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

∈ decision-making under uncertainty

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Applications:
Hyperparameter tuning
Drug discovery
Control design

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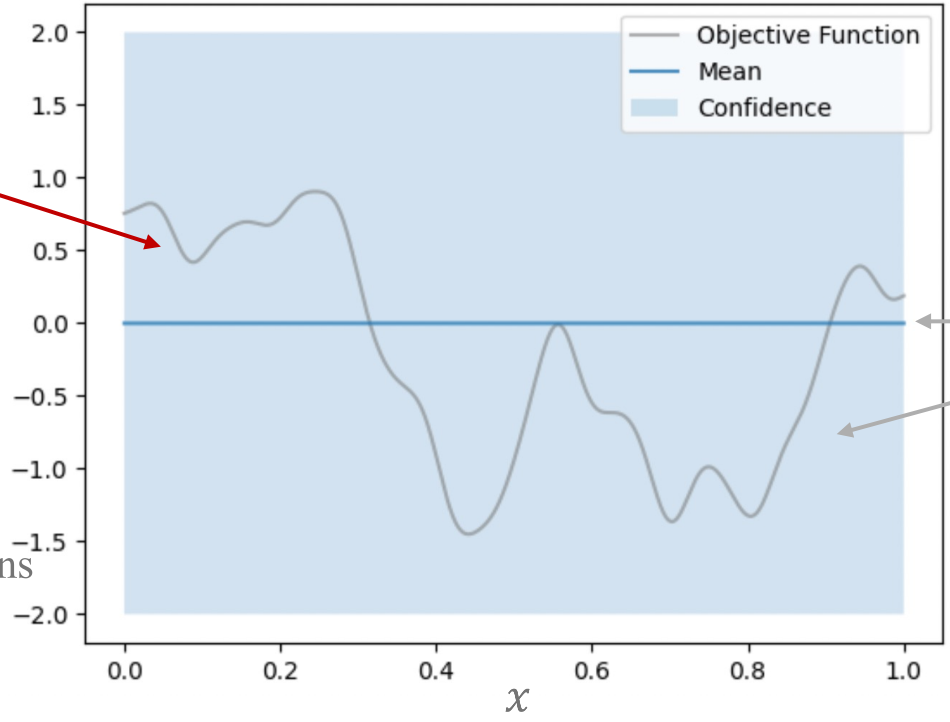
An unknown random function $f: \mathcal{X} \to \mathbb{R}$ drawn from a Gaussian process prior

Gaussian process: infinite-dimensional generalization of multivariate normal distributions



Applications:
Hyperparameter tuning
Drug discovery
Control design

x: hyperparameter/configuration

mean: prediction

variance: confidence/uncertainty

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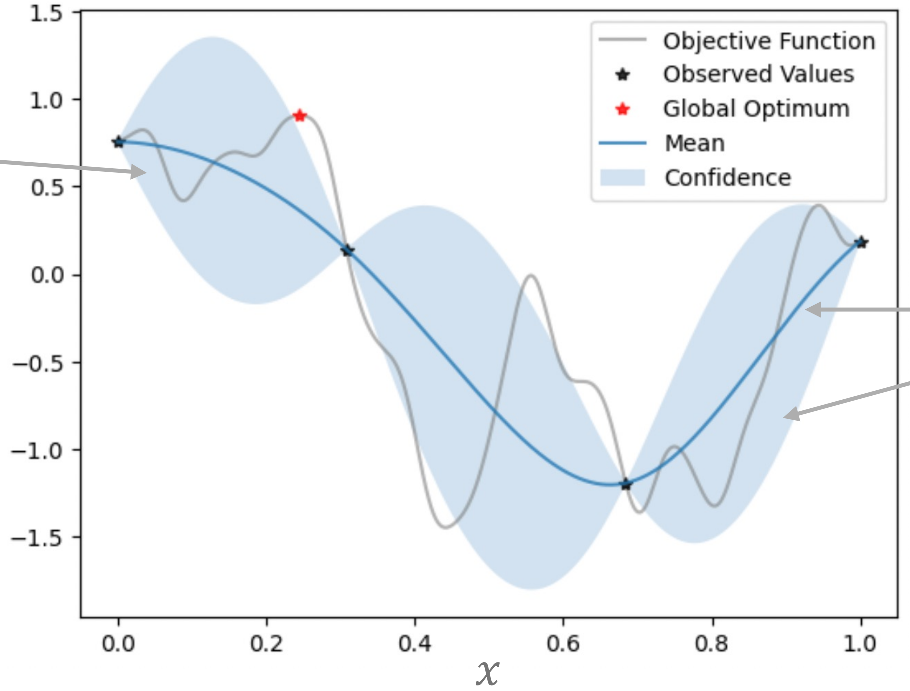

mean: prediction

variance: confidence/uncertainty

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

Decision: evaluate a set of points

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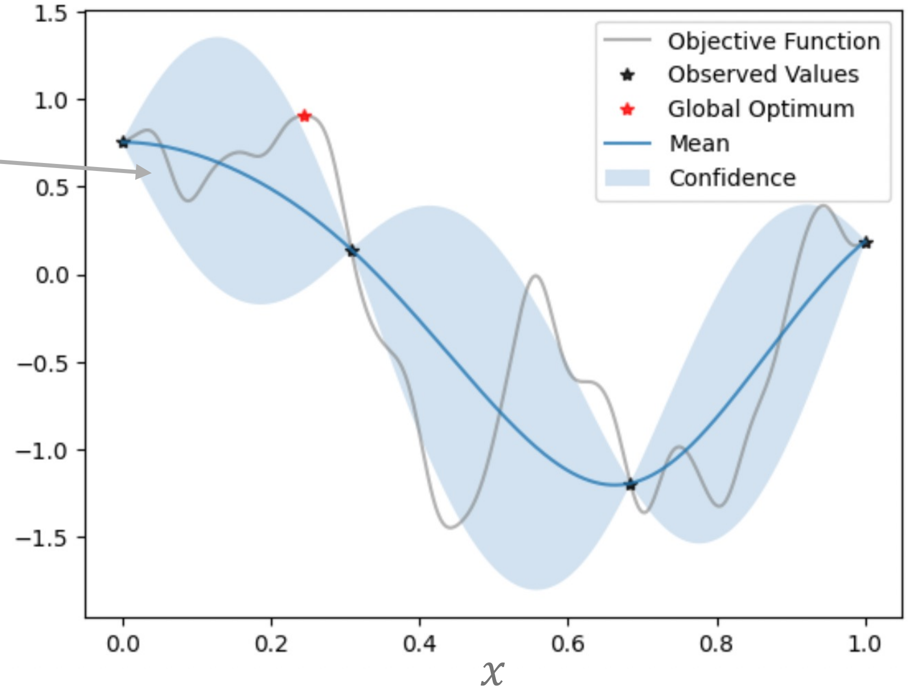

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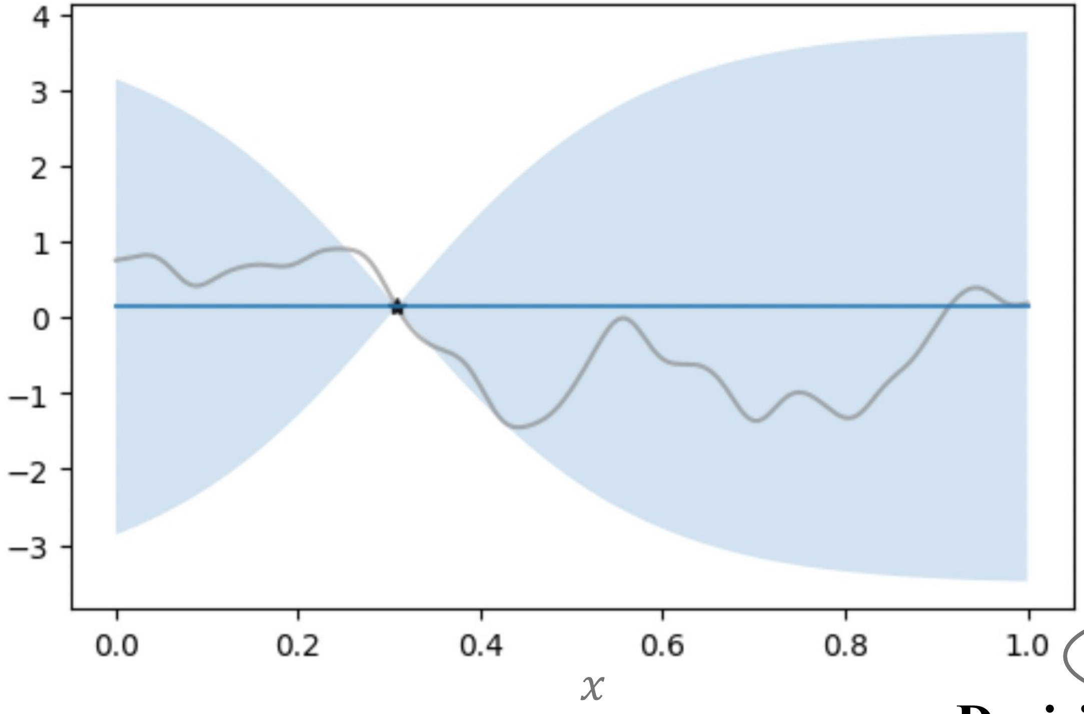

Applications:
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x: hyperparameter/configuration

adaptively

Decision: evaluate a set of points

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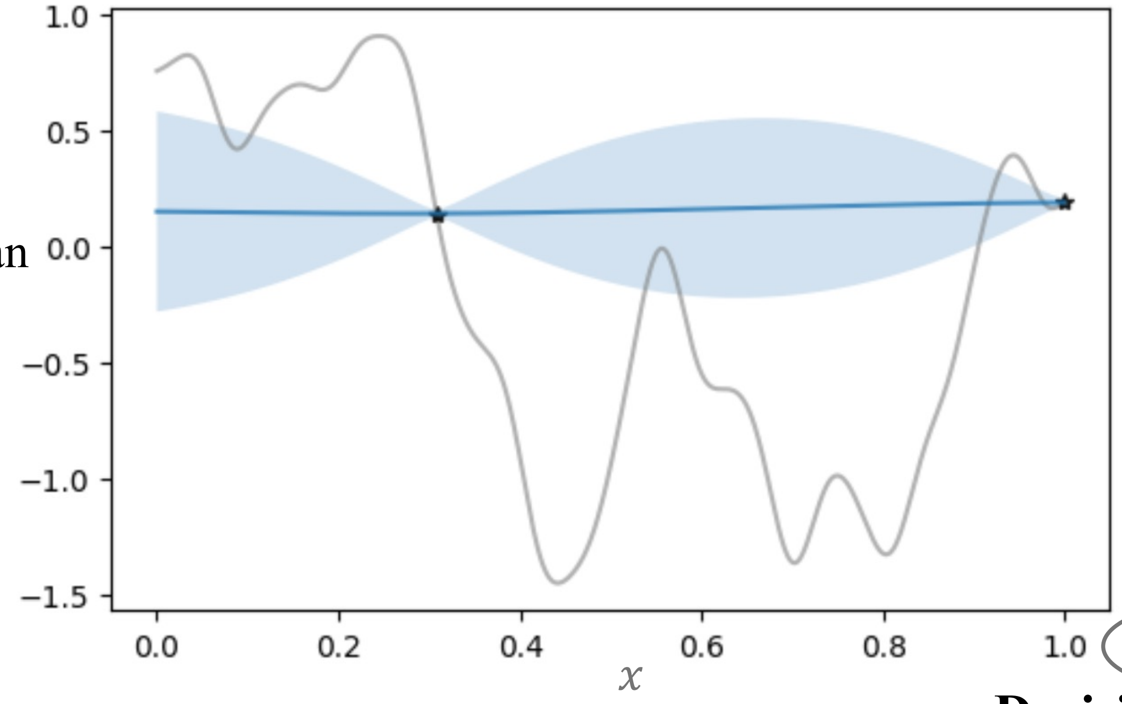

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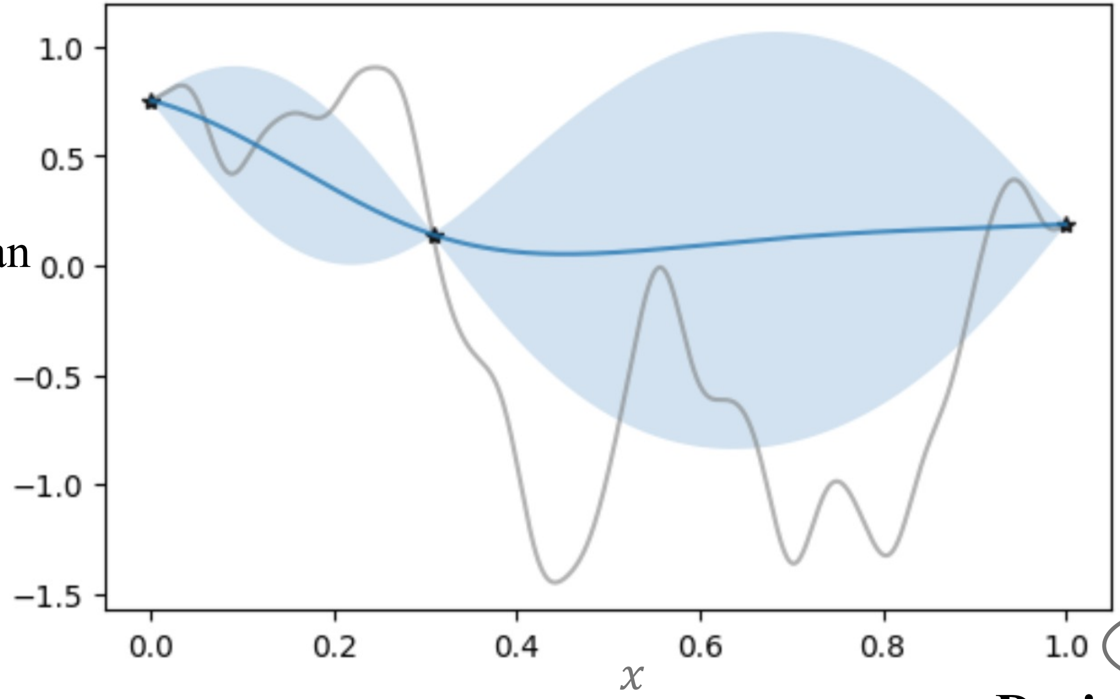

adaptively
Decision: evaluate a set of points

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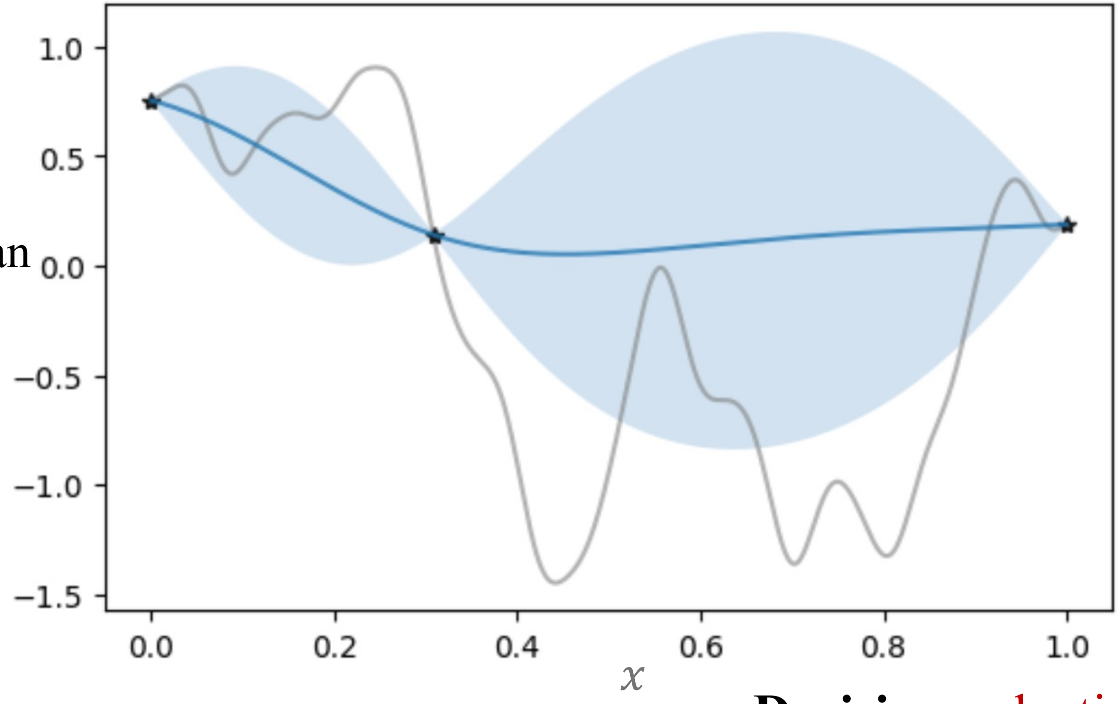

