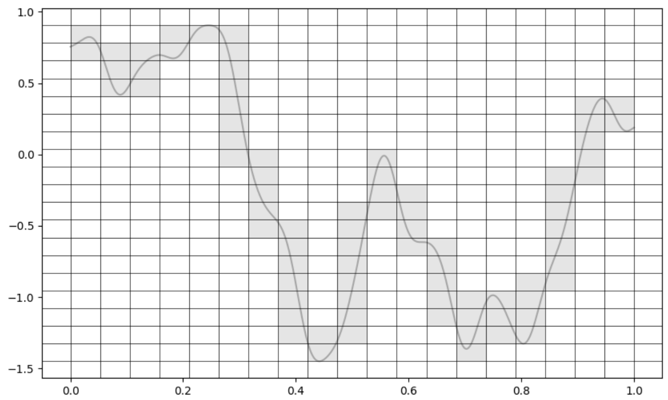


Continuous ⟹ Discrete

Correlated

Hard budget constraint

Bayesian Optimization

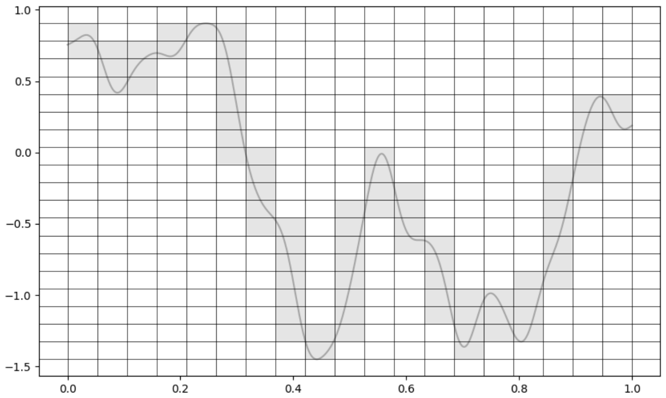


Continuous $\Longrightarrow$ Discrete

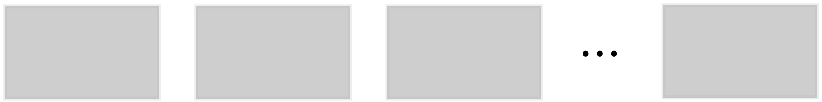
Correlated

Hard budget constraint

Bayesian Optimization



$\Longrightarrow$

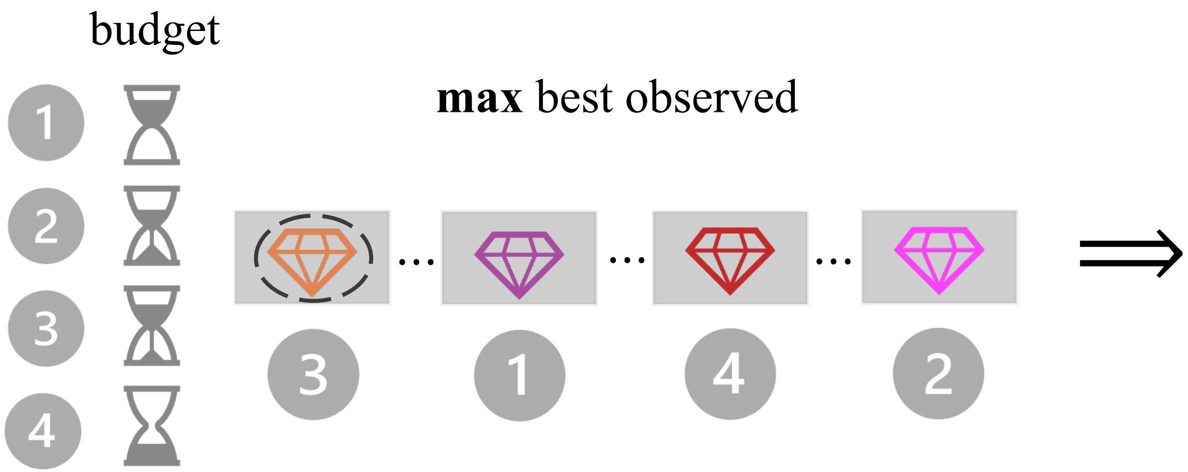


Continuous $\Longrightarrow$ Discrete

Correlated $\Longrightarrow$ Independent

Hard budget constraint

Bayesian Optimization

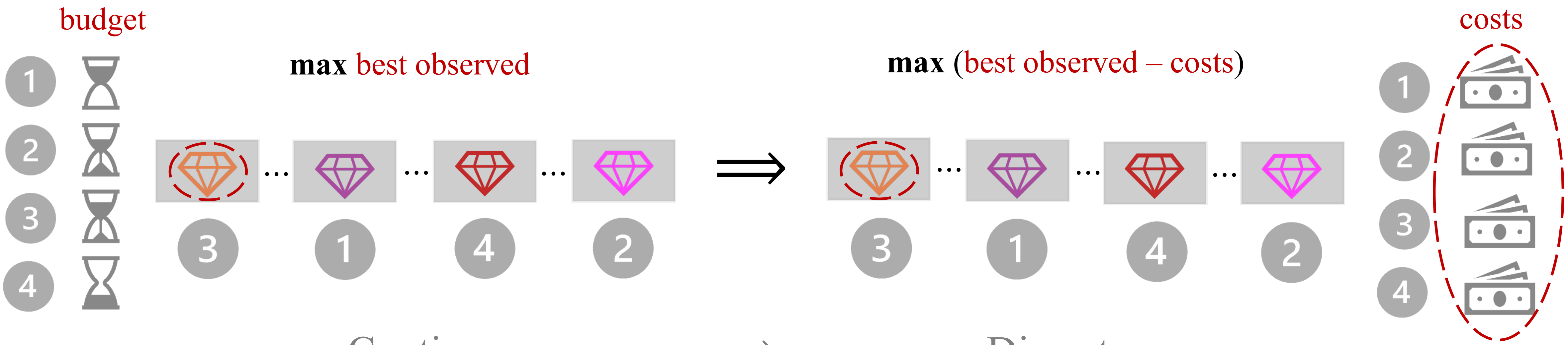


Continuous $\Longrightarrow$ Discrete

Correlated $\Longrightarrow$ Independent

Hard budget constraint

Bayesian Optimization



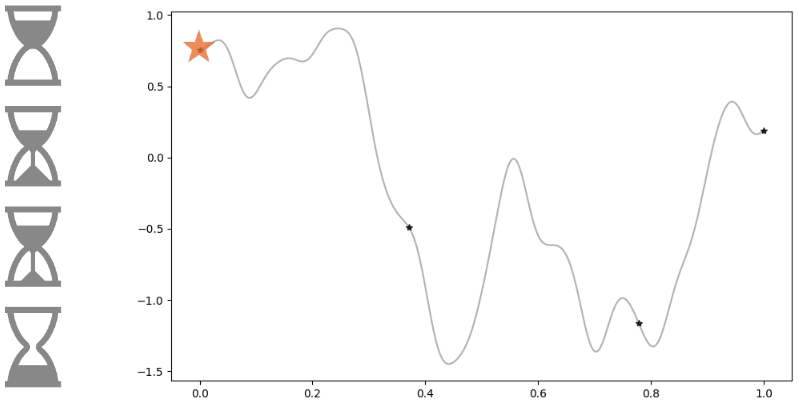
Continuous ⟹ Discrete

Correlated ⟹ Independent

Hard budget constraint $\overset{\text{Lagrangian relaxation}}{\Longrightarrow}$ Cost per sample

Bayesian Optimization ⟹ Pandora's Box

[Weitzman'79]



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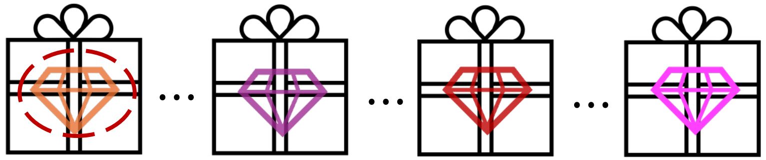
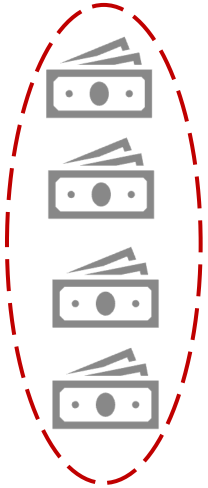
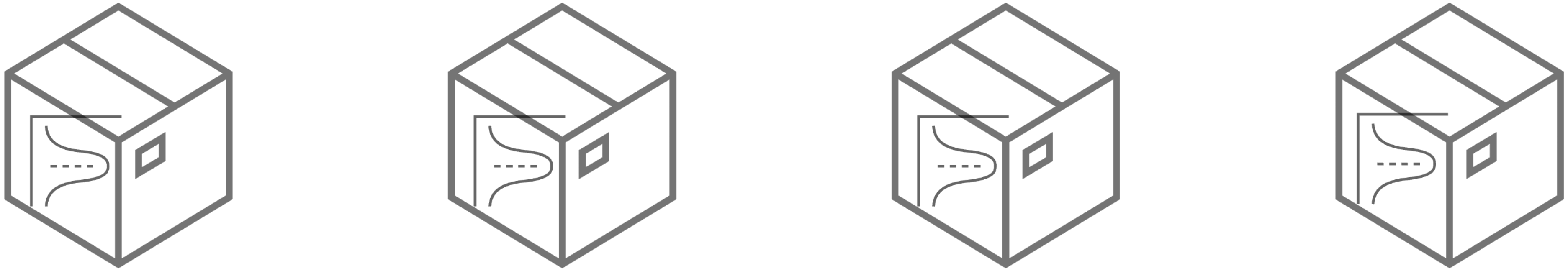




Continuous	⟹	Discrete
Correlated	⟹	Independent
Hard budget constraint	⟹	Cost per sample