Applications:
Hyperparameter tuning
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Control design

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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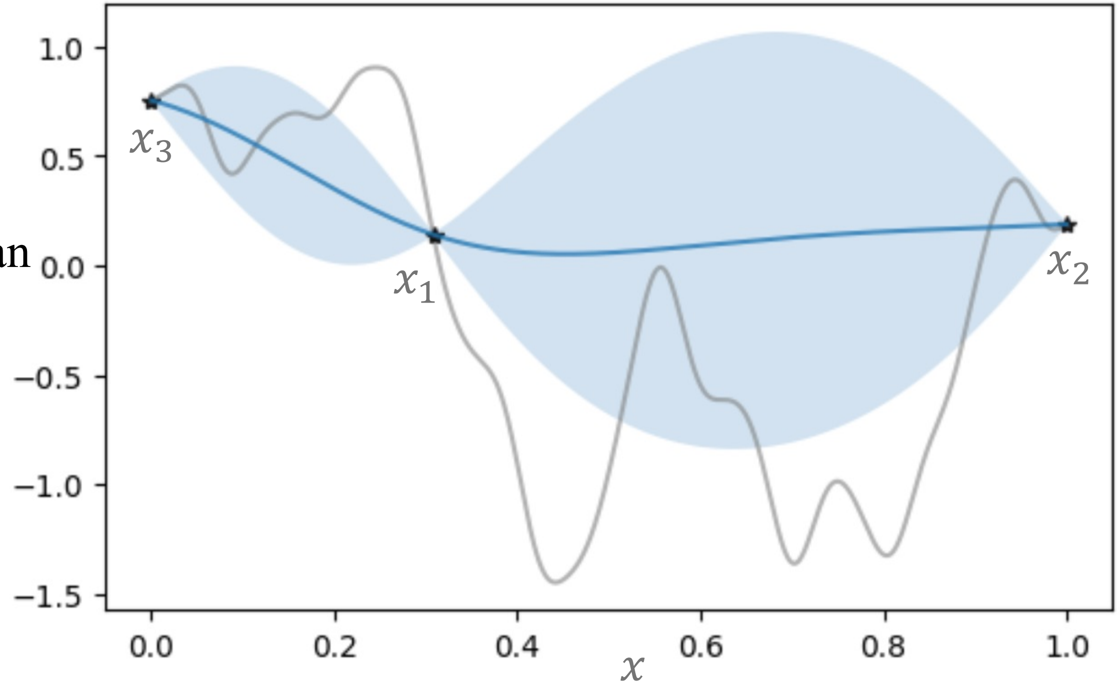


Applications:
Hyperparameter tuning
Drug discovery
Control design

x: hyperparameter/configuration

Objective: optimize best observed value at time T

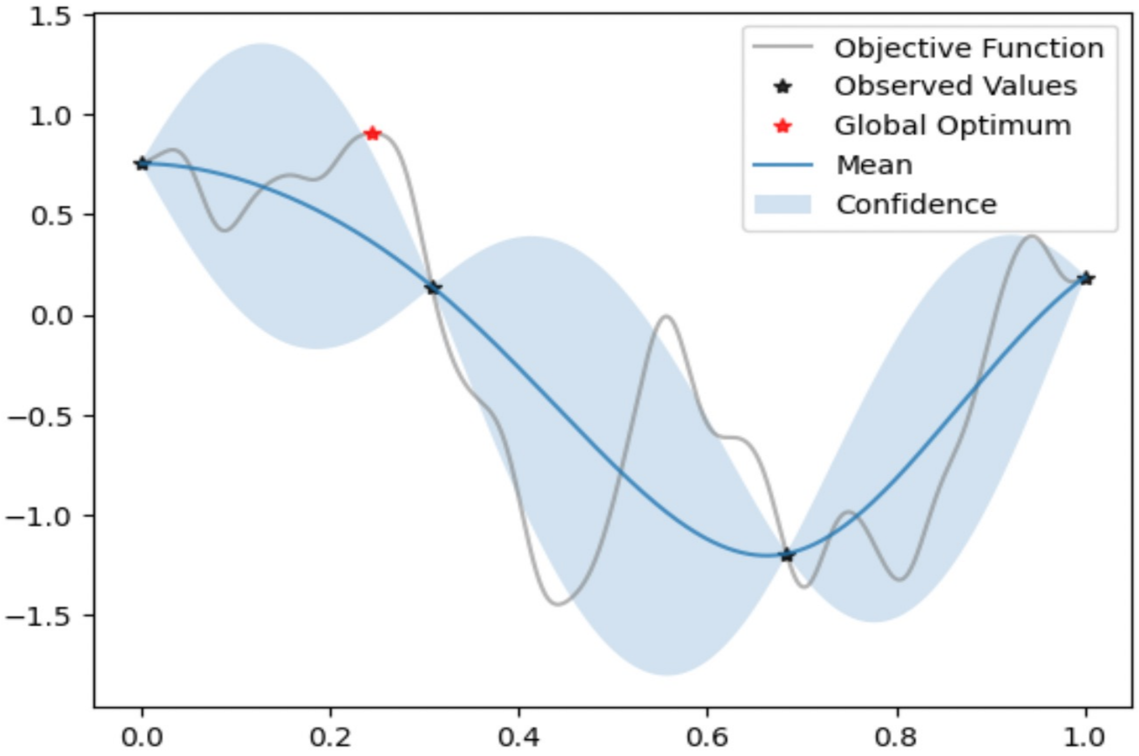
$$\max_{\text{policy}} \mathbb{E} \max_{t=1,2,\ldots,T} f(x_t)$$

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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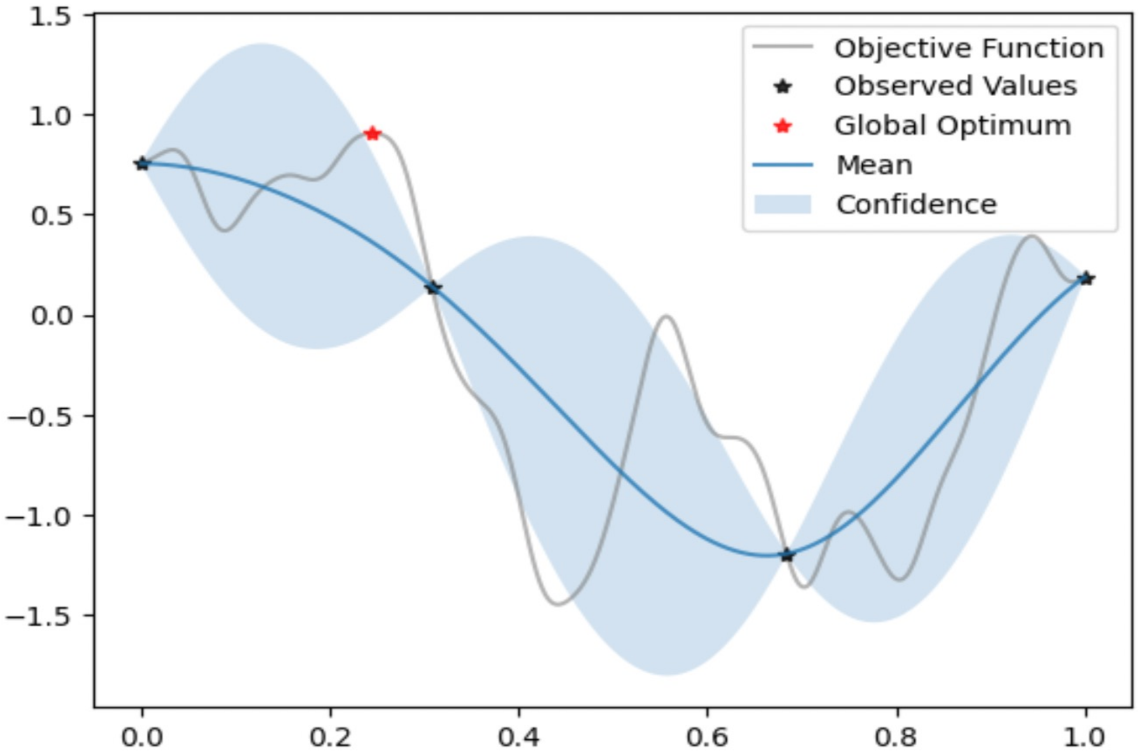
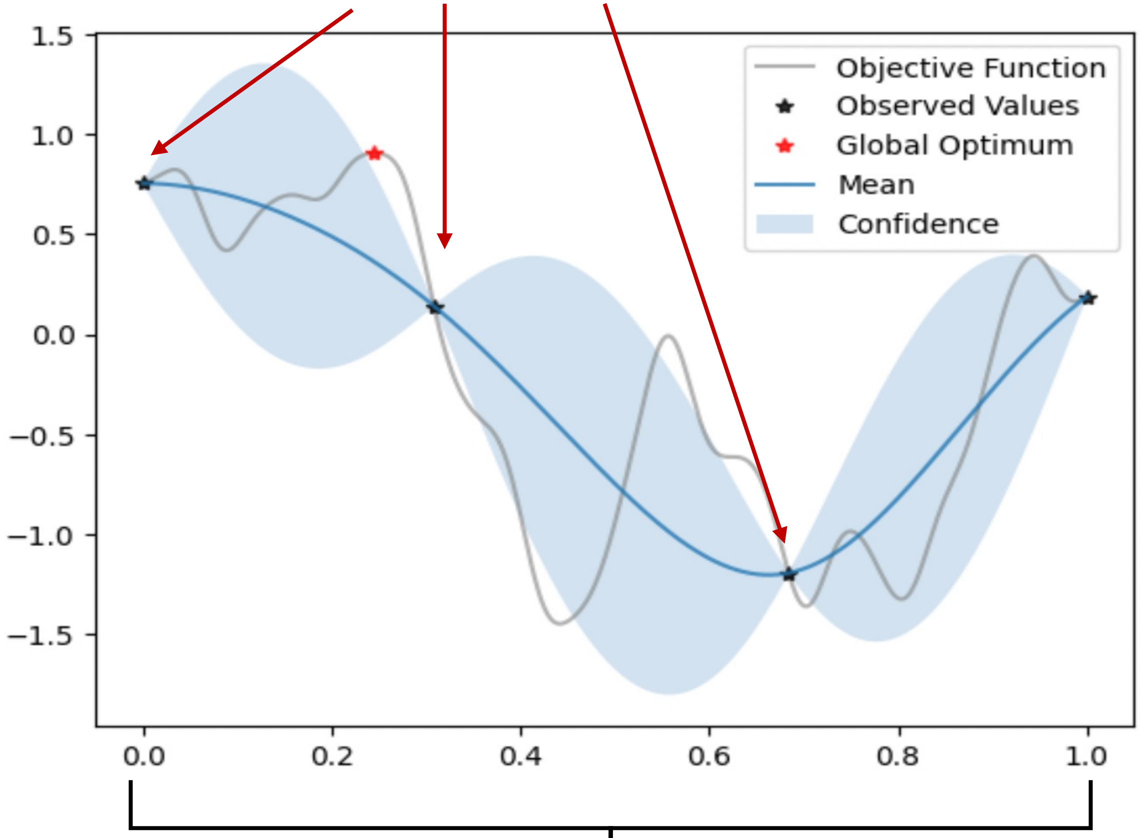


Continuous search domain

Why is it hard?

Correlated values



Continuous search domain

Why is it hard?

Hard budget constraint

$\cancel{t = 1}$

$\cancel{t = 2}$

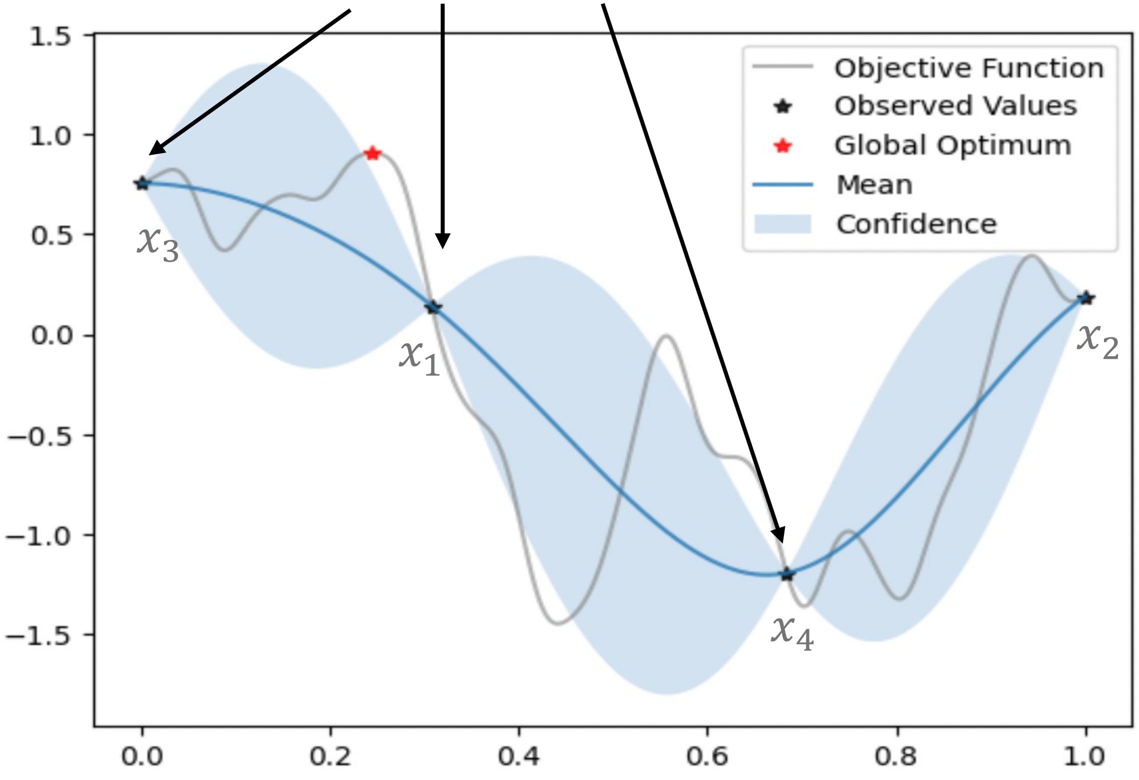
$\cancel{t = 3}$

$\cancel{t = 4}$

$\vdots$

$t = T$

Correlated values



Continuous search domain

Why is it hard?

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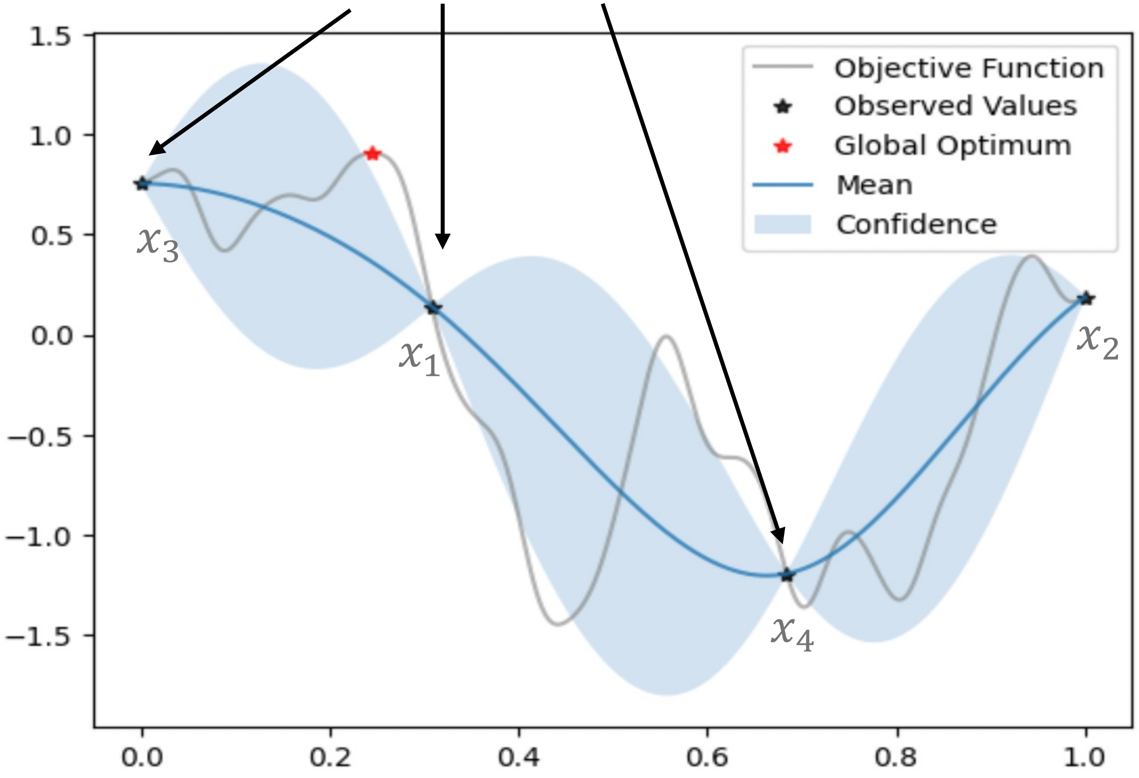
Correlated values



Continuous search domain

Evaluation costs handling

cheap	expensive
risk-seeking	risk-averse
exploration	exploitation

uniform	heterogeneous

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Hard budget constraint

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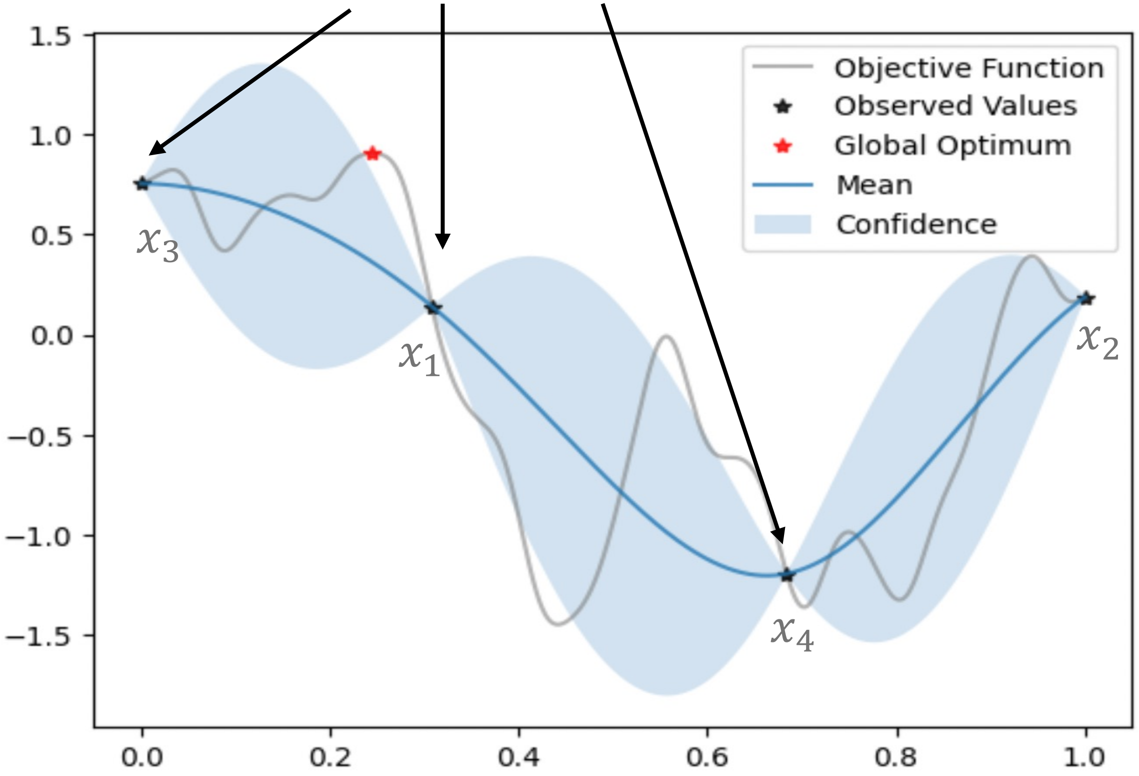
$\vdots$

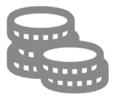
$t = T$

Correlated values



Continuous search domain

Evaluation costs handling



cheap | expensive

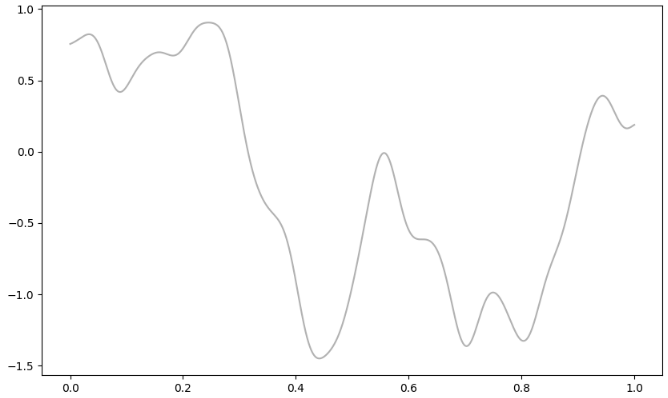
risk-seeking | risk-averse

exploration | exploitation

uniform | heterogeneous

$\Longrightarrow$ Optimal policy unknown!

Bayesian Optimization

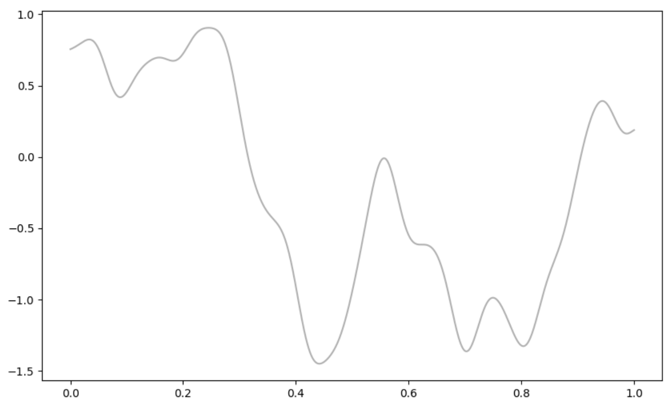


Continuous

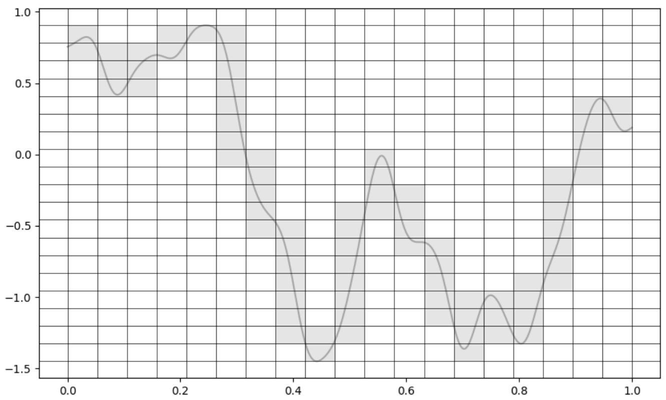
Correlated

Hard budget constraint

Bayesian Optimization



$\Longrightarrow$

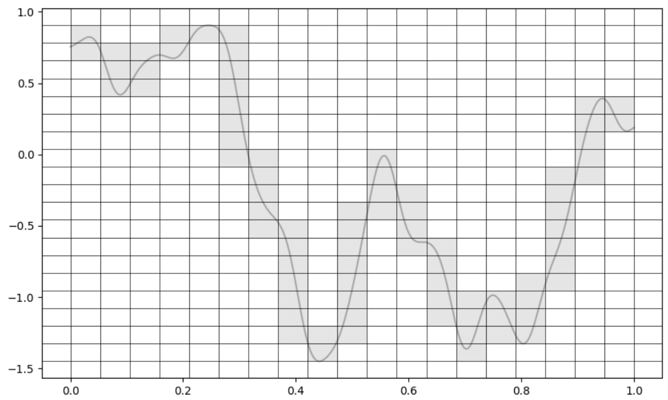


Continuous $\Rightarrow$ Discrete

Correlated

Hard budget constraint

Bayesian Optimization

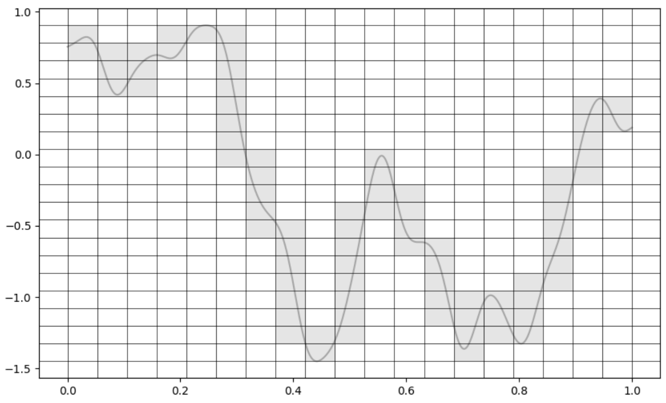


Continuous $\Longrightarrow$ Discrete

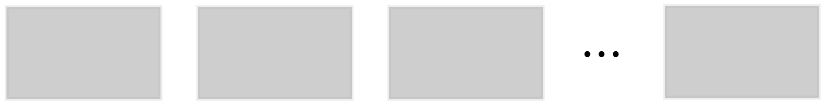
Correlated

Hard budget constraint

Bayesian Optimization

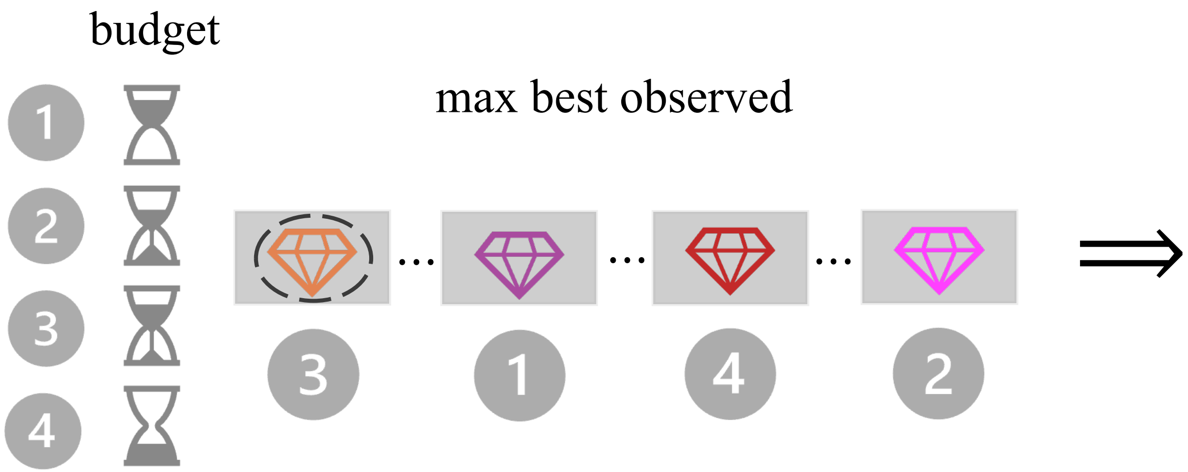


$\Longrightarrow$



Continuous	$\Longrightarrow$	Discrete
Correlated	$\Longrightarrow$	Independent
Hard budget constraint		

Bayesian Optimization

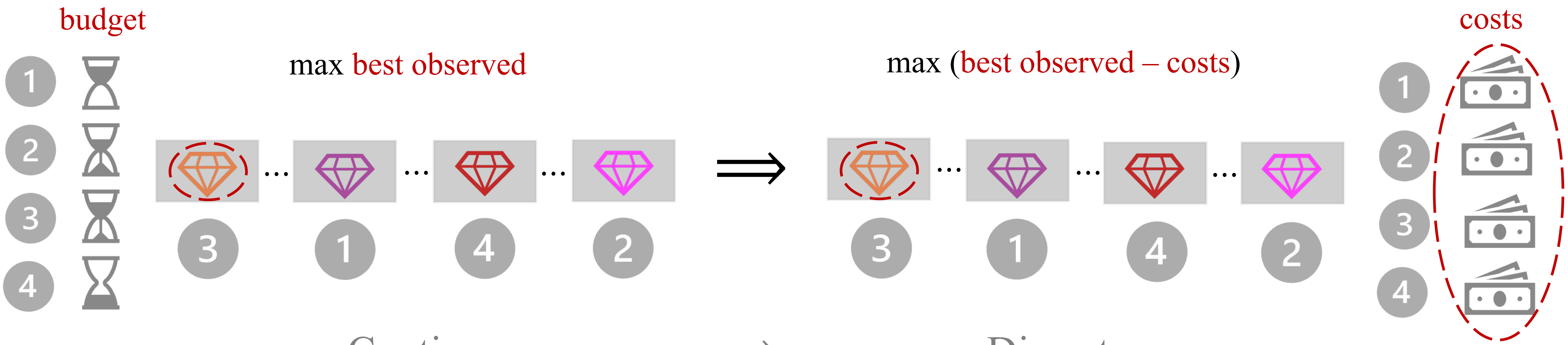


Continuous $\Longrightarrow$ Discrete

Correlated $\Longrightarrow$ Independent

Hard budget constraint

Bayesian Optimization



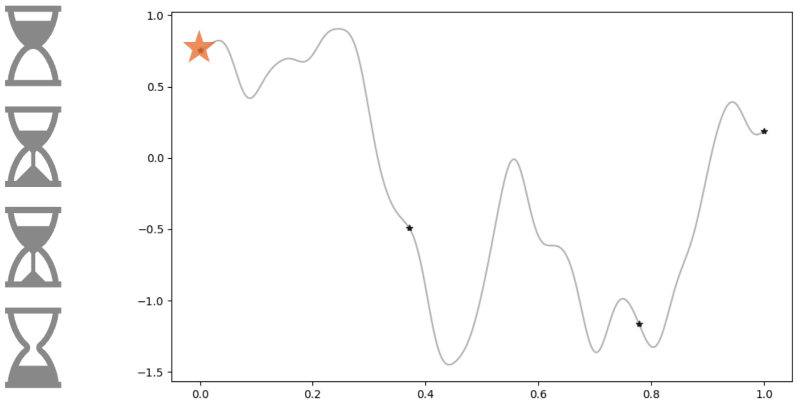
Continuous ⟹ Discrete

Correlated ⟹ Independent

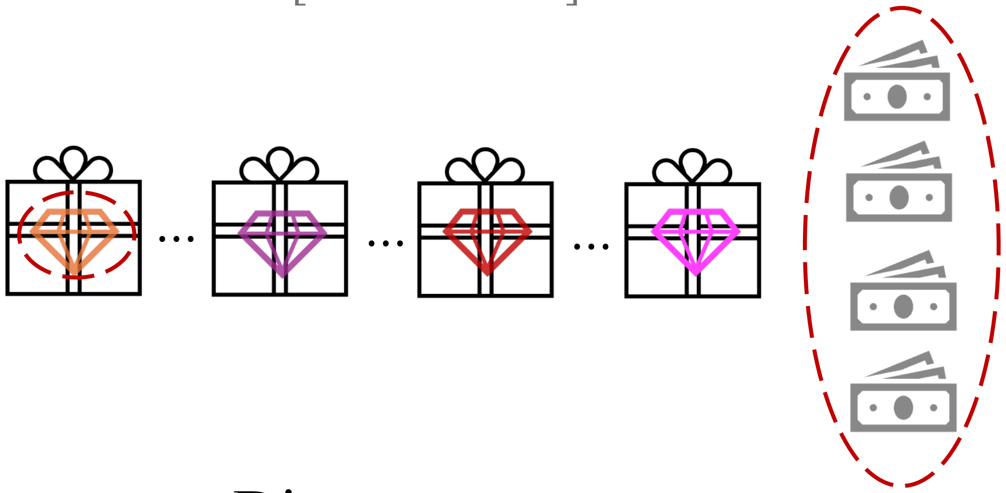
Hard budget constraint $\overset{\text{Lagrangian relaxation}}{\Longrightarrow}$ Cost per sample