Pandora’s Box

$t = 0$

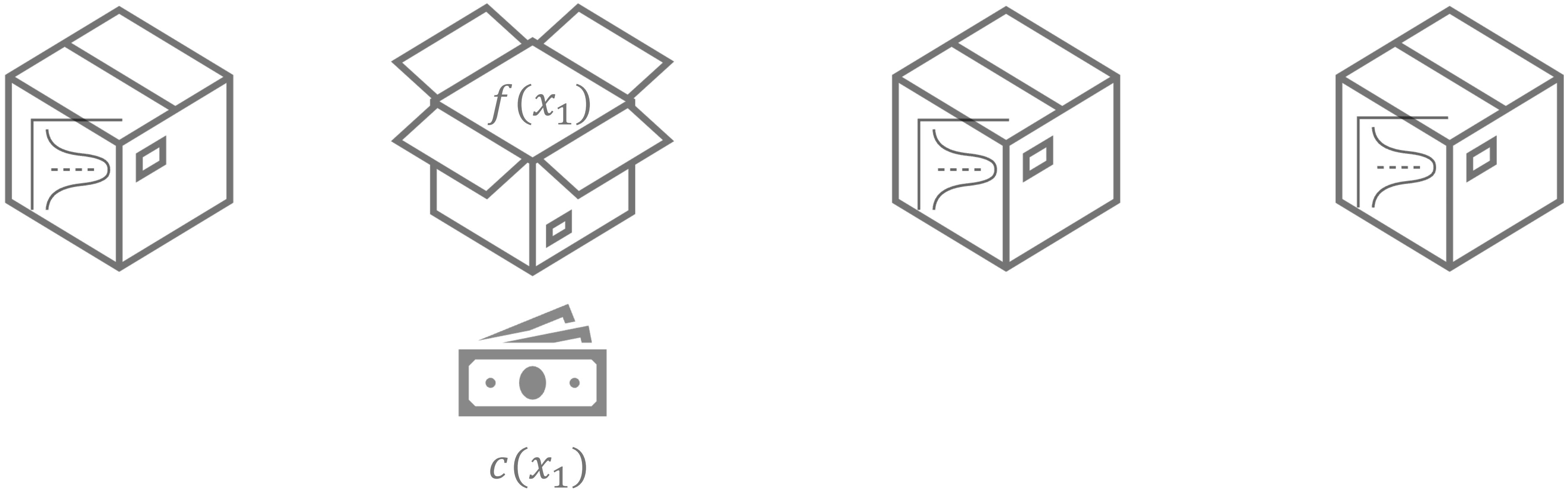


Objective: maximize net utility

Decision: adaptively evaluate a set of points

Pandora's Box

$t = 1$

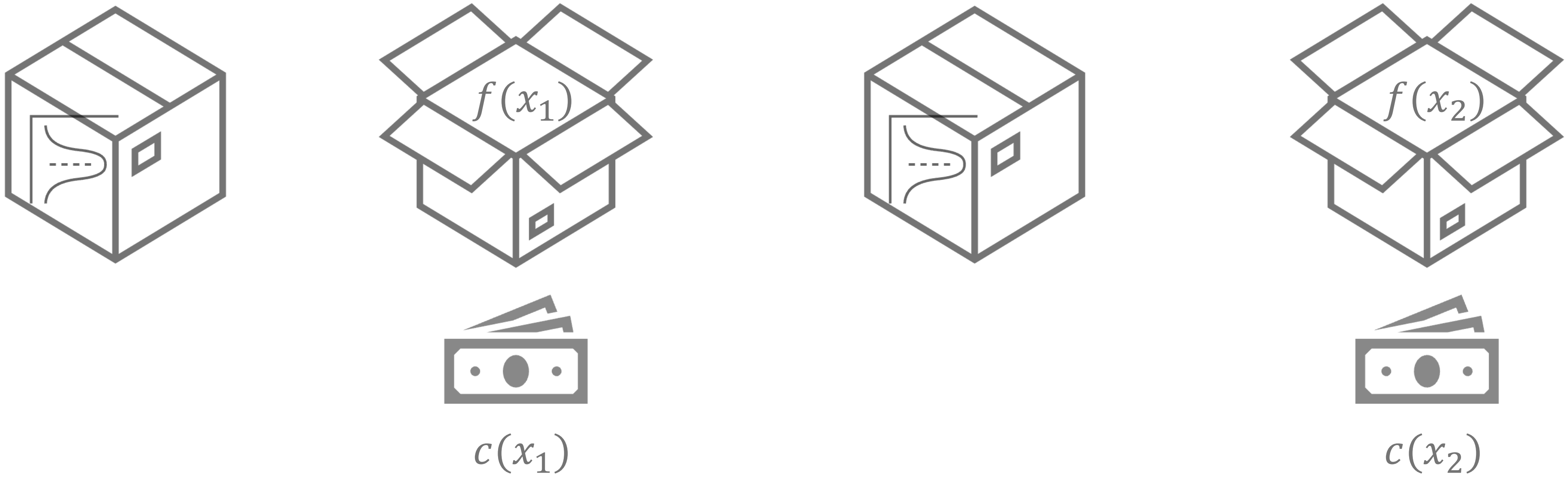


Objective: maximize net utility

Decision: adaptively evaluate a set of points

Pandora's Box

$t = 2$

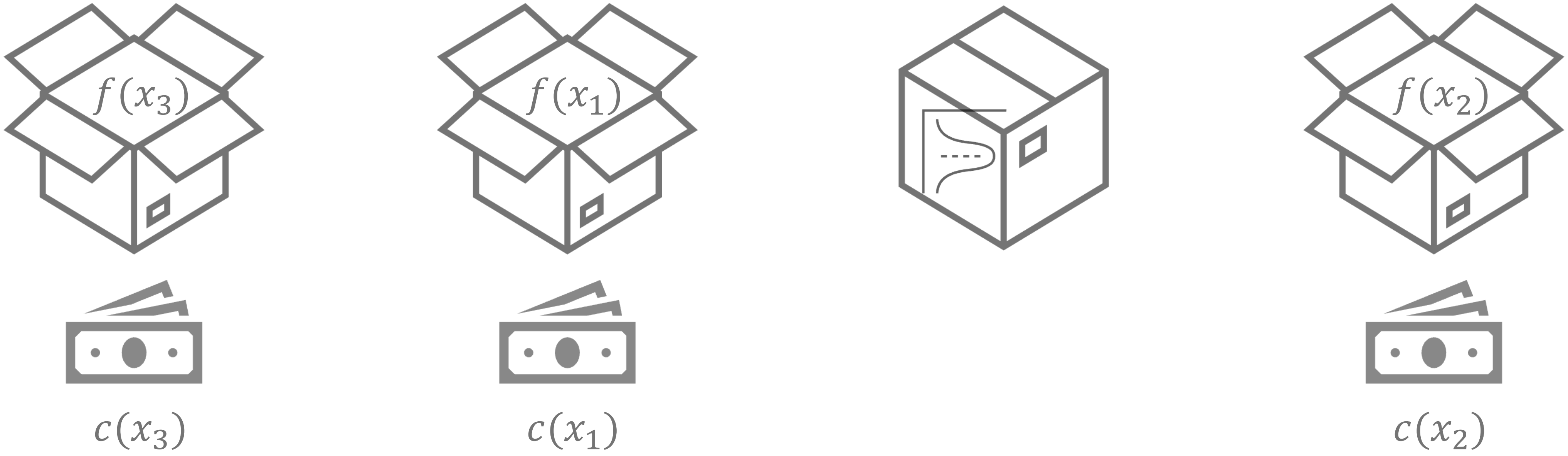


Objective: maximize net utility

Decision: adaptively evaluate a set of points

Pandora's Box

$t = 3$

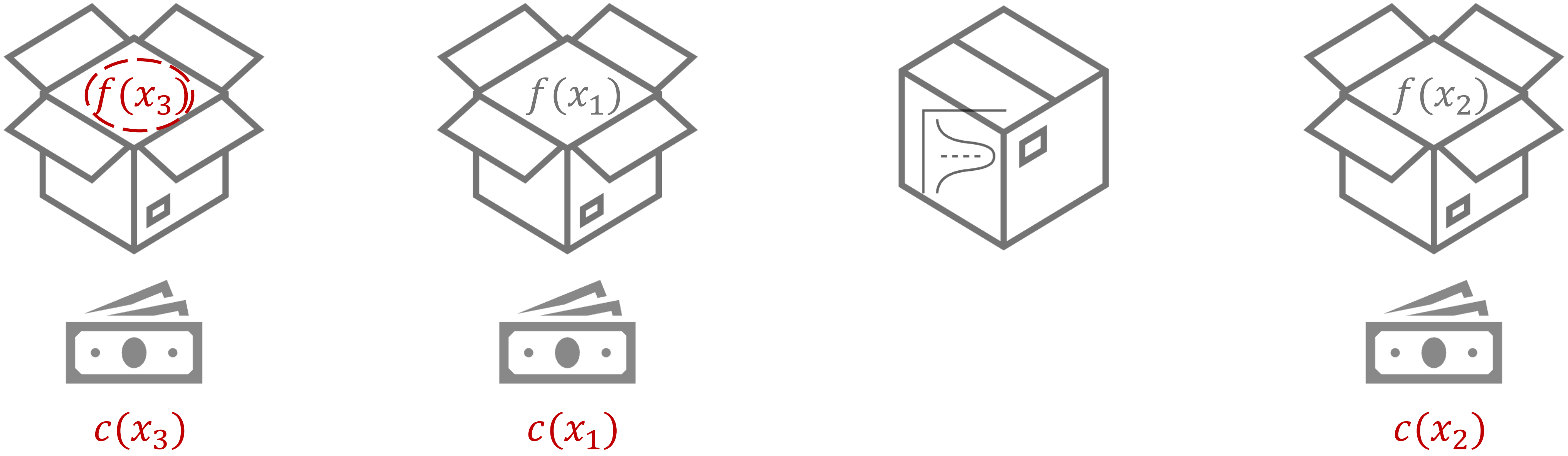


Objective: maximize net utility

Decision: adaptively evaluate a set of points

Pandora's Box

$t = 3$



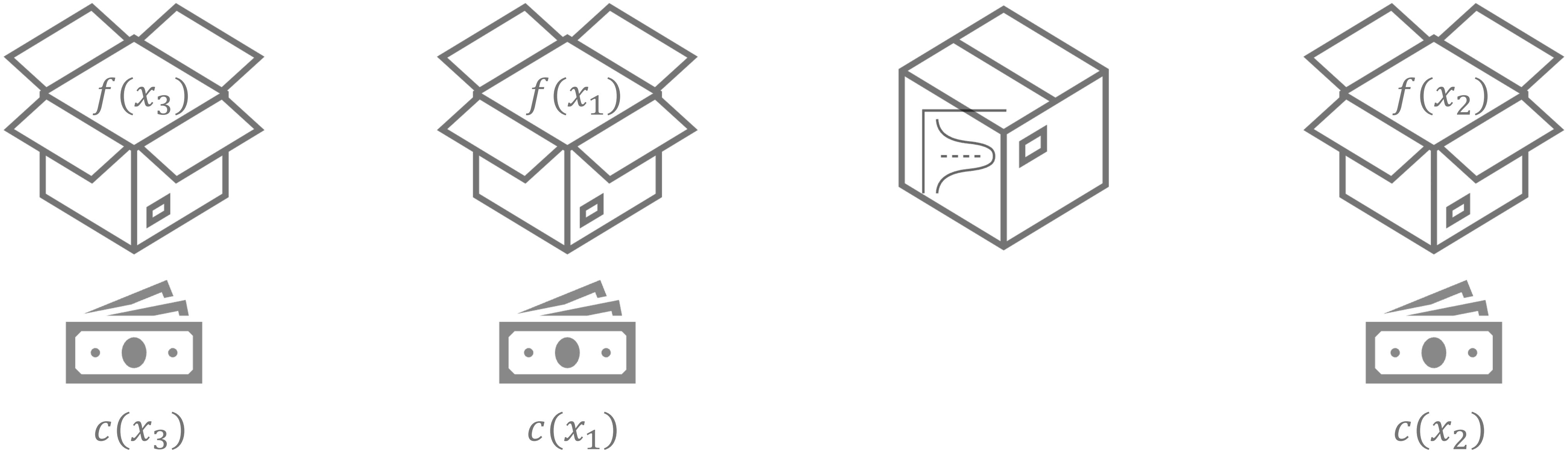
Objective: maximize net utility

max (best observed value – total costs)

Decision: adaptively evaluate a set of points

Pandora's Box

$t = 3$



Objective: maximize net utility

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

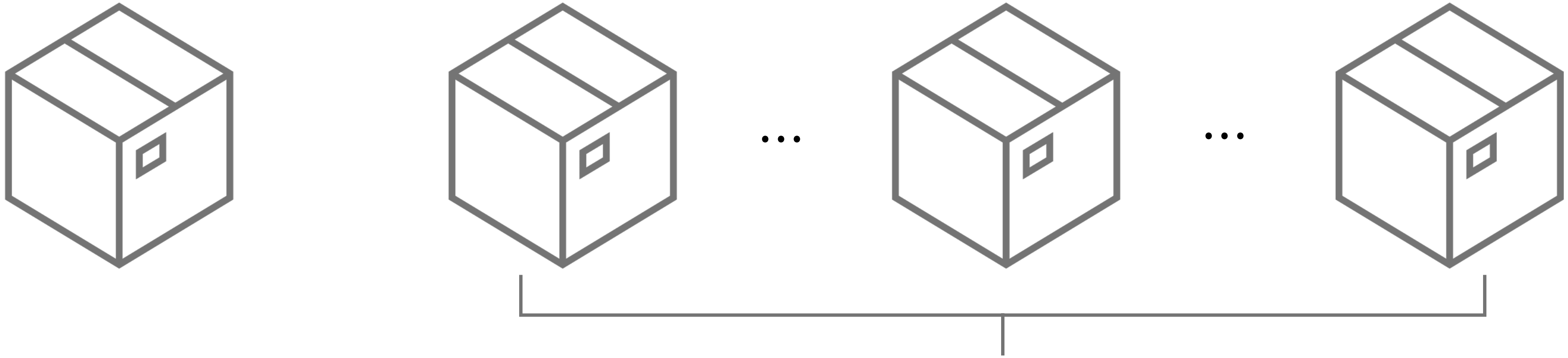
Decision: adaptively evaluate a set of points

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

$\mathcal{X}$: discrete

T: random stopping time

Greedy policy can fail [Singla'18]