Bayesian Optimization ⟹ Pandora's Box

[Weitzman'79]



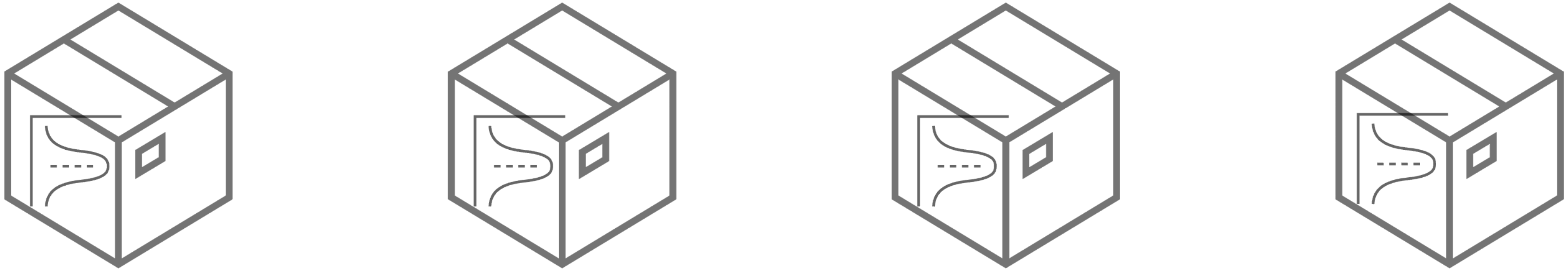
⟹



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

Pandora's Box

$t = 0$

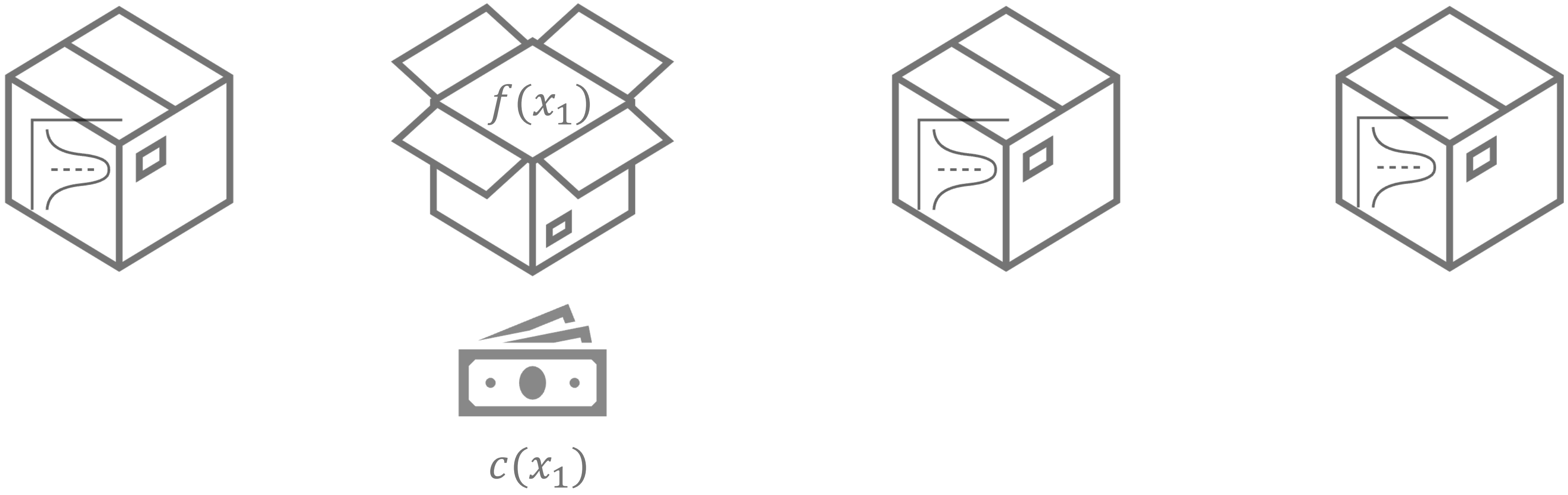


Objective: maximize net utility

Decision: adaptively evaluate a set of points

Pandora's Box

$t = 1$

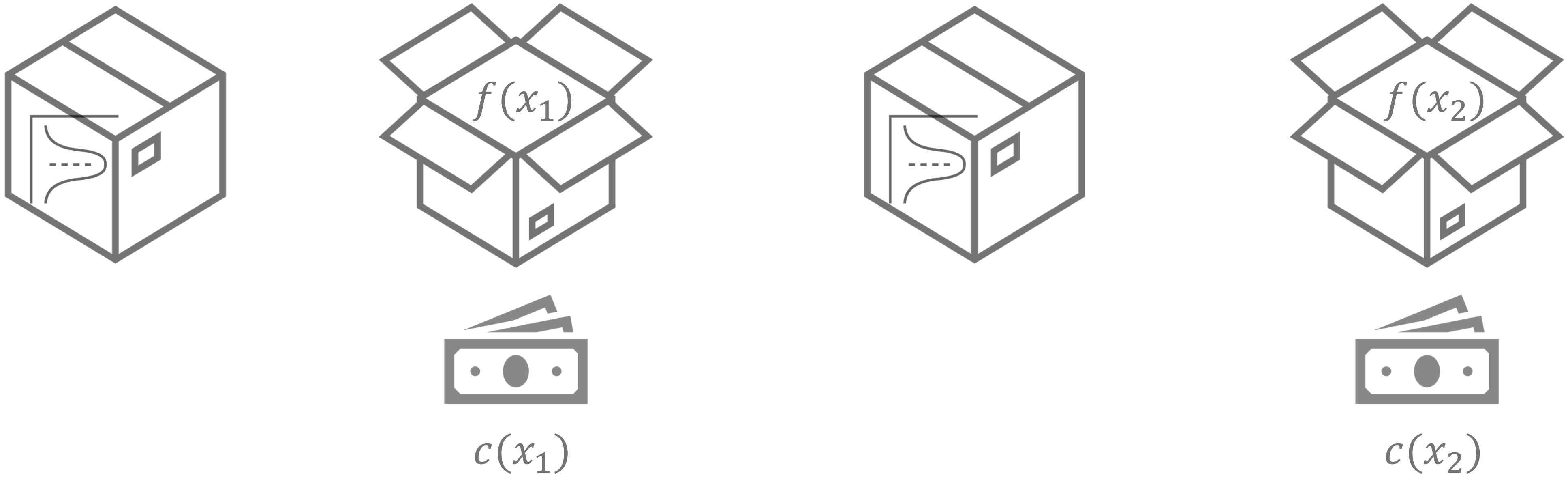


Objective: maximize net utility

Decision: adaptively evaluate a set of points

Pandora's Box

$t = 2$

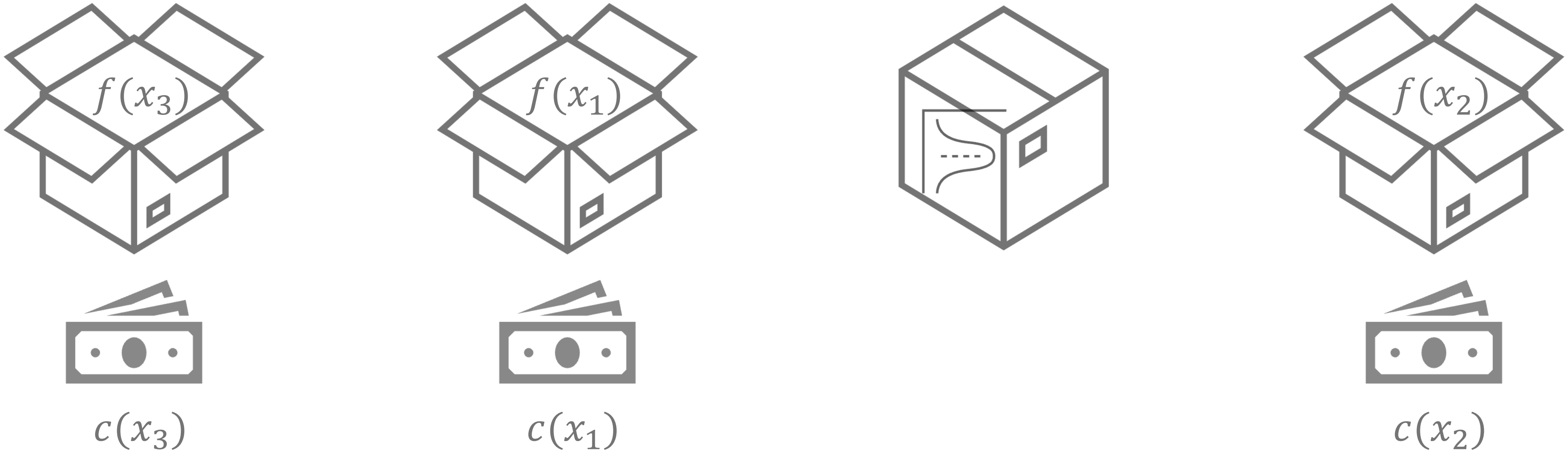


Objective: maximize net utility

Decision: adaptively evaluate a set of points

Pandora's Box

$t = 3$

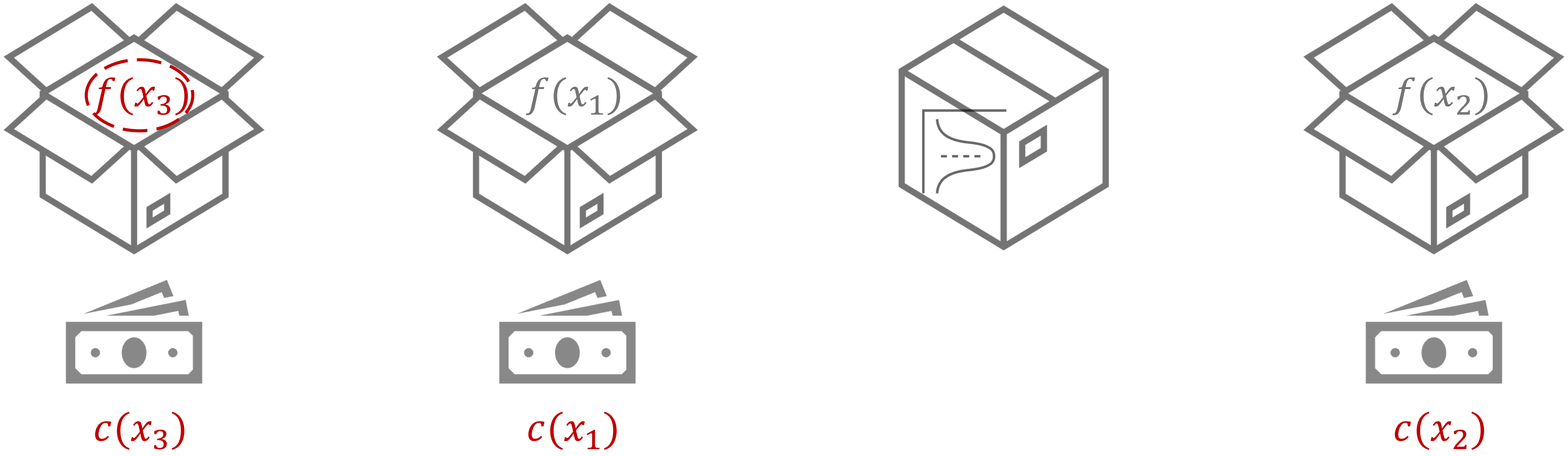


Objective: maximize net utility

Decision: adaptively evaluate a set of points

Pandora’s Box

$t = 3$



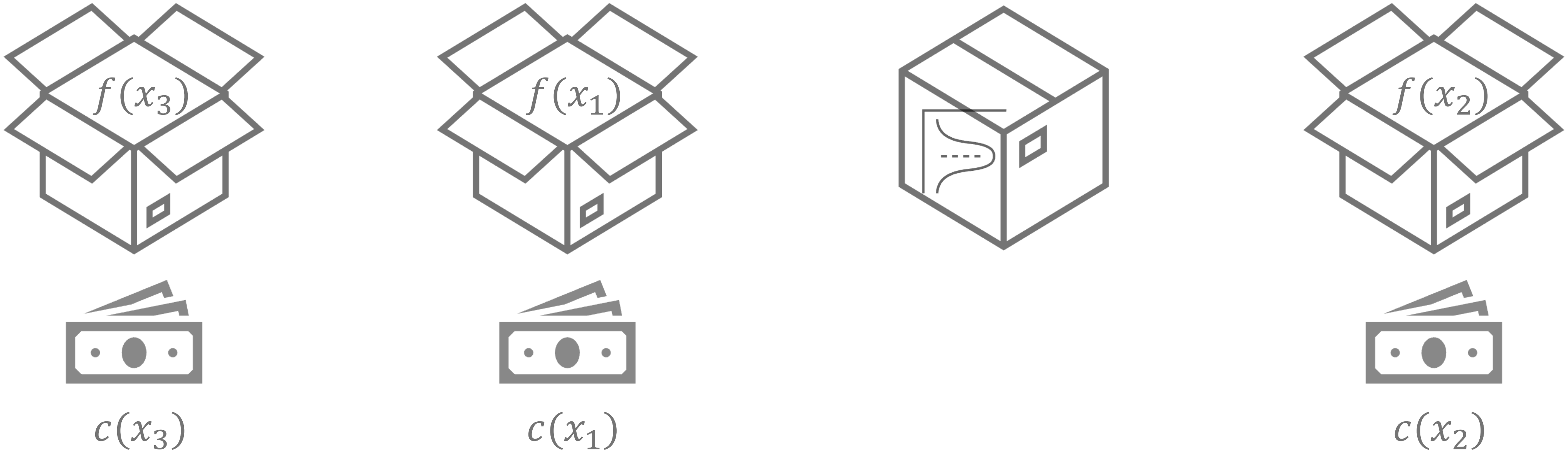
Objective: maximize net utility

Decision: adaptively evaluate a set of points

max $\mathbb{E}$(best observed value – total costs)