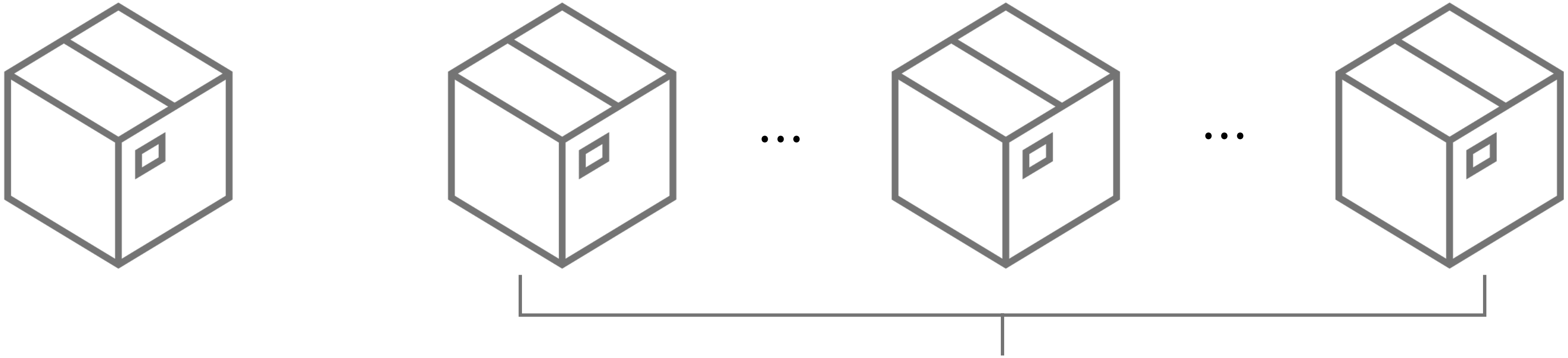
$f(1) = 200 \text{ w.p. } 1$

$c(1) = 198$

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

Greedy policy can fail [Singla'18]

Greedy policy



$f(1) = 200$ 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: $\operatorname{argmax}_x \left(\mathrm{EI}_f(x; y_{\text{best}}) - c(x)\right)$
expected improvement - cost

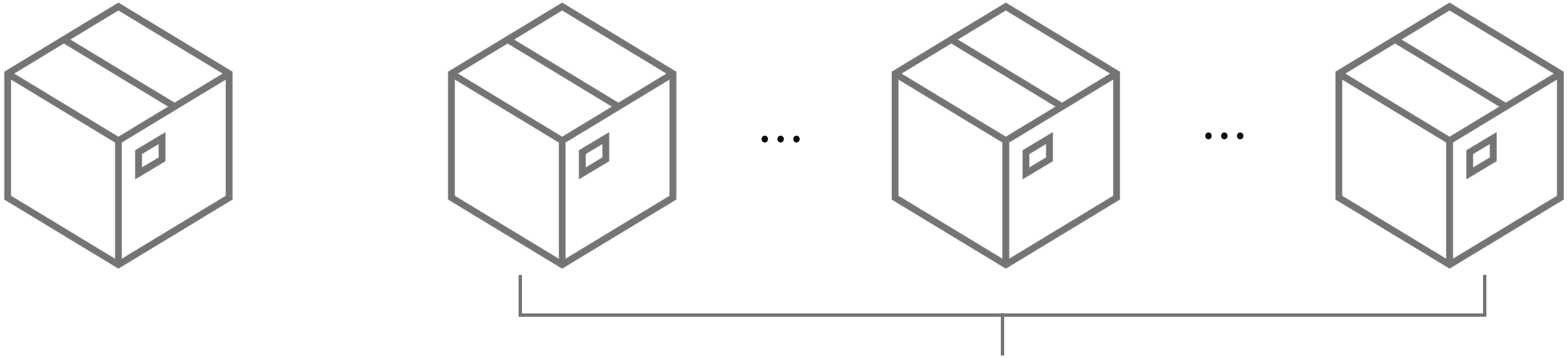
Stopping rule: $\mathrm{EI}_f(x; y_{\text{best}}) \le c(x), \forall x \in \mathcal{X}$
expected improvement $\le$ cost

y_{best}: current best observed value
$\mathrm{EI}_f(x; y) = \mathbb{E}[(f(x) - y)^+]$

Greedy policy can fail [Singla'18]

$t = 0$

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



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

$c(1) = 198$

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

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

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

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

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

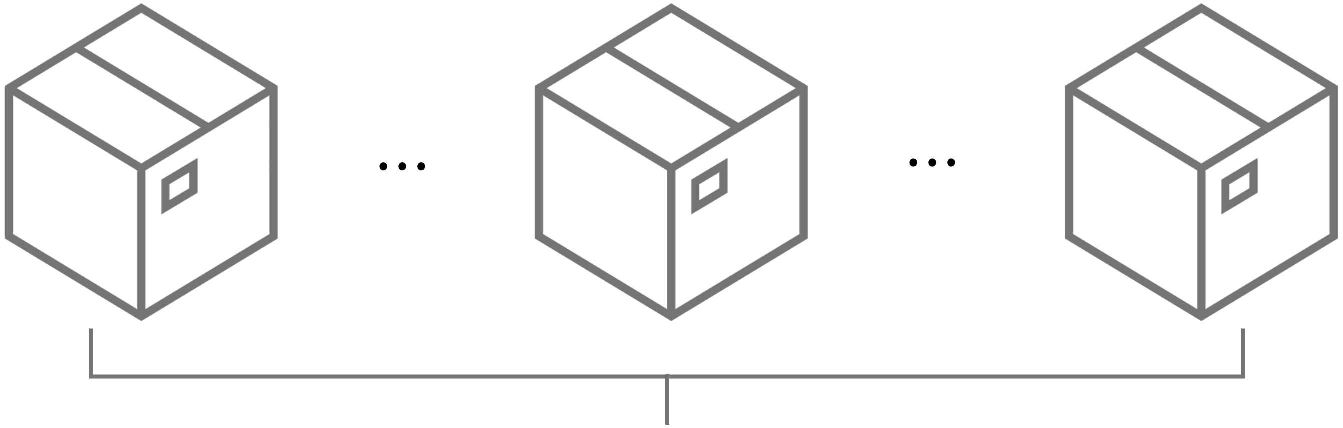
Greedy policy can fail [Singla'18]

$t = 1$

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

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

$c(1) = 198$



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

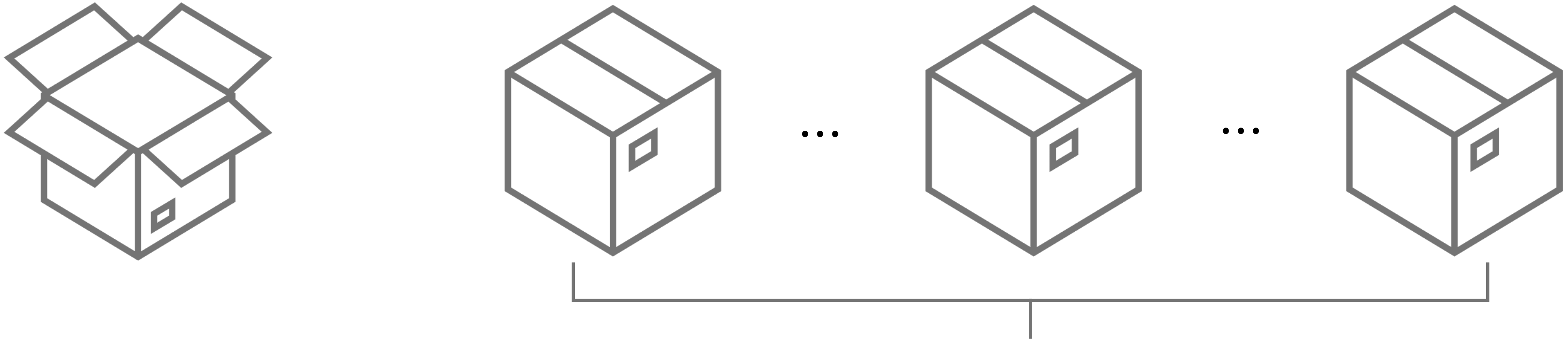
$\mathrm{EI}_f(x; 200) - c(x)$
$= 0 - 1 = -1 < 0$

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

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

Greedy policy can fail [Singla'18]

$t = 1$



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

$c(1) = 198$

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

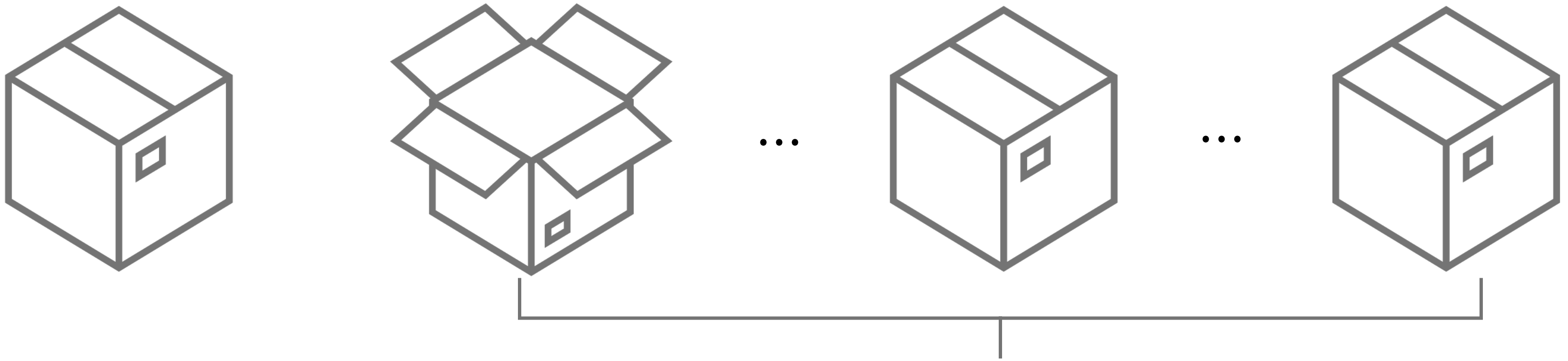
Inspection rule: $\mathrm{argmax}_x \left(\mathrm{EI}_f(x; y_{\mathrm{best}}) - c(x)\right)$ **Stopping rule:** $\mathrm{EI}_f(x; y_{\mathrm{best}}) \leq c(x), \forall x \in \mathcal{X}$

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

Greedy policy can fail [Singla'18]

$t \approx 100$

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



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

$c(1) = 198$

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

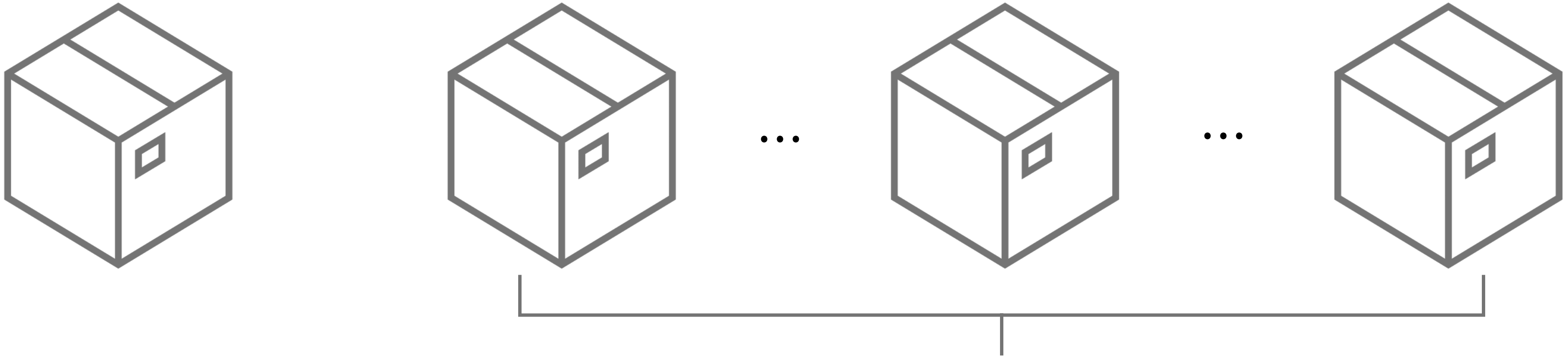
Inspection rule: $x \in \{2, 3, \ldots, 1000\}$