Pandora's Box

$t = 3$



Objective: maximize net utility

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

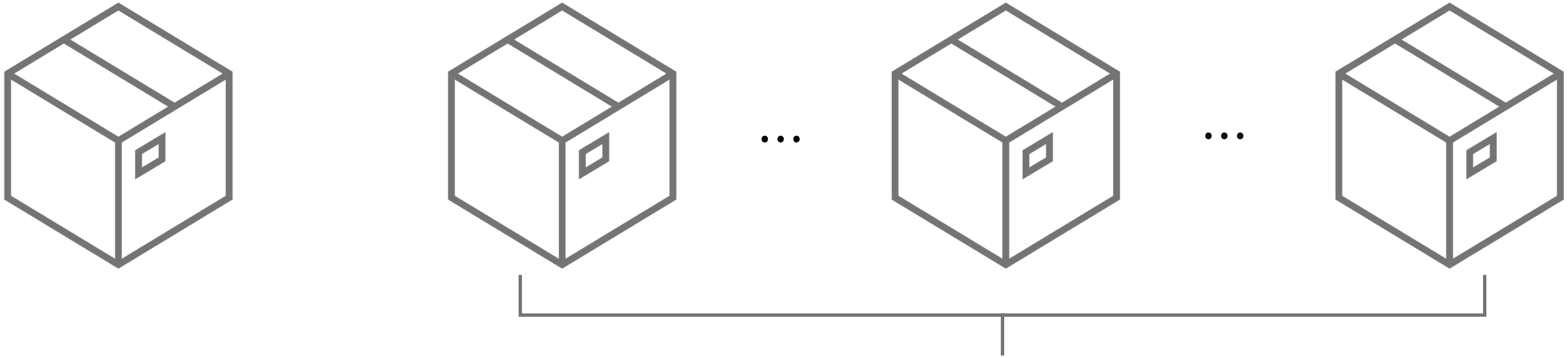
Decision: adaptively evaluate a set of points

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

$\mathcal{X}$: discrete

T: random stopping time

Greedy policy can fail [Singla'18]



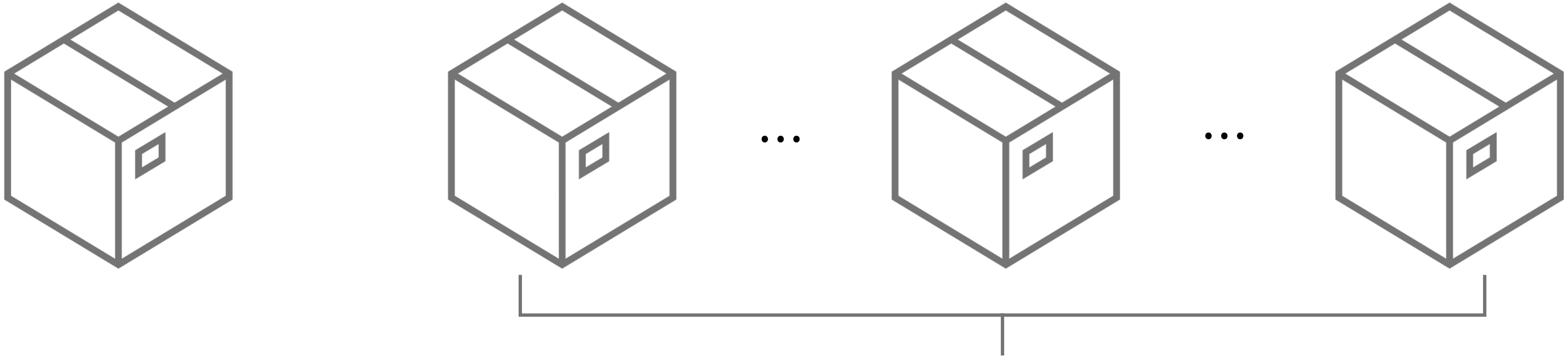
$f(1) = 200 \text{ w.p. } 1$

$c(1) = 198$

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

Greedy policy can fail [Singla'18]

Greedy policy



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

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

expected improvement - cost

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

expected improvement $\leq$ cost

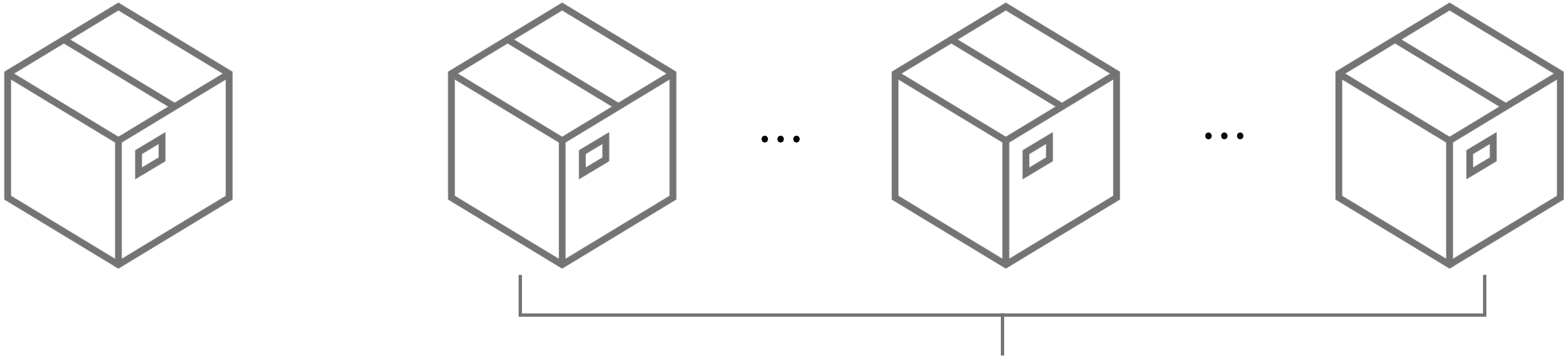
y_{best}: current best observed value

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

Greedy policy can fail [Singla'18]

$t = 0$

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



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

$c(1) = 198$

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

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

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

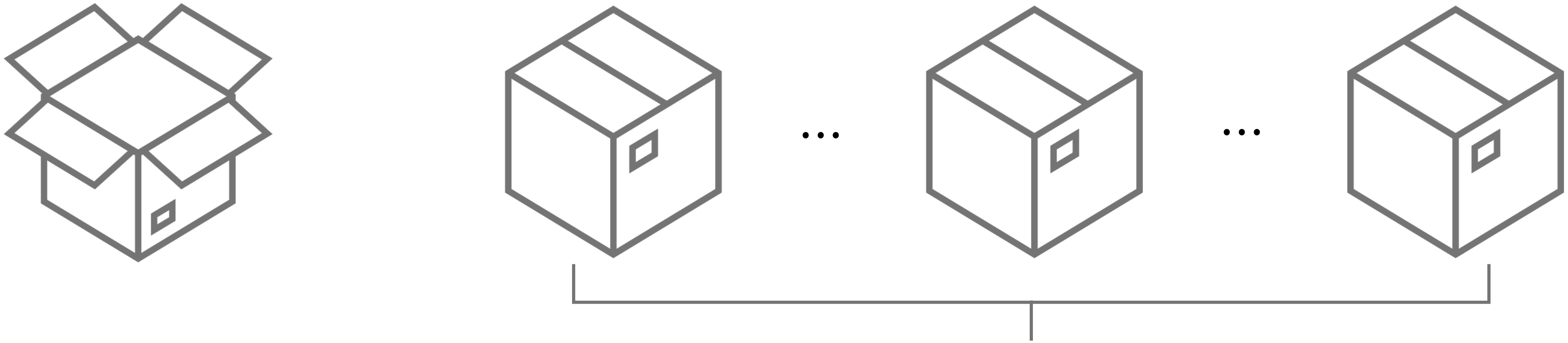
Inspection rule: $\mathrm{argmax}_x \left(\mathrm{EI}_f(x; y_{\text{best}}) - c(x)\right)$ **Stopping rule:** $\mathrm{EI}_f(x; y_{\text{best}}) \leq c(x), \forall x \in \mathcal{X}$

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

Greedy policy can fail [Singla'18]

$t = 1$

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



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

$c(1) = 198$

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

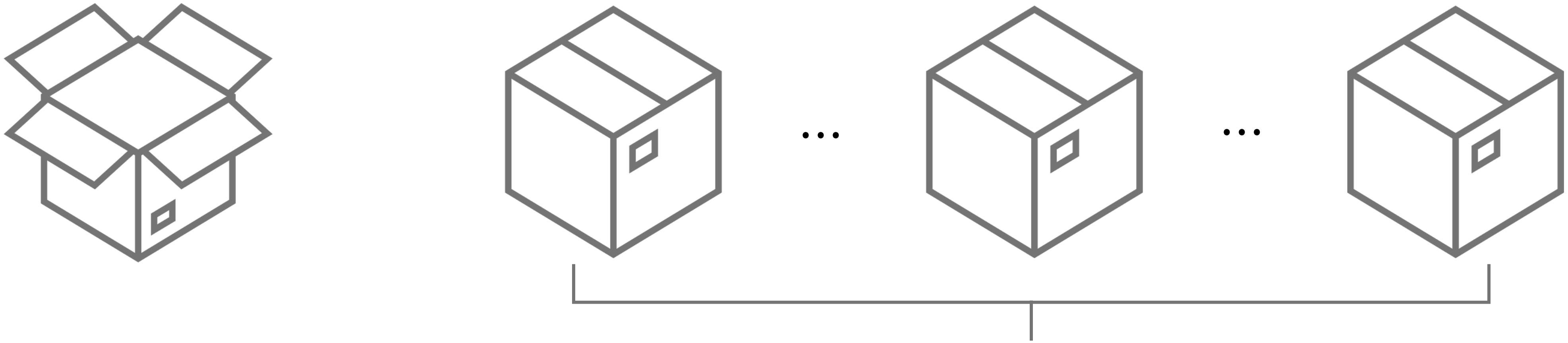
$\mathrm{EI}_f(x; 200) - c(x)$
$= 0 - 1 = -1 < 0$

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

$t = 1$



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

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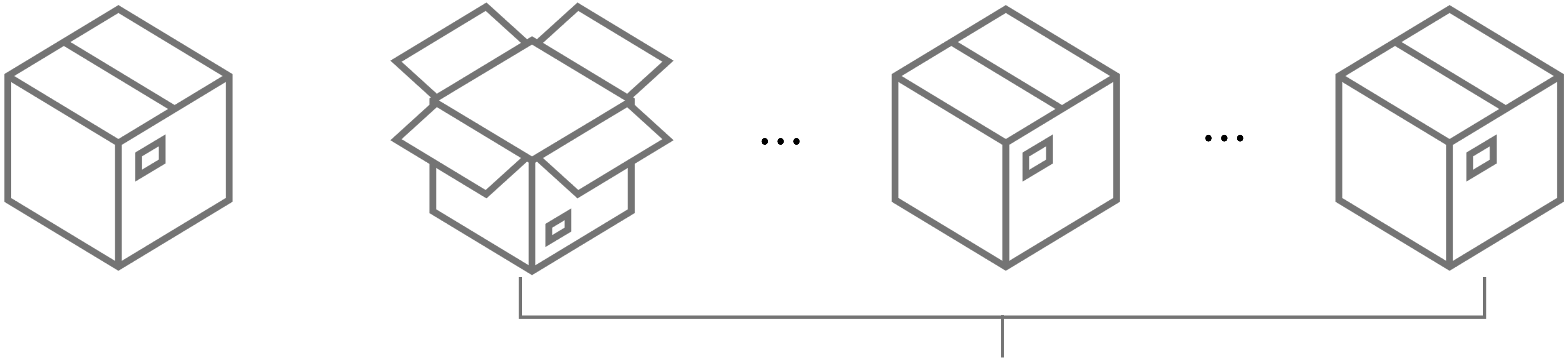
$$f(x) = \begin{cases} 200 & \text{w.p. } 0.01 \\ 0 & \text{otherwise} \end{cases}, c(x) = 1, x \in \{2, 3, \dots, 1000\}$$

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

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

Greedy policy can fail [Singla'18]

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



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

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

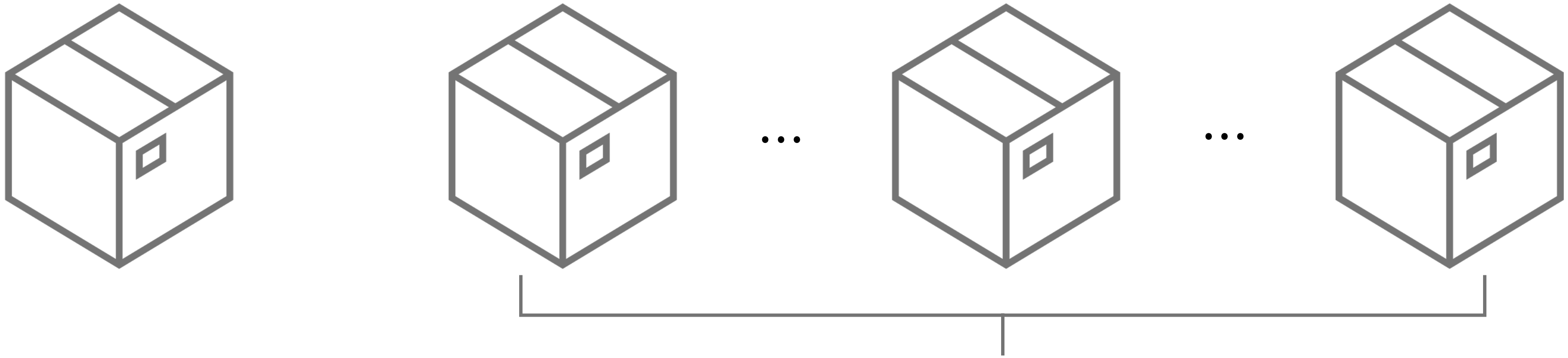
Inspection rule: $x \in \{2, 3, \dots, 1000\}$