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

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

Optimal policy: Gittins policy

Gittins policy



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

$c(1) = 198$

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

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

solution to expected improvement = cost

Stopping rule: $\alpha^*(x) \le y_{\text{best}}, \forall x \in \mathcal{X}$

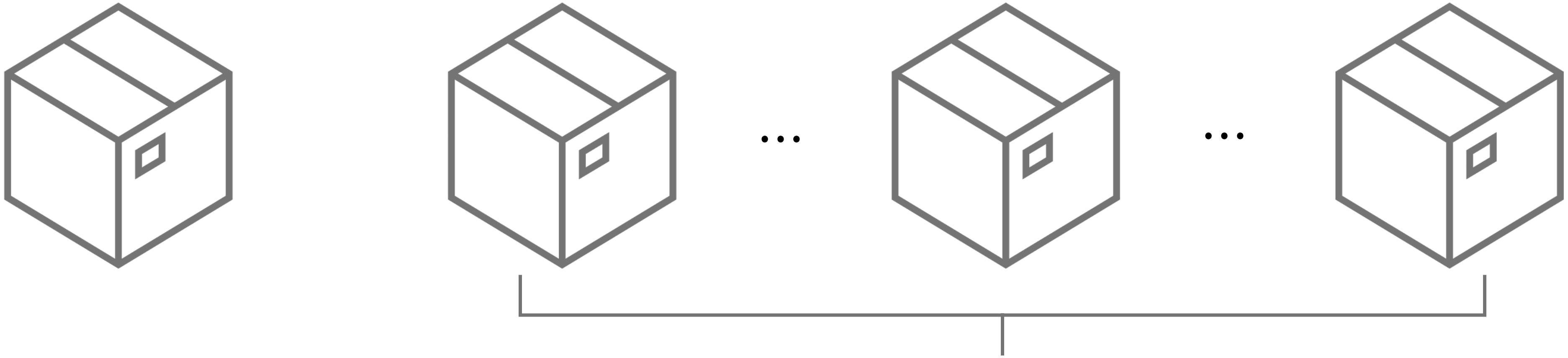
Gittins index $\le$ current best

y_{best}: current best observed value

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

Optimal policy: Gittins policy

$t = 0$



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

$c(1) = 198$

$\alpha^*(1) = 2$

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

$\alpha^*(x) = 100$

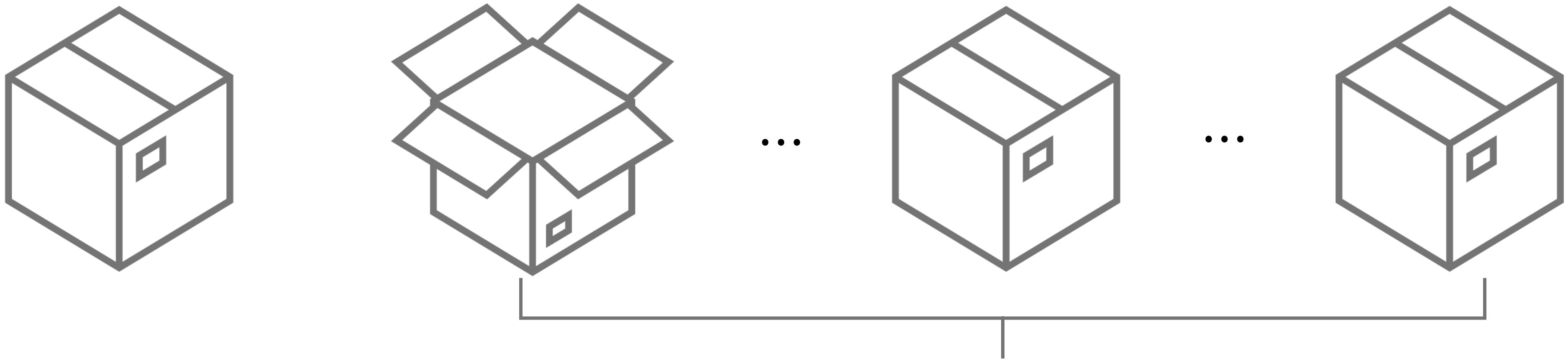
Inspection rule: $\text{argmax}_x\, \alpha^*(x)$ s.t. $\text{EI}_f(x; \alpha^*(x)) = c(x)$ **Stopping rule:** $\alpha^*(x) \le y_{\text{best}}, \forall x \in \mathcal{X}$

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

Optimal policy: Gittins policy

$t = 1$

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



$f(1) = 200$ w. p. 1

$c(1) = 198$

$\alpha^*(1) = 2$

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

$\alpha^*(x) = 100$

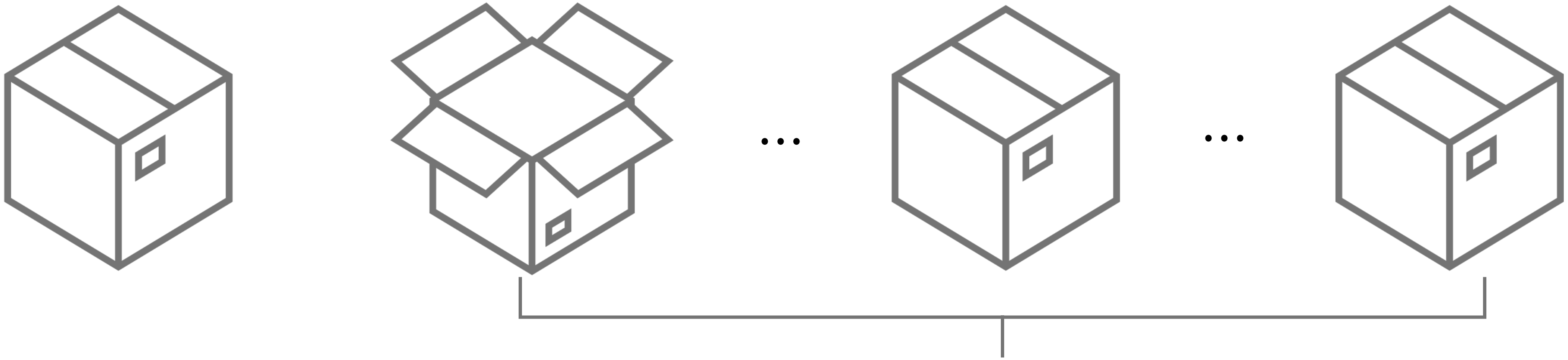
Inspection rule: $\text{argmax}_x\ \alpha^*(x)$ s.t. $\text{EI}_f(x; \alpha^*(x)) = c(x)$ **Stopping rule:** $\alpha^*(x) \leq y_{\text{best}}, \forall x \in \mathcal{X}$

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

Optimal policy: Gittins policy

$t \approx 100$

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



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

$c(1) = 198$

$\alpha^*(1) = 2$

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

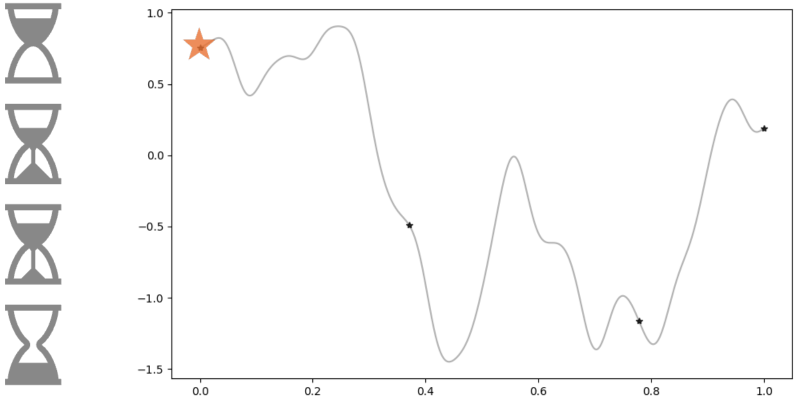
$\alpha^*(x) = 100$

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

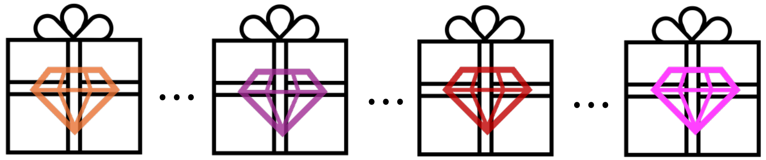
Expected utility: $\mathbb{E}[\text{Gittins}] = 200 - 100 * 1 = 100$

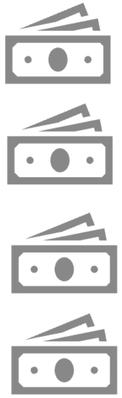
Bayesian Optimization ⟹ Pandora's Box

Special case of Markovian/
Bayesian multi-armed bandits



⟹

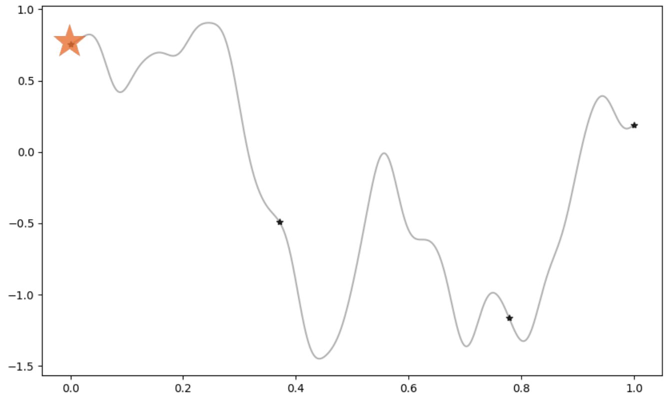




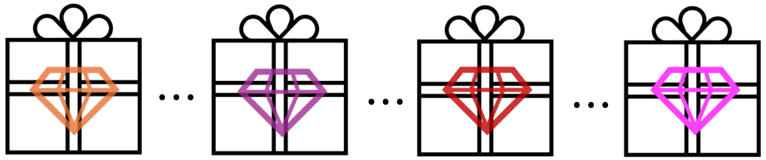
Continuous	⟹	Discrete
Correlated	⟹	Independent
Hard budget constraint	⟹	Cost per sample

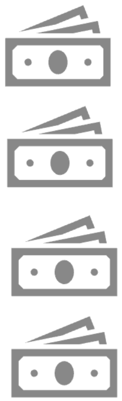
Optimal policy: Gittins index [Weitzman'79]

Bayesian Optimization $\Longrightarrow$ Pandora's Box



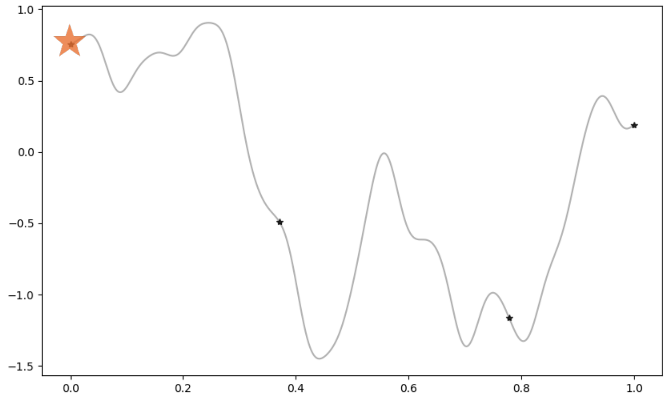
$\Longrightarrow$



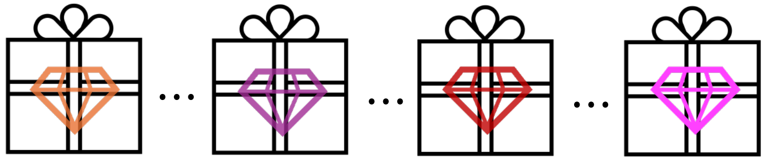


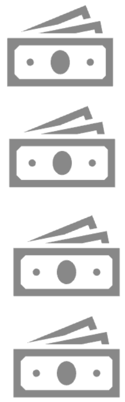
Continuous	$\Longrightarrow$	Discrete
Correlated	$\Longrightarrow$	Independent
Hard budget constraint	$\Longrightarrow$	Cost per sample
Is Gittins index good?	$\Longleftarrow$	Optimal policy: Gittins index

Bayesian Optimization $\Longrightarrow$ Pandora's Box



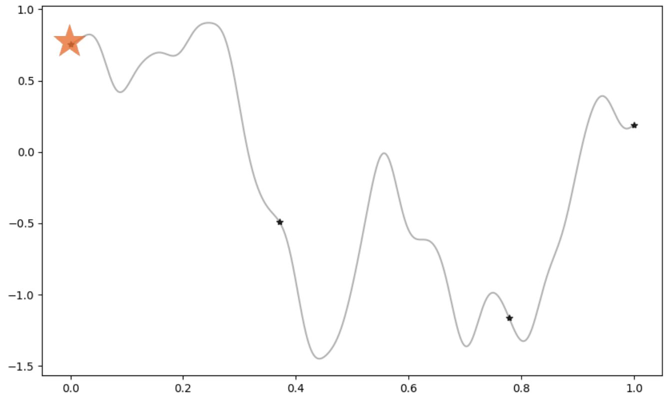
$\Longrightarrow$



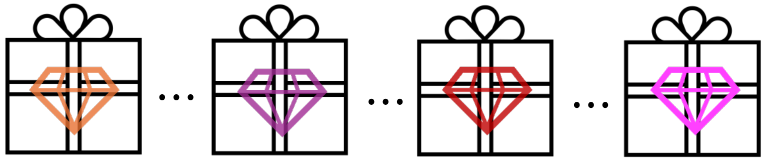


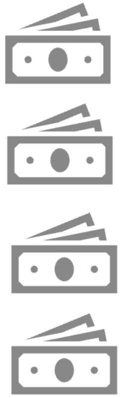
Continuous	$\Longrightarrow$	Discrete
Correlated	$\Longrightarrow$	Independent
Hard budget constraint	$\Longrightarrow$	Cost per sample
Is Gittins index good?	How to translate? $\Longleftarrow$	Optimal policy: Gittins index

Bayesian Optimization $\Longrightarrow$ Pandora's Box



$\Longrightarrow$





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

max best observed
s.t. budget constraint

Pandora's box

costs

max (best observed – costs)

Expected budget constraint $\Longleftrightarrow$ Cost per sample

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

Expected budget constraint $\Longleftrightarrow$ Cost per sample

budget

max best observed
s.t. budget constraint

Pandora's box

scaled costs

max (best observed – λ_B^* costs))

λ_B^*: budget-dependent scaling factor

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

Expected budget constraint $\Longleftrightarrow$ Cost per sample

max best observed
s.t. budget constraint

Pandora's box

max (best observed – λ_B^* costs))

λ_B^*: budget-dependent scaling factor

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

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

Expected budget constraint ⟺ Cost per sample

Constrained

budget

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

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

Lagrangian relaxation

$\Longleftrightarrow$

Unconstrained

costs

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

λ: Lagrange multiplier

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

Extension to [Aminian et al.'24]

Expected budget constraint $\Longleftrightarrow$ Cost per sample

Constrained

budget

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

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

Lagrangian relaxation

$\Longleftrightarrow$

Lagrange multiplier theorem

$\Longleftrightarrow$

Unconstrained

costs

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

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

Extension to [Aminian et al.'24]

Expected budget constraint $\Longleftrightarrow$ Cost per sample

Constrained

budget

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

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

Unconstrained

costs

Lagrangian relaxation

$\Longleftrightarrow$

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

Lagrange multiplier theorem

$\Longleftrightarrow$

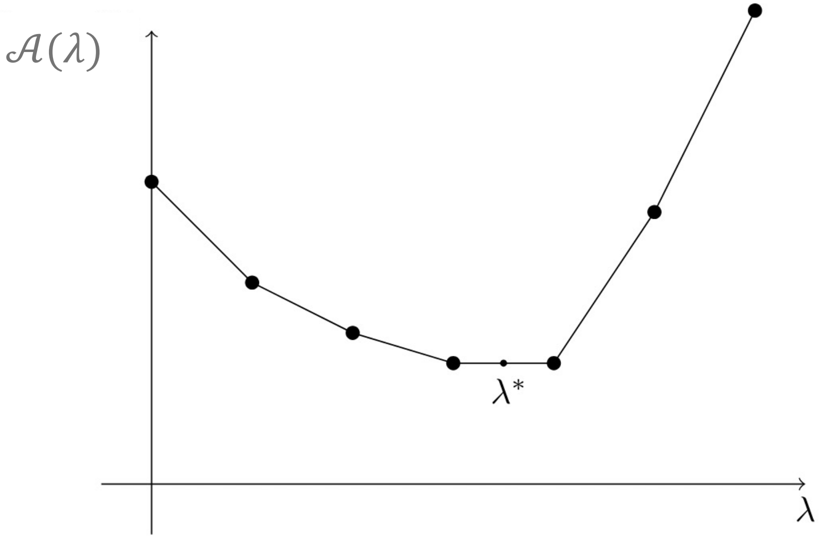
$$\inf_{\lambda \ge 0} \sup_{\text{policy}} \underbrace{\mathbb{E}\left(\max_{t=1,2,\dots,T} f(x_t) + \lambda \left(B - \mathbb{E} \sum_{t=1}^{T} c(x_t) \right) \right)}_{\mathcal{A}(\lambda)}$$

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

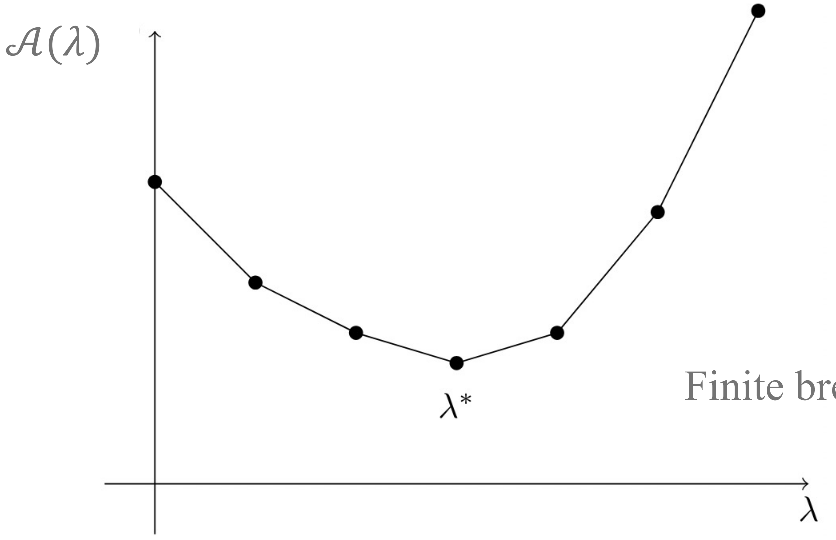
Optimal policy: Gittins solution to Pandora's box with scaled costs $\Longleftarrow$ Optimal policy: Gittins index

Extension to [Aminian et al.'24]

Expected budget constraint $\Leftrightarrow$ Cost per sample



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



Finite breakpoints

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

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

Envelope Theorem

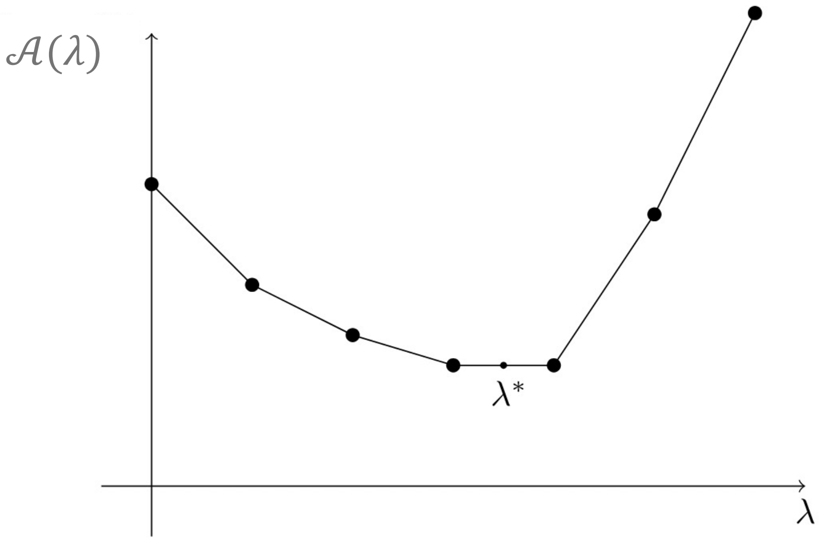
λ_B^*: nonzero infimum of $\mathcal{A}(\lambda)$ exists $\Longleftarrow$ $\mathcal{A}(\lambda)$: convex (possibly non-differentiable) in λ

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

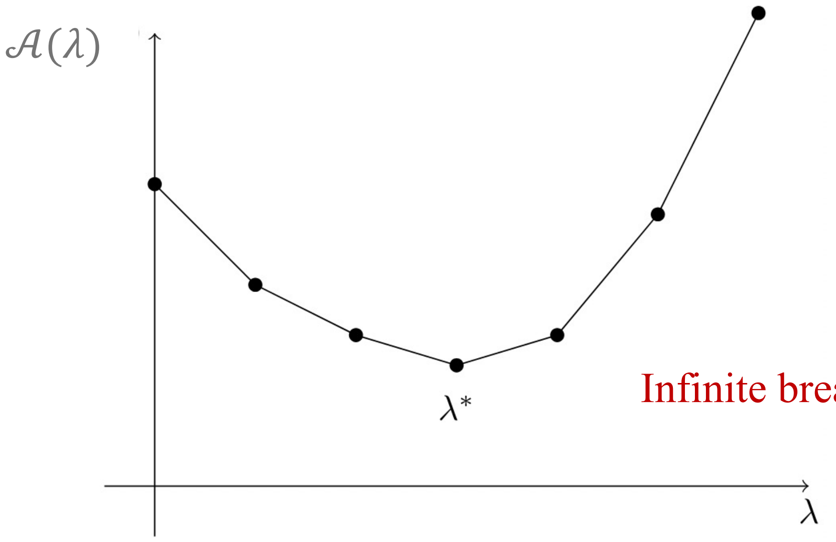
Extension to [Aminian et al.'24]

Figure from [Aminian et al.'24]

Expected budget constraint $\Longleftrightarrow$ Cost per sample



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



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

Infinite breakpoints?

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

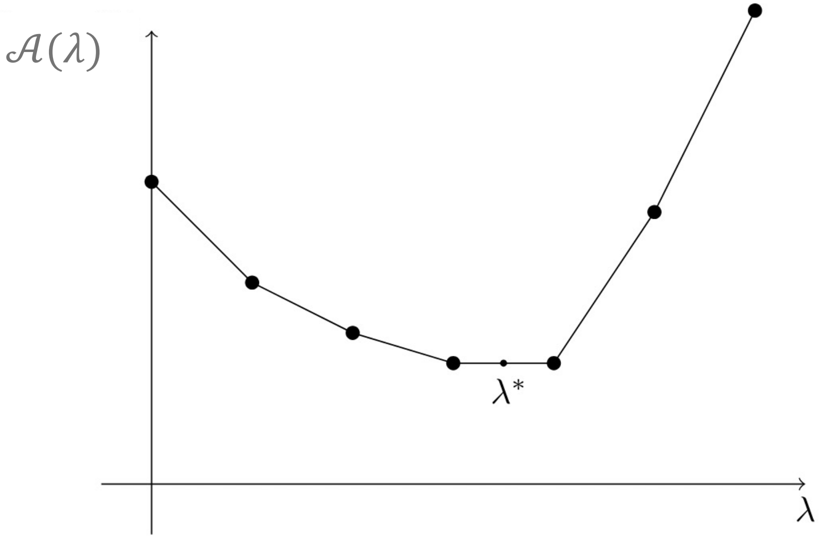
λ_B^*: nonzero infimum of $\mathcal{A}(\lambda)$ exists $\Longleftarrow$ $\mathcal{A}(\lambda)$: convex (possibly non-differentiable) in λ

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

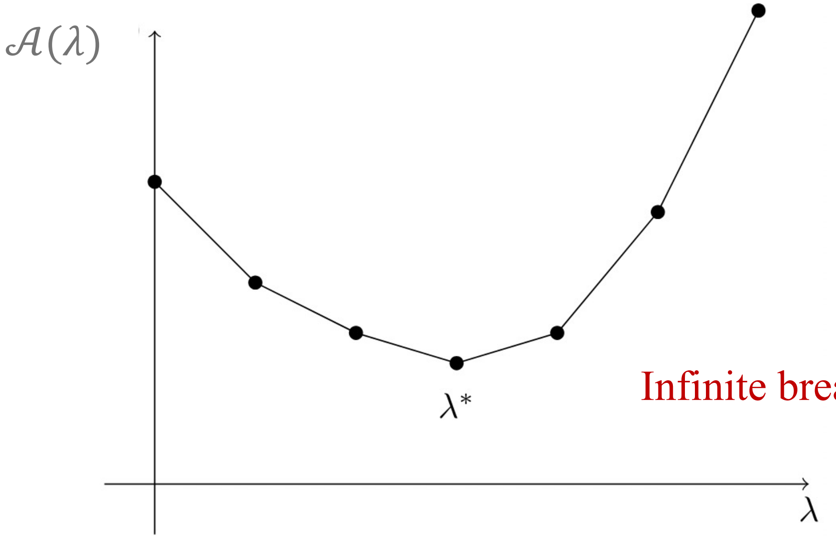
Extension to [Aminian et al.'24]

Figure from [Aminian et al.'24]

Expected budget constraint $\Longleftrightarrow$ Cost per sample



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



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

Infinite breakpoints?