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

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

Optimal policy: Gittins policy

Gittins policy



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

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

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

solution to expected improvement = cost

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

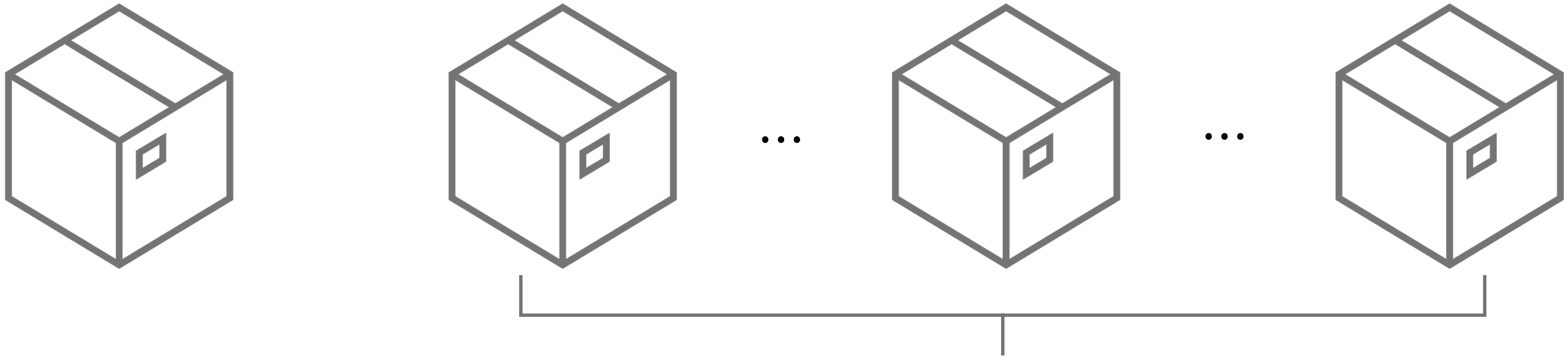
Gittins index ≤ current best

y_{best}: current best observed value

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

Optimal policy: Gittins policy

$t = 0$



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

$c(1) = 198$

$\alpha^*(1) = 2$

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

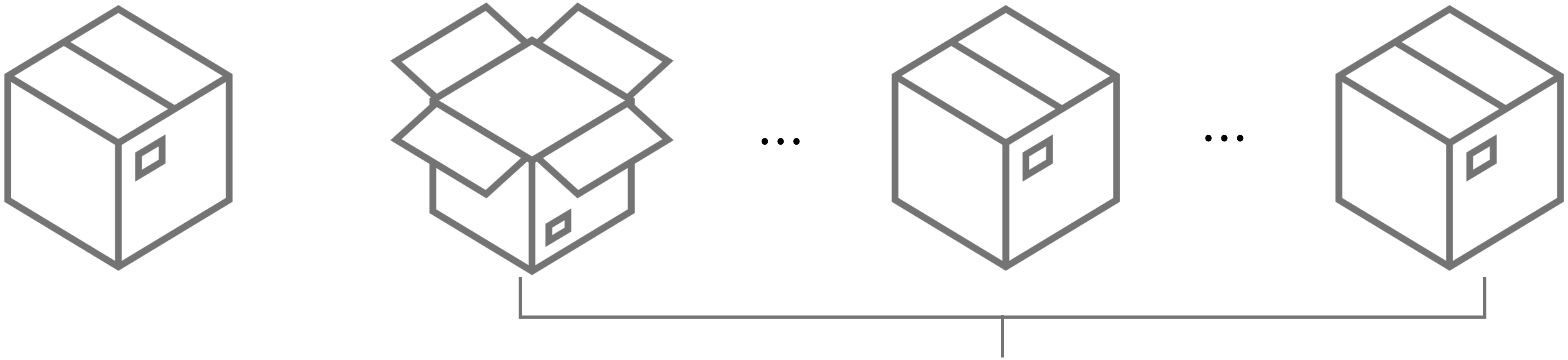
$\alpha^*(x) = 100$

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

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

Optimal policy: Gittins policy

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



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$\alpha^*(x) = 100$

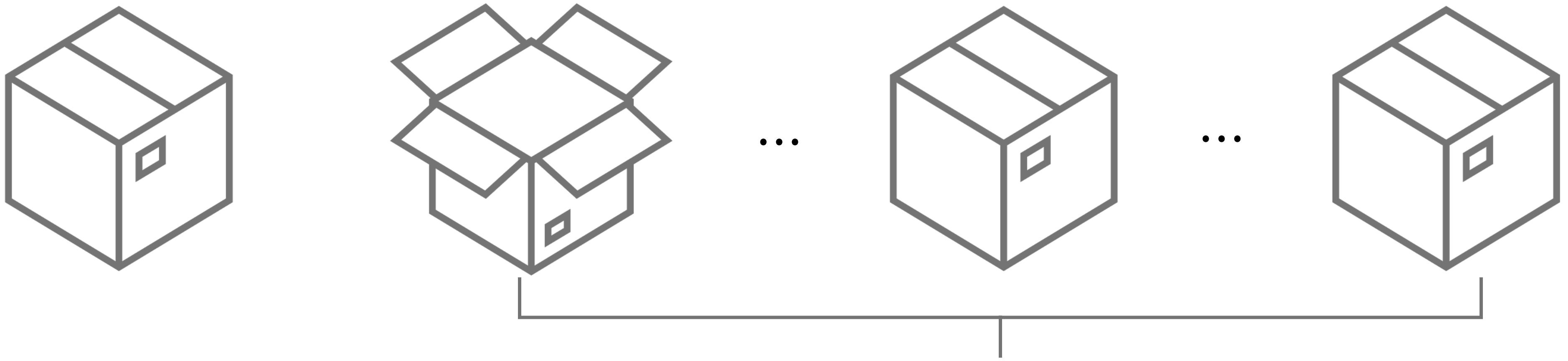
Inspection rule: $\text{argmax}_x\, \alpha^*(x)$ s.t. $\text{EI}_f(x; \alpha^*(x)) = c(x)$ **Stopping rule:** $\alpha^*(x) \le y_{\text{best}}, \forall x \in \mathcal{X}$

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

Optimal policy: Gittins policy

$t \approx 100$

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



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

$c(1) = 198$

$\alpha^*(1) = 2$

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

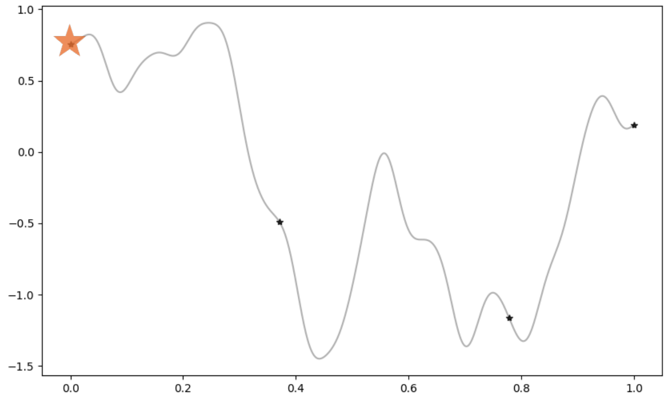
$\alpha^*(x) = 100$

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

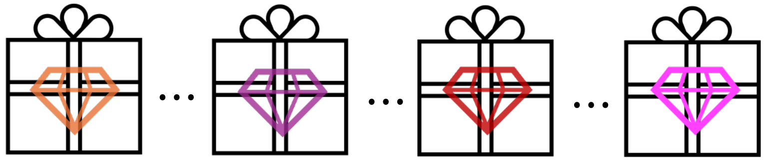
Expected utility: $\mathbb{E}[\text{Gittins}] = 200 - 100 * 1 = 100$

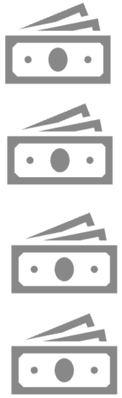
Bayesian Optimization $\Longrightarrow$ Pandora's Box

Special case of Markovian/
Bayesian multi-armed bandits



$\Longrightarrow$

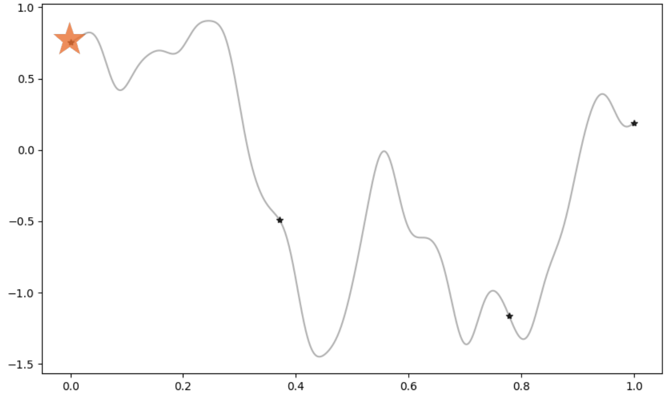




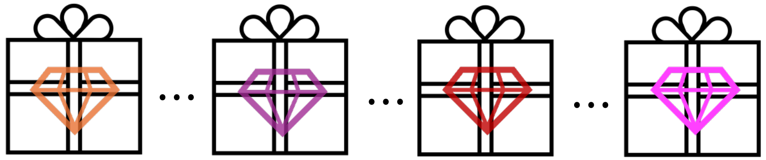
Continuous	$\Longrightarrow$	Discrete
Correlated	$\Longrightarrow$	Independent
Hard budget constraint	$\Longrightarrow$	Cost per sample

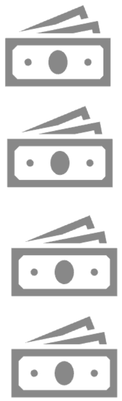
Optimal policy: Gittins index [Weitzman'79]

Bayesian Optimization $\Longrightarrow$ Pandora’s Box



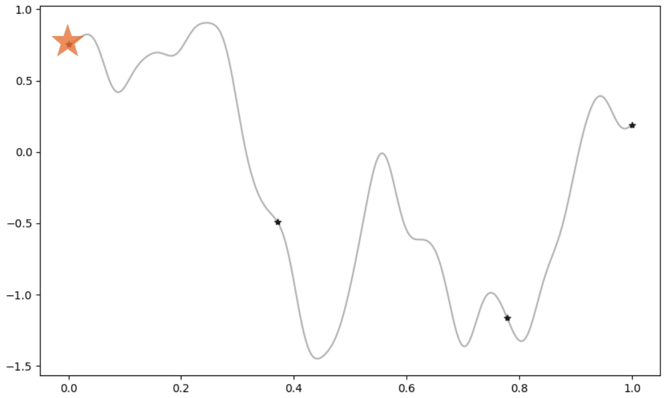
$\Longrightarrow$



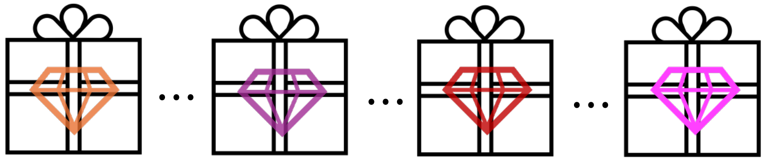


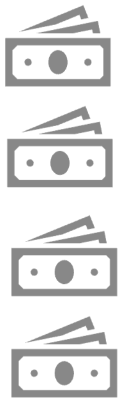
Continuous	$\Longrightarrow$	Discrete
Correlated	$\Longrightarrow$	Independent
Hard budget constraint	$\Longrightarrow$	Cost per sample
Is Gittins index good?	$\Longleftarrow$	Optimal policy: Gittins index

Bayesian Optimization $\Longrightarrow$ Pandora's Box



$\Longrightarrow$





Continuous $\Longrightarrow$ Discrete

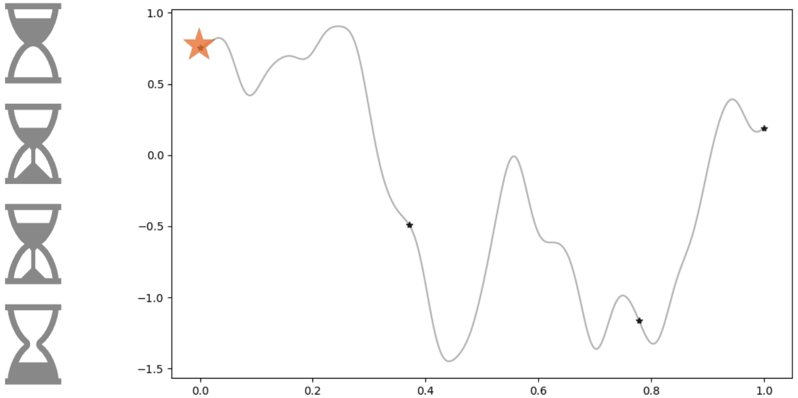
Correlated $\Longrightarrow$ Independent

Hard budget constraint $\Longrightarrow$ Cost per sample

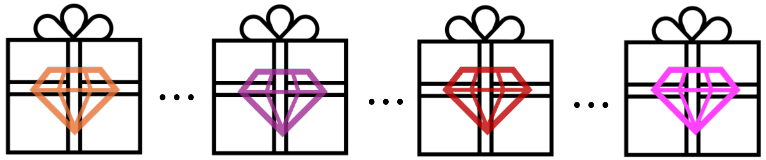
How to translate?

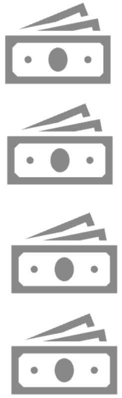
Is Gittins index good? $\Longleftarrow$ Optimal policy: Gittins index

Bayesian Optimization $\Longrightarrow$ Pandora's Box



$\Longrightarrow$





Continuous $\Longrightarrow$ Discrete

Correlated $\Longrightarrow$ Independent

Hard budget constraint $\Longrightarrow$ Cost per sample

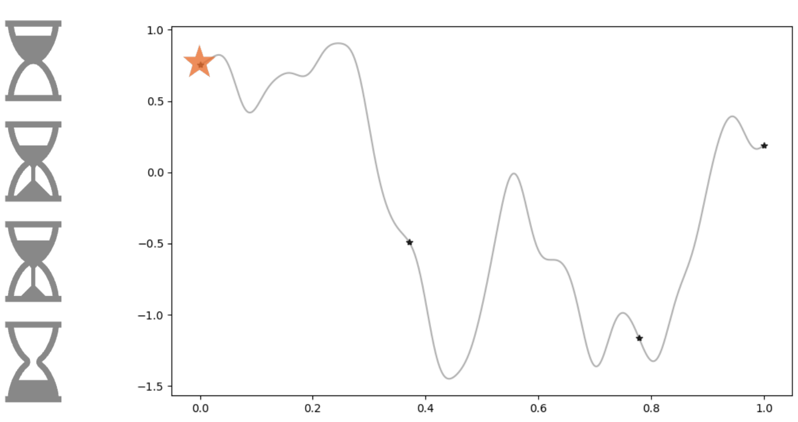
How to translate?

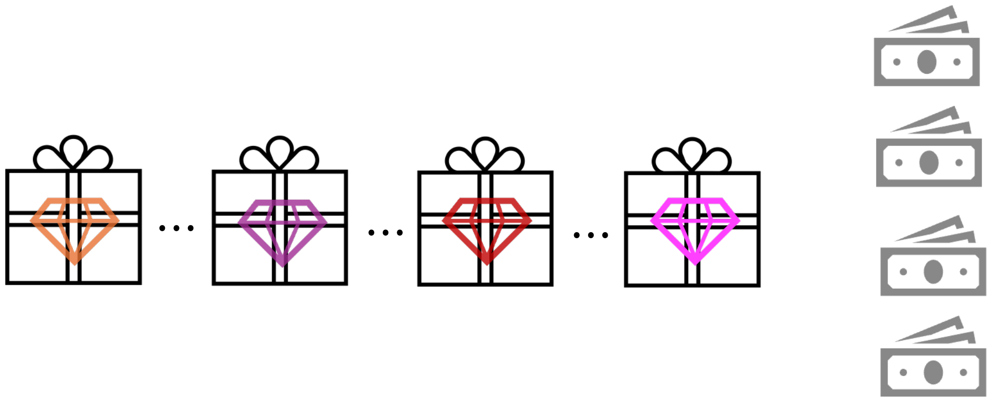
Is Gittins index good? $\Longleftarrow$ Optimal policy: Gittins index

Our contributions!