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

sharp Envelope Theorem

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

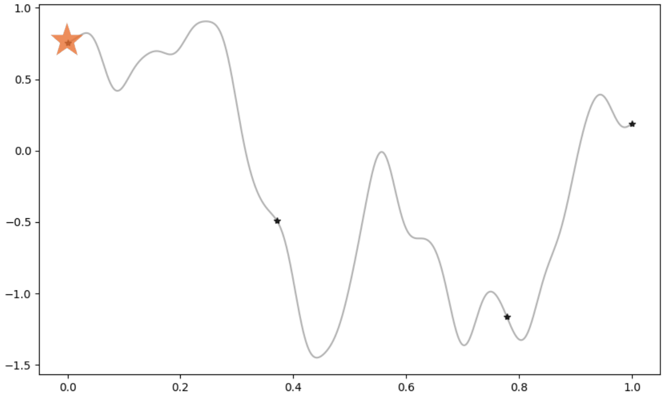
Optimal policy: Gittins solution to Pandora's box with scaled costs $\Longleftarrow$ Optimal policy: Gittins index

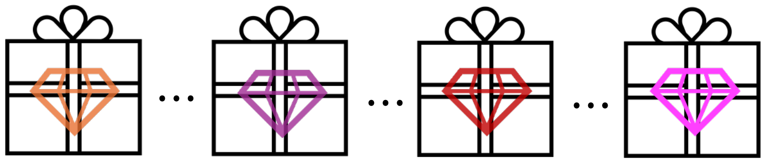
Extension to [Aminian et al.'24]

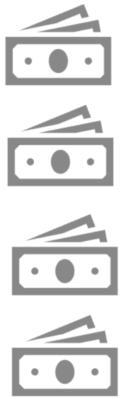
Figure from [Aminian et al.'24]

Our Contributions

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



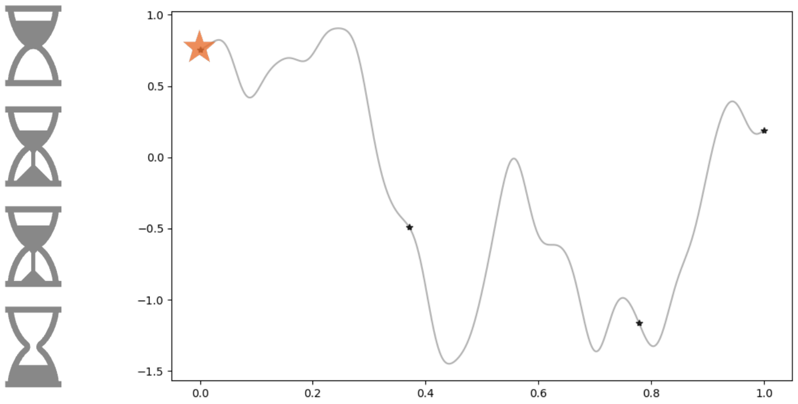


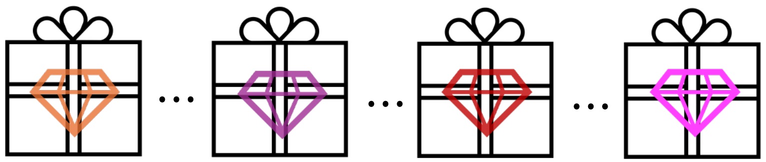


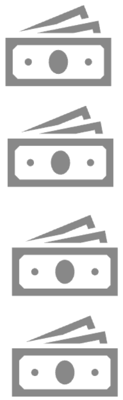
? $\Longleftarrow$ Pandora's Box Gittins index

Our Contributions

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



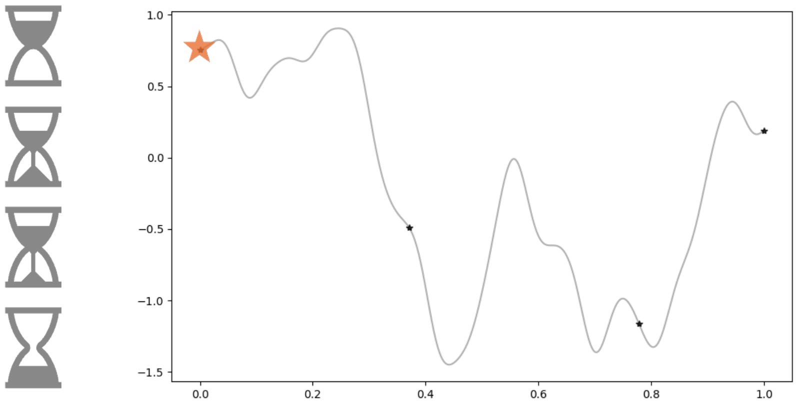


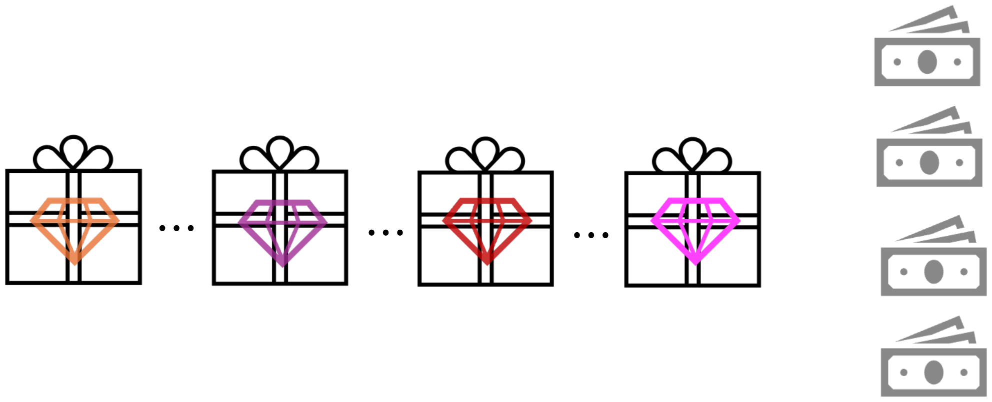


Our work $\Longleftarrow$ Pandora's Box Gittins index

Our Contributions

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

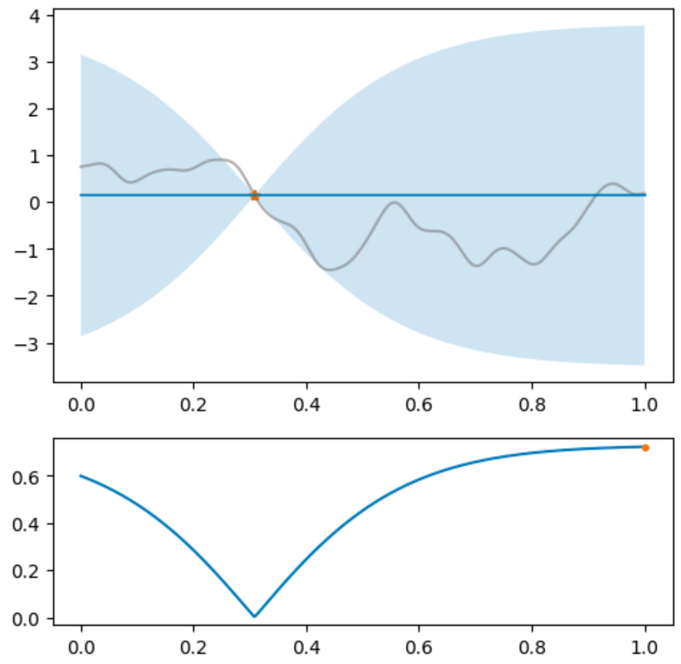




Our work $\Longleftarrow$ Pandora’s Box Gittins index

How is our PBGI policy different from baselines?

Popular One-step Heuristic: EI



mean: prediction

variance: confidence/uncertainty

Trade-off between
- exploitation (high mean) and
- exploration (high uncertainty)

Expected improvement

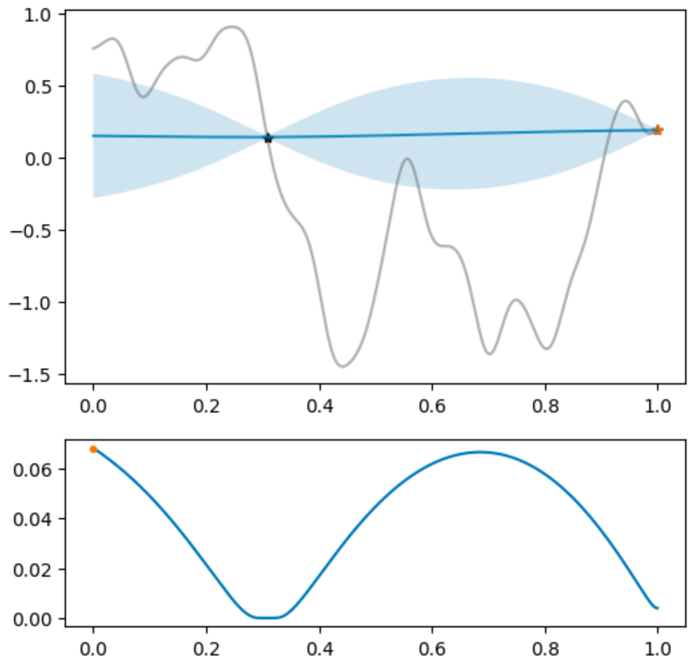
$$\mathrm{EI}_{f|D}(x; y) = \mathbb{E}[((f|D)(x) - y)^+]$$

D: observed data

y_{best}: current best observed value

EI policy: evaluate $\mathrm{argmax}_x \mathrm{EI}_{f|D}(x; y_{\mathrm{best}})$

Popular One-step Heuristic: EI



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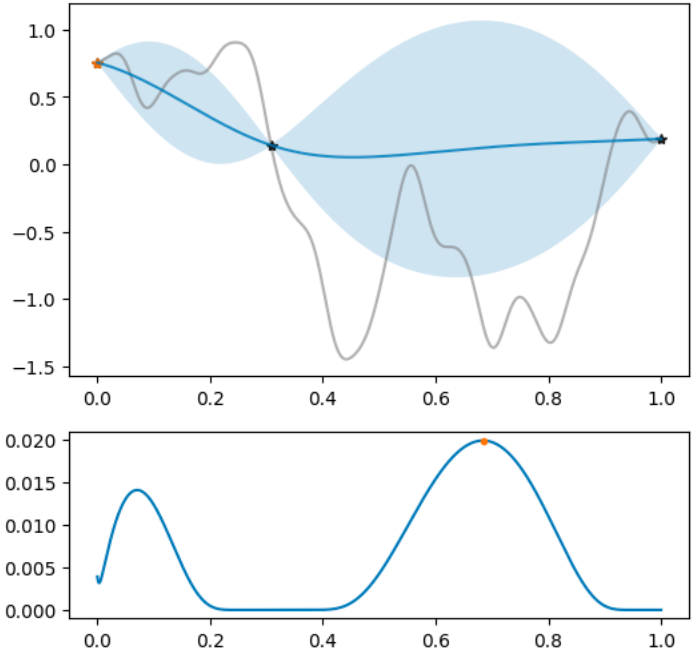
Popular One-step Heuristic: EI



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EI policy: evaluate $\text{argmax}_x \, \mathrm{EI}_{f|D}(x; y_{\text{best}})$

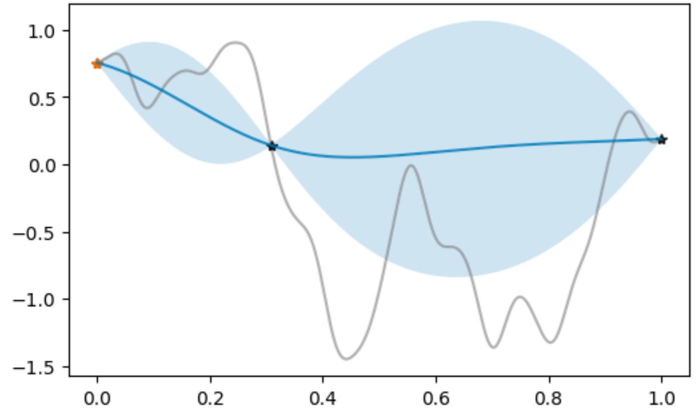
Popular One-step Heuristic: EI

Other heuristics:

simple

- Upper Confidence Bound
- Thompson Sampling (TS)
- Predictive Entropy Search
- Knowledge Gradient
- Multi-step Lookahead EI

slow



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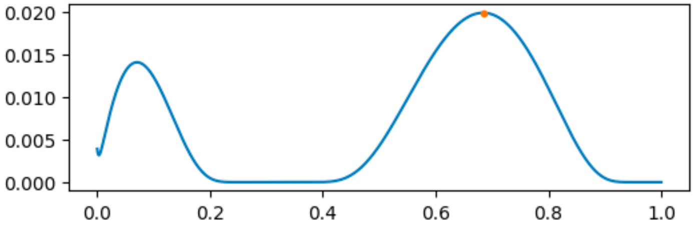