Our Contributions

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

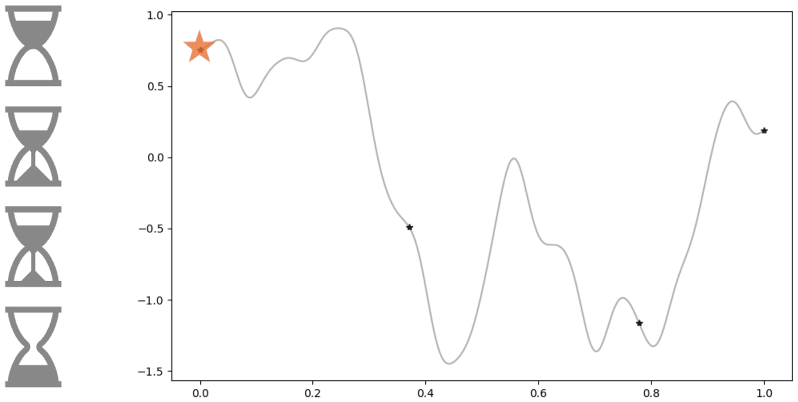


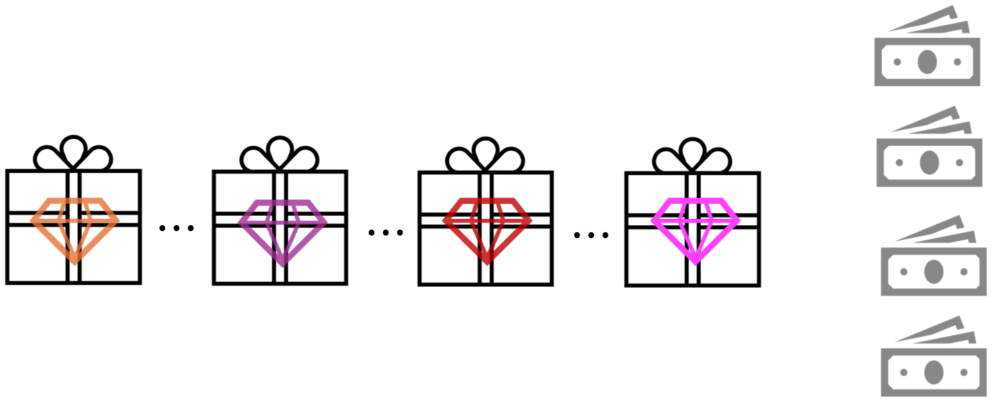


? $\Longleftarrow$ Pandora's Box Gittins index

Our Contributions

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

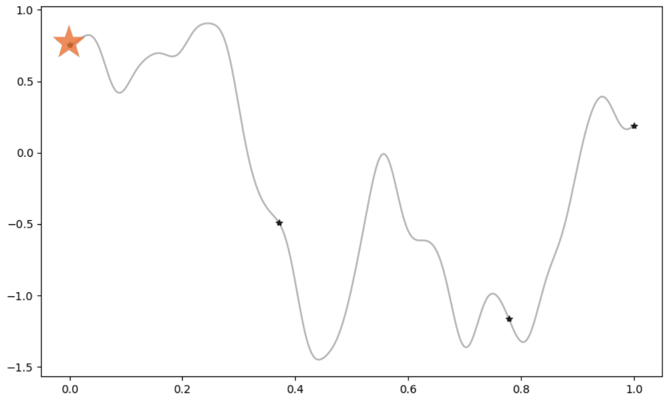


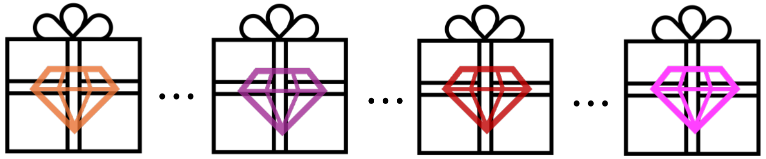


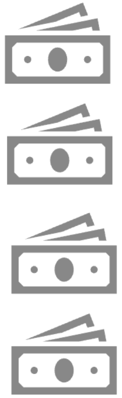
Our work $\Longleftarrow$ Pandora's Box Gittins index

Our Contributions

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



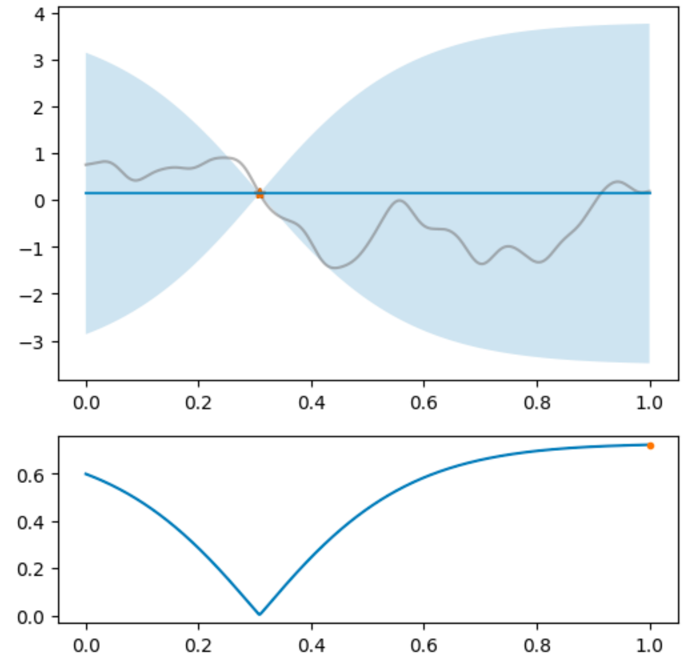




Our work $\Longleftarrow$ Pandora's Box Gittins index

How is our PBGI policy different from baselines?

Popular One-step Heuristic: EI



Expected improvement

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

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

mean: prediction

variance: confidence/uncertainty

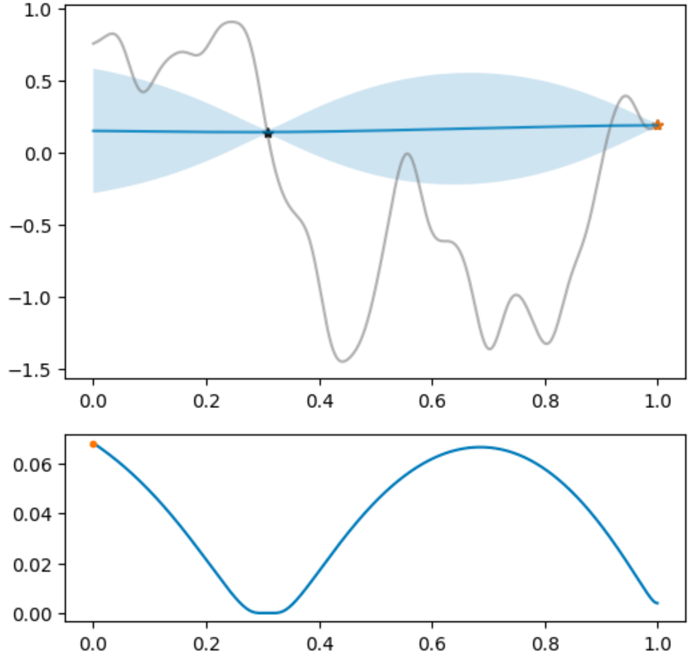
Trade-off between

- exploitation (high mean) and
- exploration (high uncertainty)

D: observed data

y_{best}: current best observed value

Popular One-step Heuristic: EI



mean: prediction

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Trade-off between

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Expected improvement

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

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

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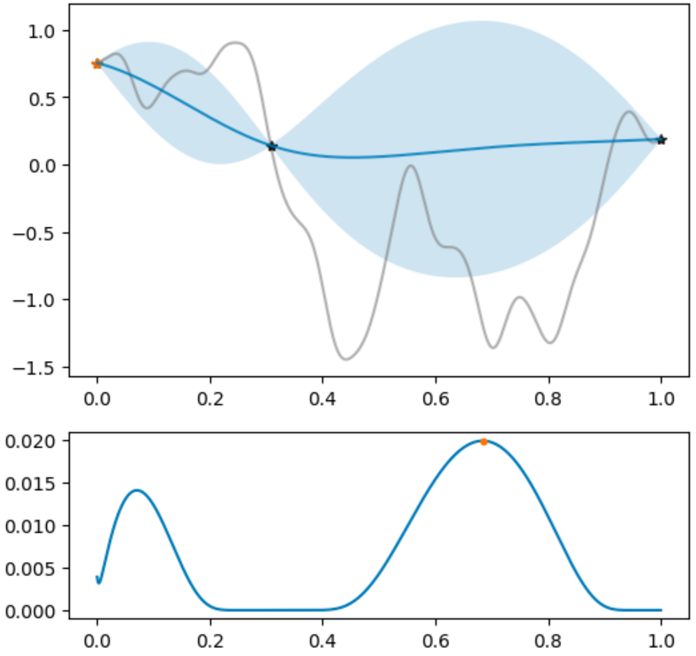
Popular One-step Heuristic: EI



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

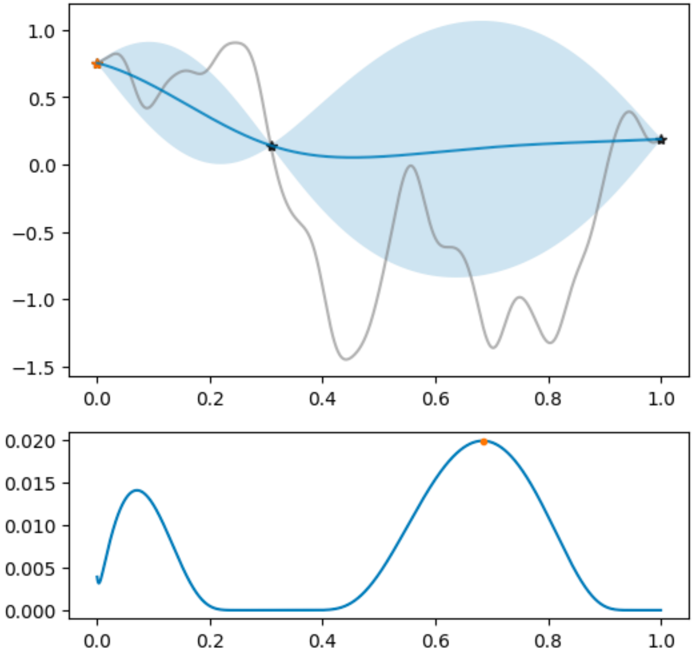
EI policy: evaluate $\arg\max_x \mathrm{EI}_{f|D}(x; y_{\text{best}})$

Popular One-step Heuristic: EI

Other heuristics:

simple
- Upper Confidence Bound
- Thompson Sampling (TS)
- Predictive Entropy Search

slow
- Knowledge Gradient
- Multi-step Lookahead 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

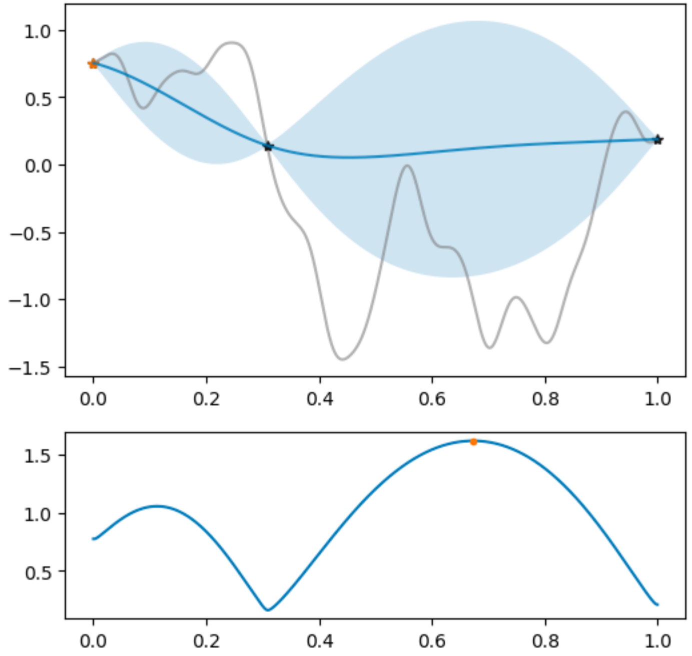
y_{best}: current best observed value

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

New One-step Heuristic: PBGI

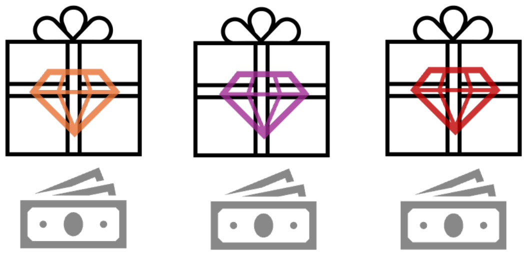
Other heuristics:

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



Pandora's box Gittins index

Pandora's box



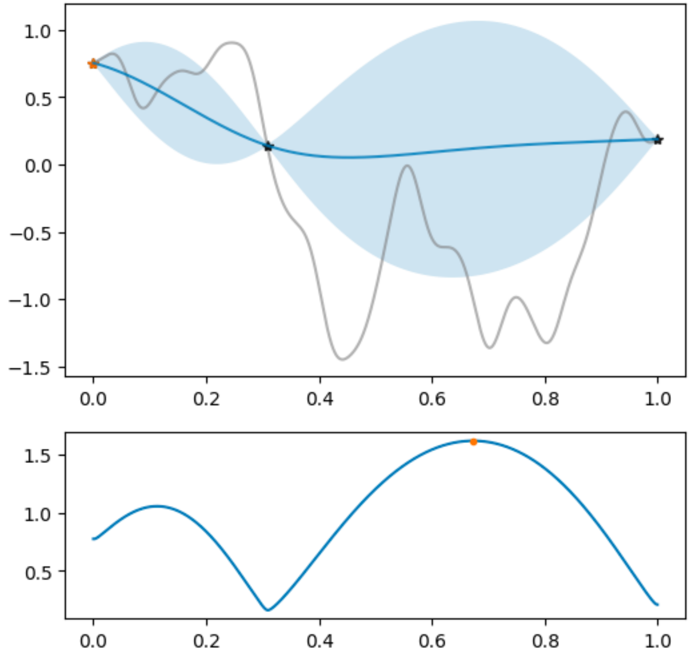
$\alpha^*(x)$: Gittins index function

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

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

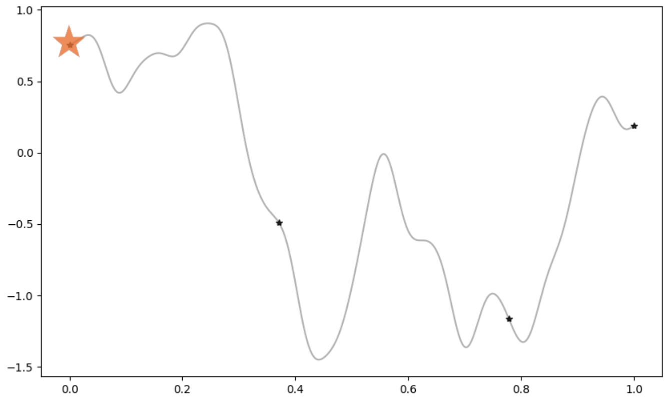
PBGI policy: evaluate $\mathrm{argmax}_x\, \alpha^*(x)$

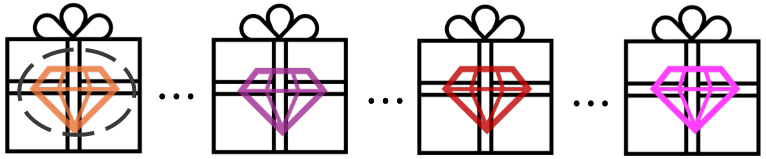
D: observed data

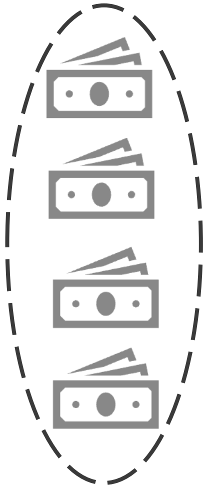
$\alpha^*(x)$: solution to $\mathrm{EI}_{f|D}(x; \alpha^*(x)) = \lambda$