Trade-off between

- exploitation (high mean) and
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Expected improvement

$$\mathrm{EI}_{f|D}(x; y) = \mathbb{E}[((f|D)(x) - y)^+]$$

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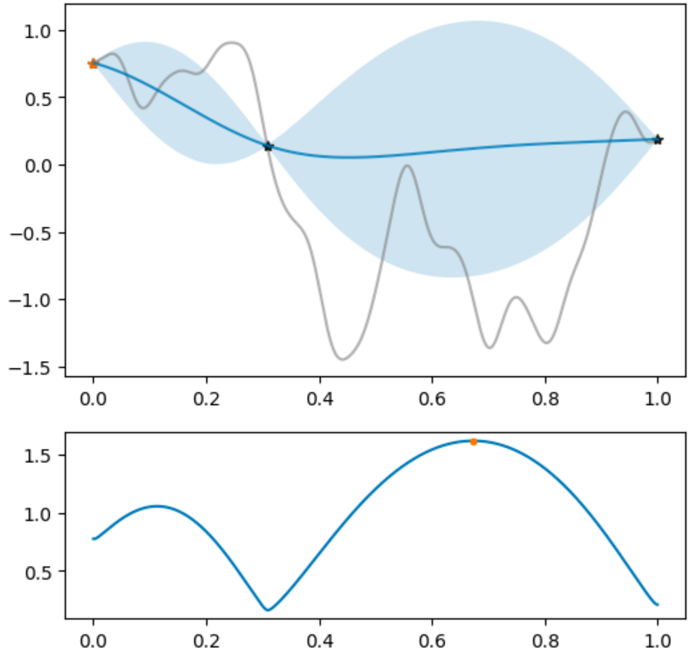
New One-step Heuristic: PBGI

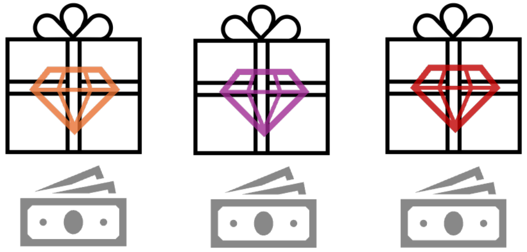
Other heuristics:

- Upper Confidence Bound
- Thompson Sampling (TS)
- Knowledge Gradient
- Predictive Entropy Search
- Multi-step Lookahead EI



Pandora's box Gittins index

Pandora's box



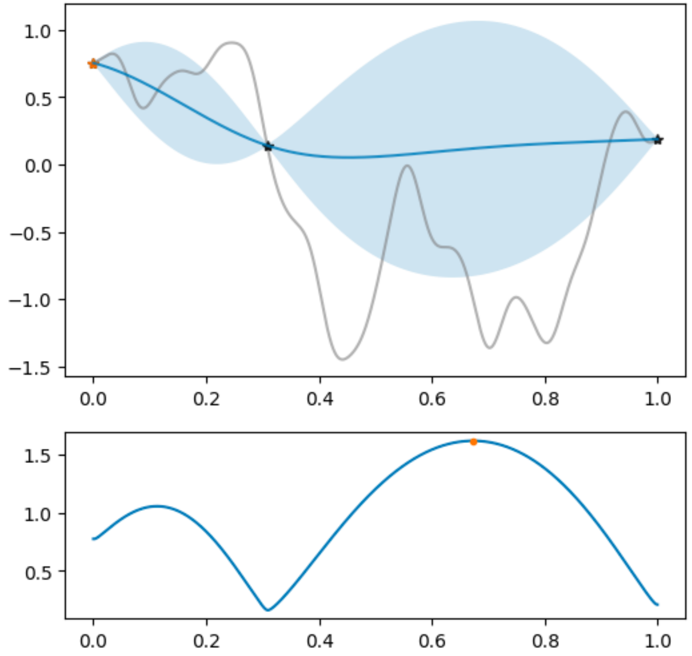
$\alpha^*(x)$: Gittins index function

PBGI policy: evaluate $\text{argmax}_x\, \alpha^*(x)$

New One-step Heuristic: PBGI

Other heuristics:

- Upper Confidence Bound
- Thompson Sampling (TS)
- Knowledge Gradient
- Predictive Entropy Search
- Multi-step Lookahead EI



Pandora's box

λ λ λ

λ: cost-per-sample
(Lagrange multiplier)

Pandora's box Gittins index

$\mathrm{EI}_{f|D}(x; y) = \mathbb{E}[((f|D)(x) - y)^+]$

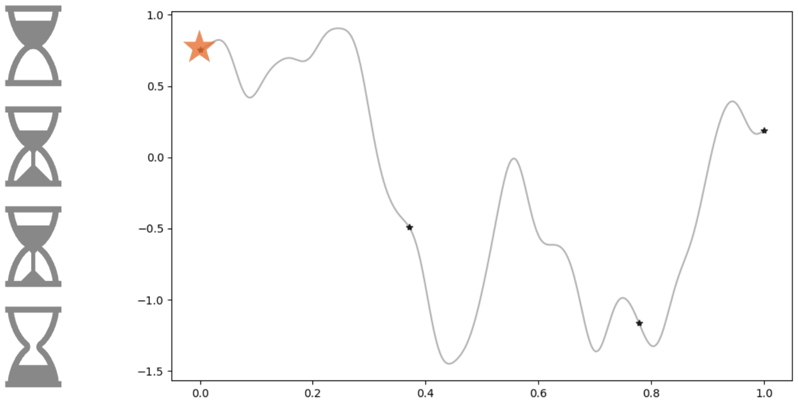
PBGI policy: evaluate $\mathrm{argmax}_x\ \alpha^*(x)$

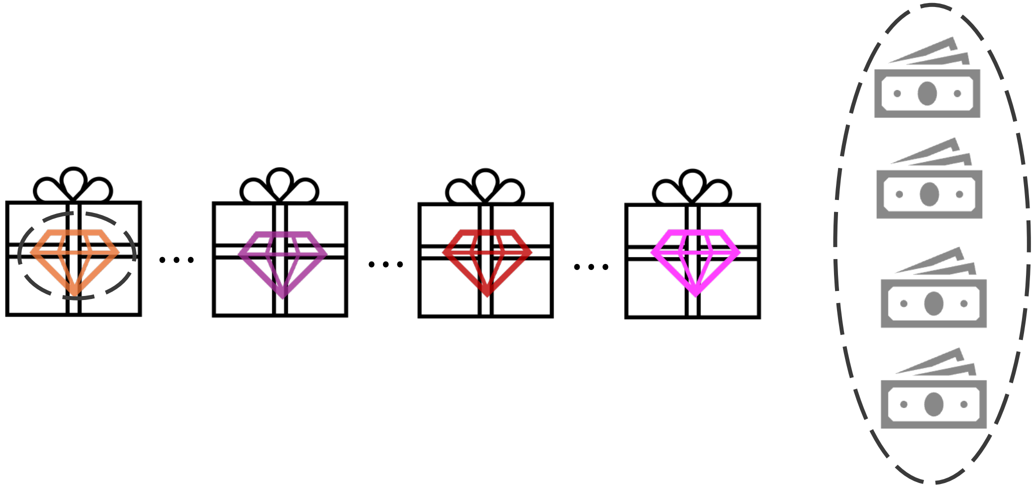
D: observed data

$\alpha^*(x)$: solution to $\mathrm{EI}_{f|D}(x; \alpha^*(x)) = \lambda$

Our Contributions

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





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

Our Contributions

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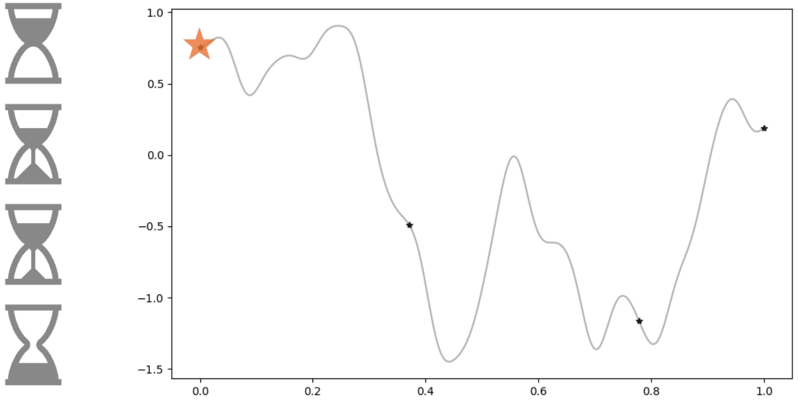
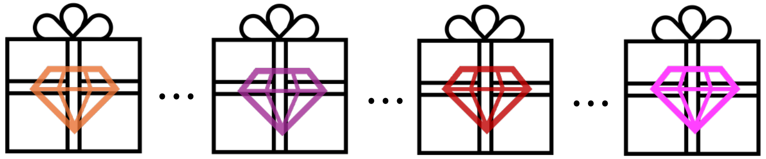
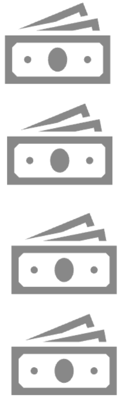
- Show performance against baselines on synthetic & empirical experiments