Our Contributions

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



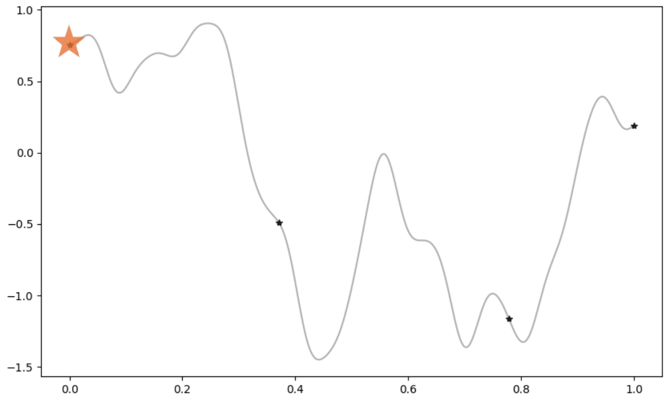


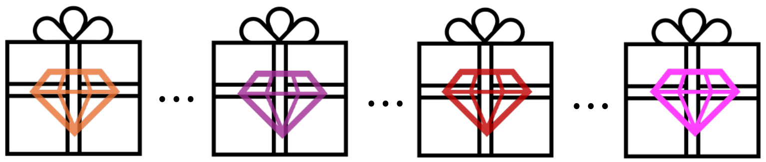


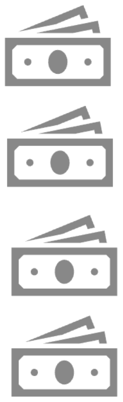
Our work ⟸ Pandora’s Box Gittins index

Our Contributions

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





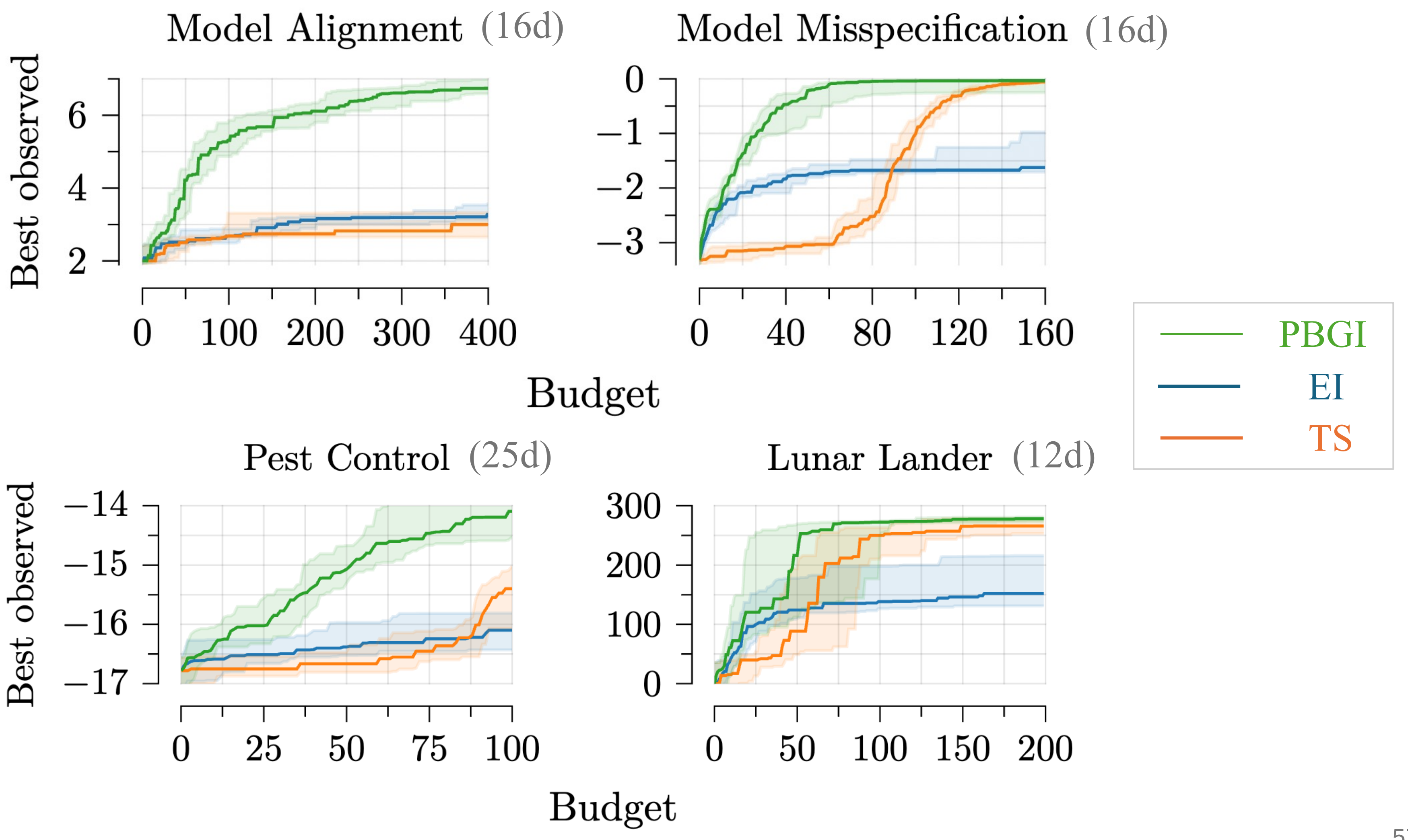


Our work $\Longleftarrow$ Pandora’s Box Gittins index

Experiment Results: PBGI vs EI vs TS

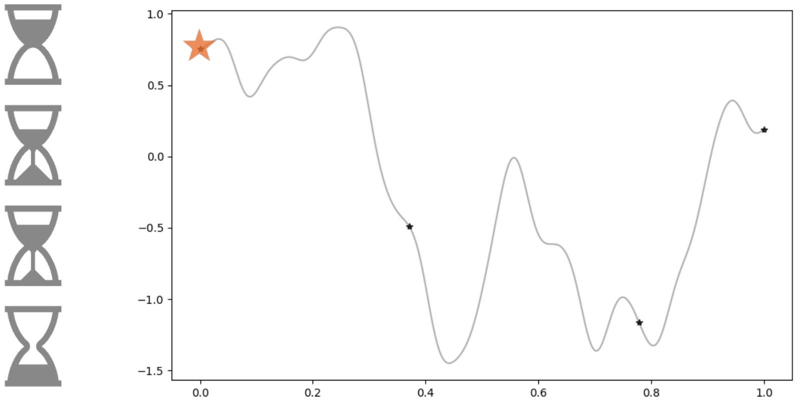
Synthetic

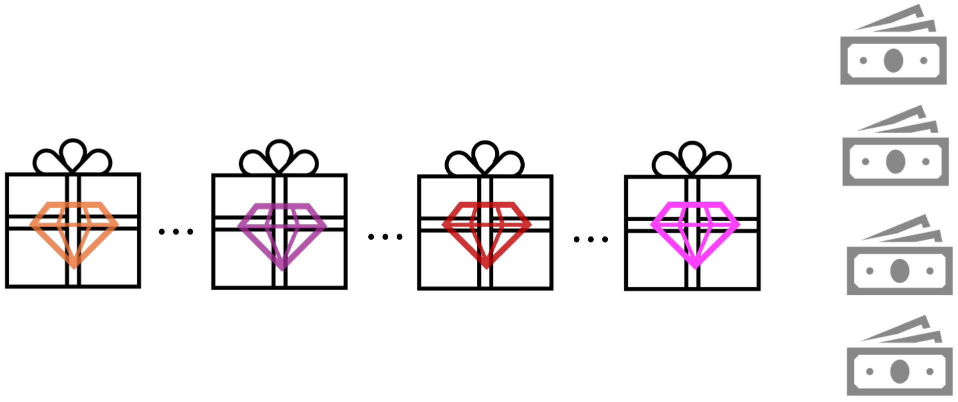
Empirical



Conclusions

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





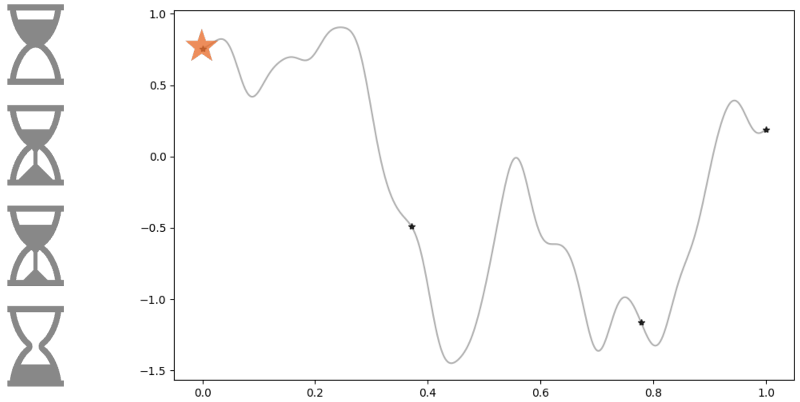
Our work $\Longleftarrow$ Pandora's box Gittins index

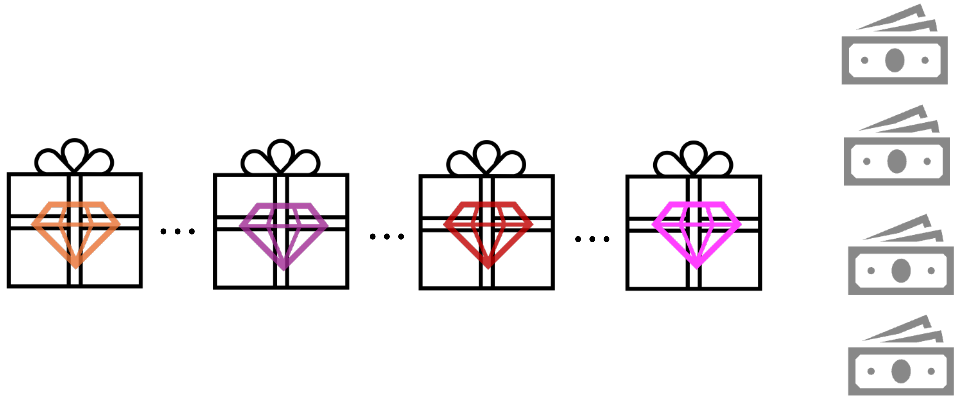
Check our preprint on arXiv!

Conclusions

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

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





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

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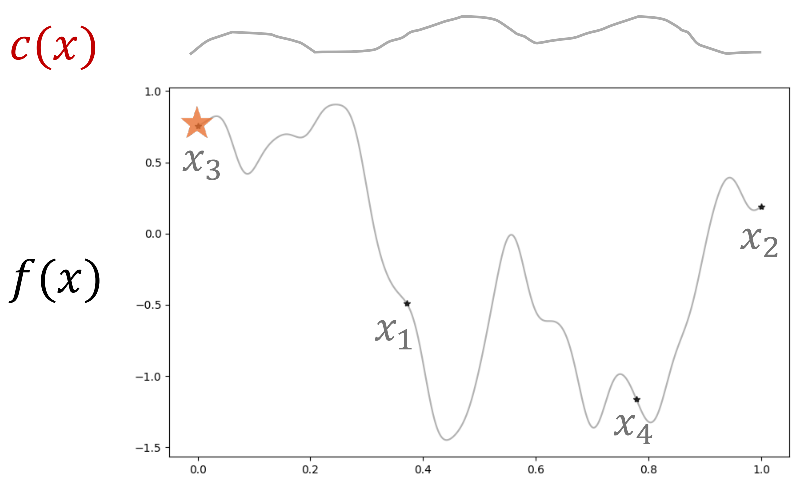
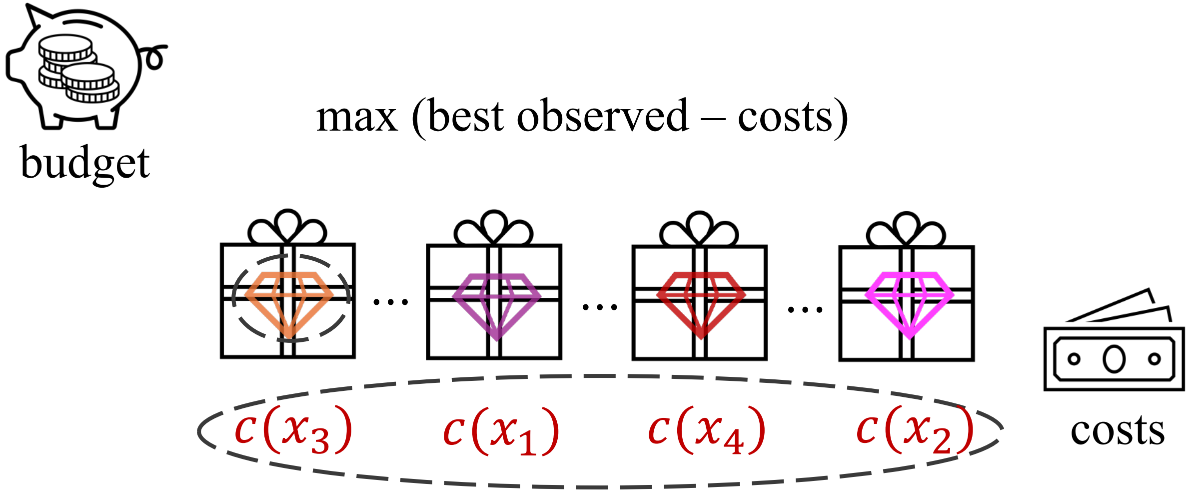
Conclusions

- 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





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

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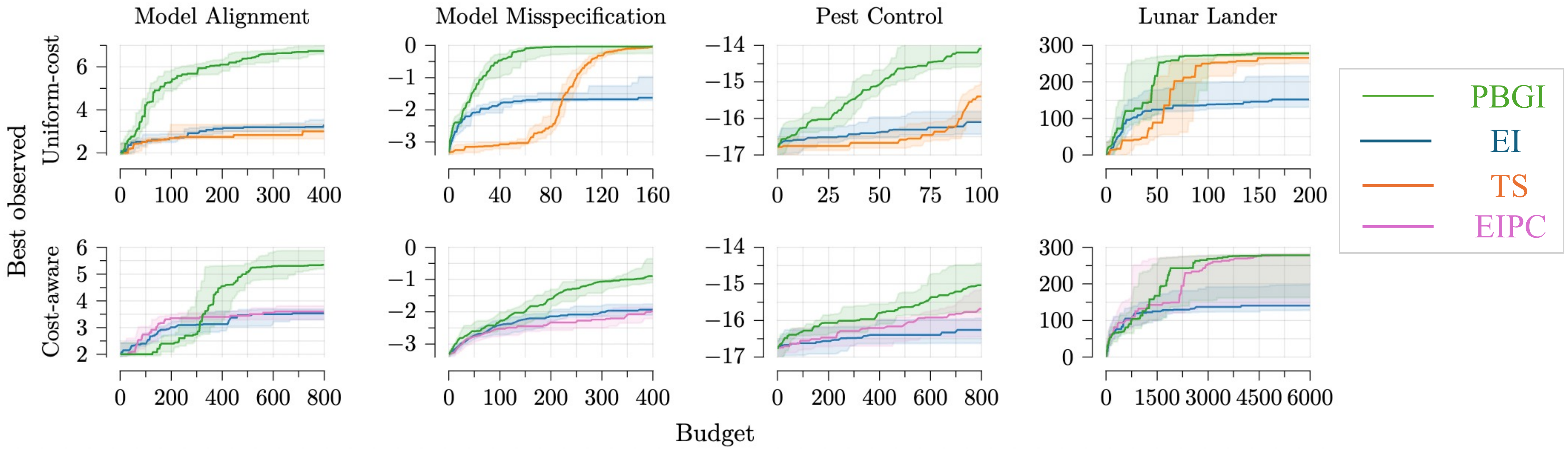
Heterogeneous-cost Experiment Results

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



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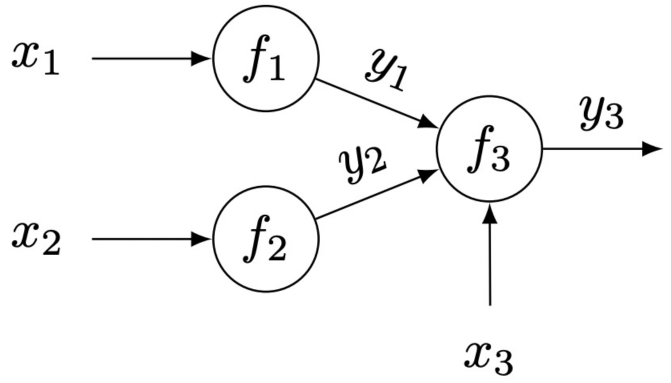
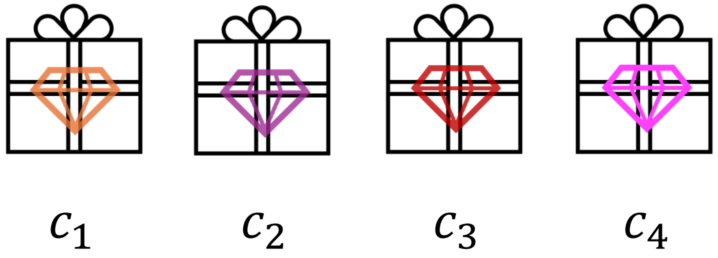
Conclusions

- 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.)





? $\Longleftarrow$ Pandora's Box Gittins index

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