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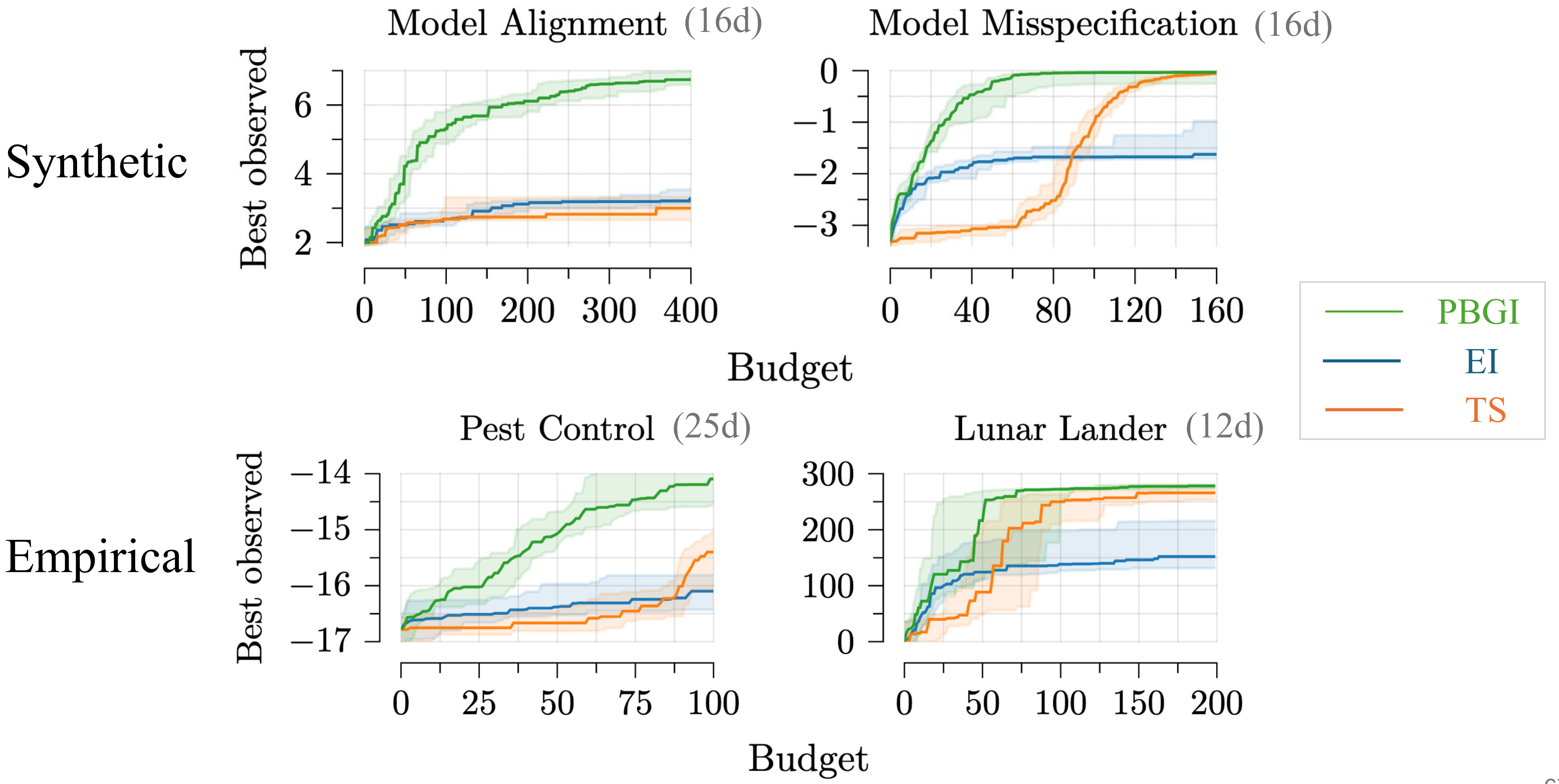
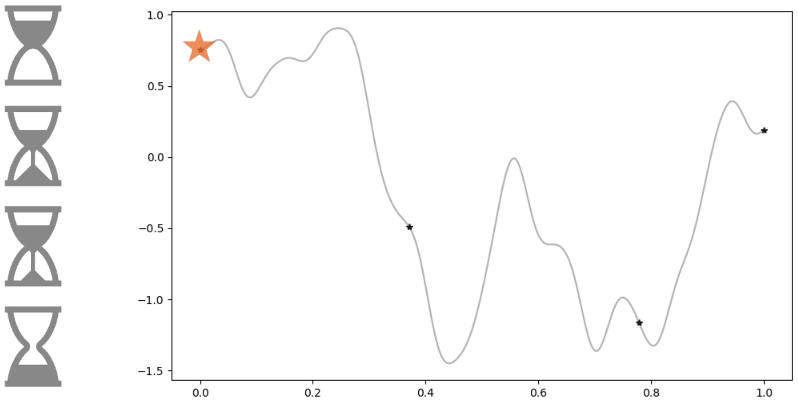
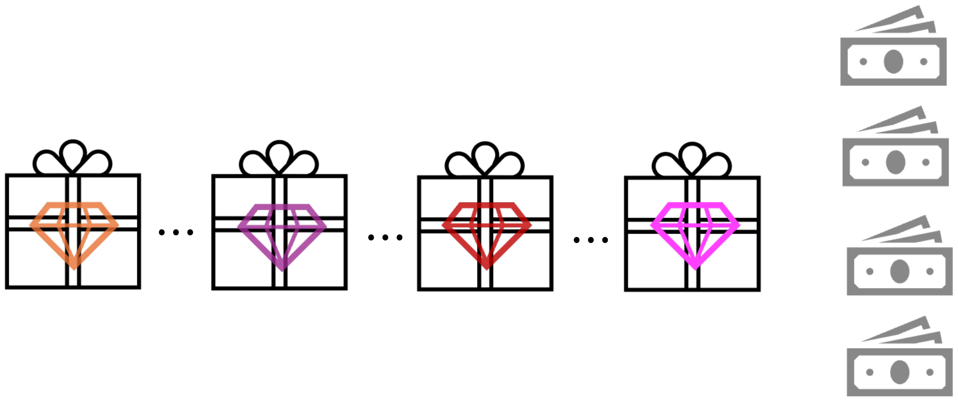
Experiment Results: PBGI vs EI vs TS



Conclusions

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





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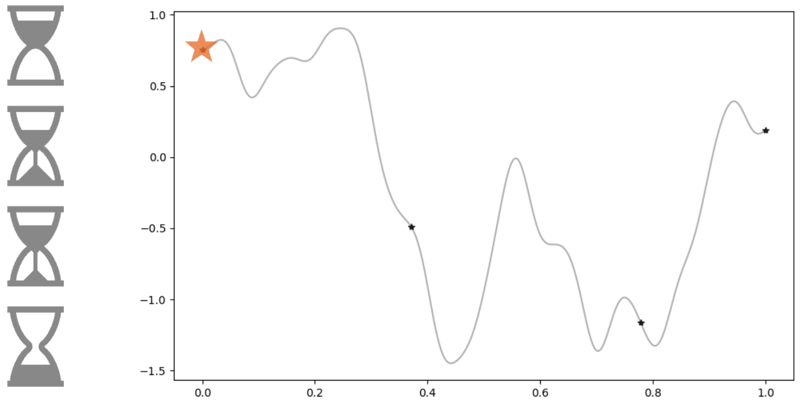
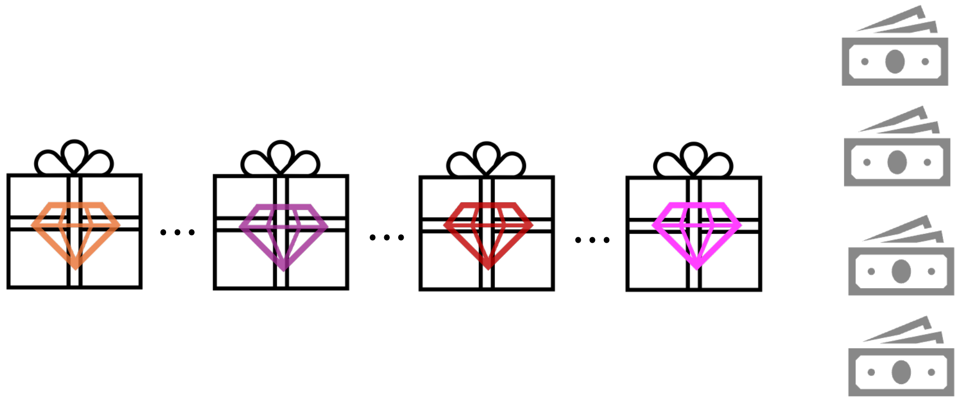
Conclusions

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

particularly on medium-high dimensions and relatively-large domains!





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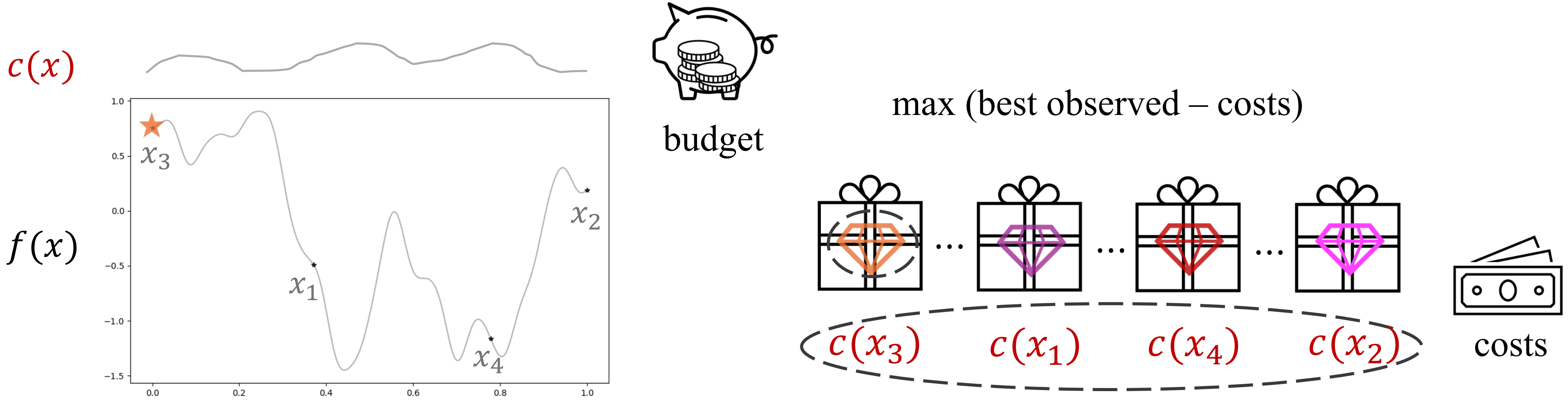
Conclusions

- Propose easy-to-compute PBGI policy for Bayesian optimization
- Show the effectiveness of PBGI on synthetic & empirical experiments
- Extend to Bayesian optimization with heterogeneous evaluation costs



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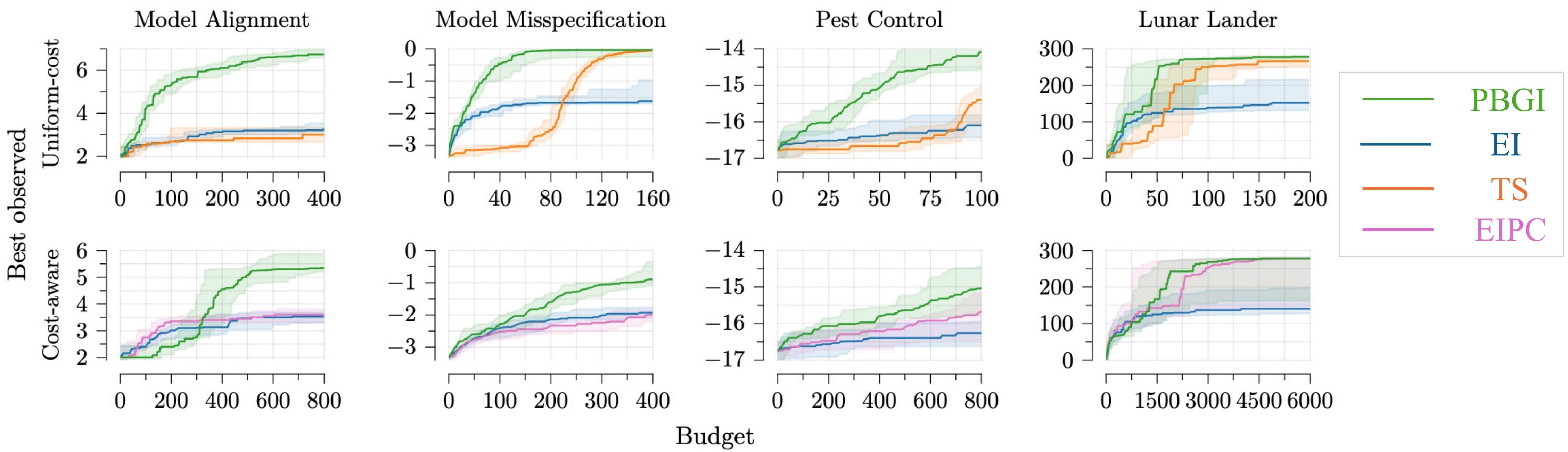
Heterogeneous-cost Experiment Results

- Show the effectiveness of PBGI on synthetic & empirical experiments
- Extend to Bayesian optimization with heterogeneous evaluation costs



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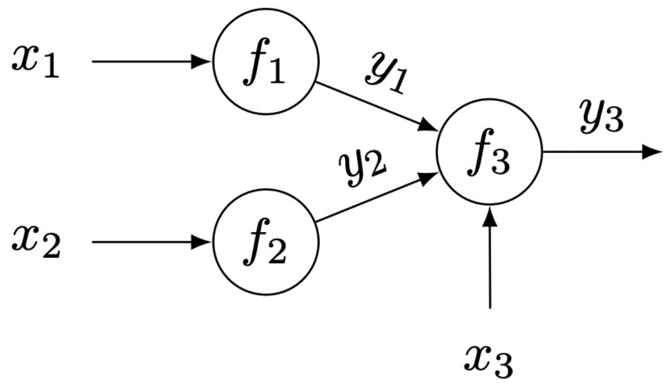
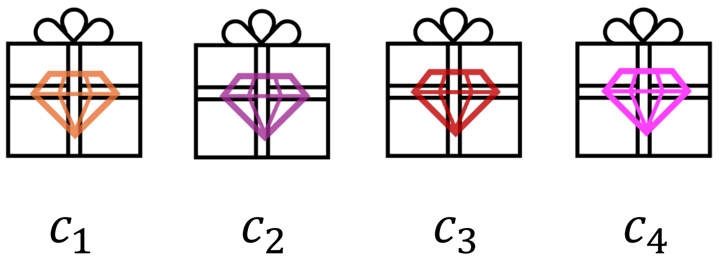
Conclusions

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





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