

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

NYC Ops Day'24 Joint PhD Colloquium

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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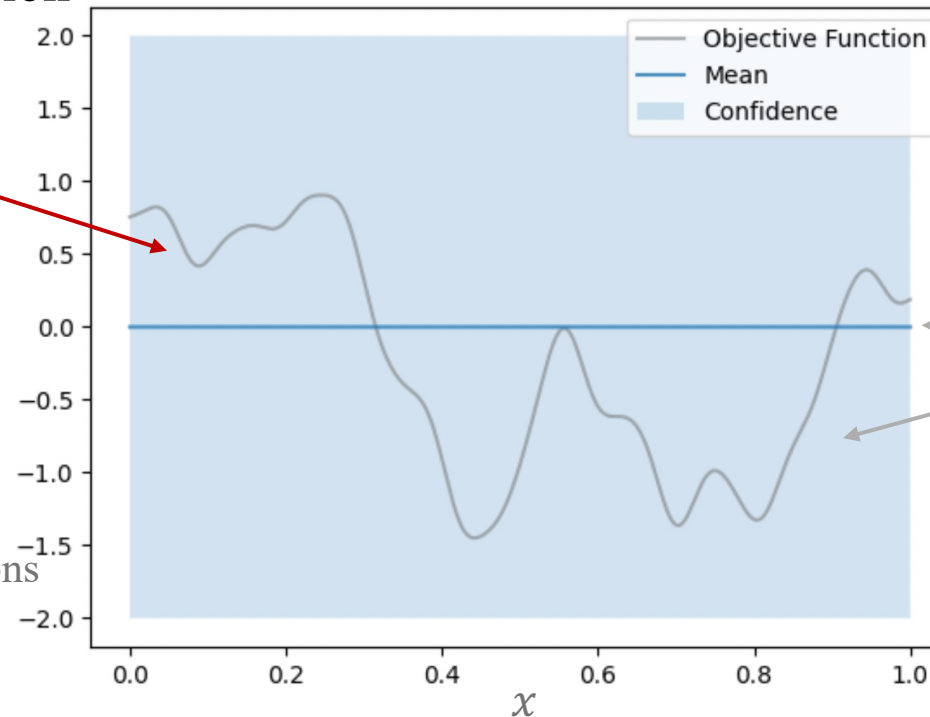
Control design

Bayesian Optimization

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

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

Gaussian process: infinite-dimensional generalization of multivariate normal distributions



Applications:

Hyperparameter tuning
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x : hyperparameter/configuration

mean: prediction

variance: confidence/uncertainty

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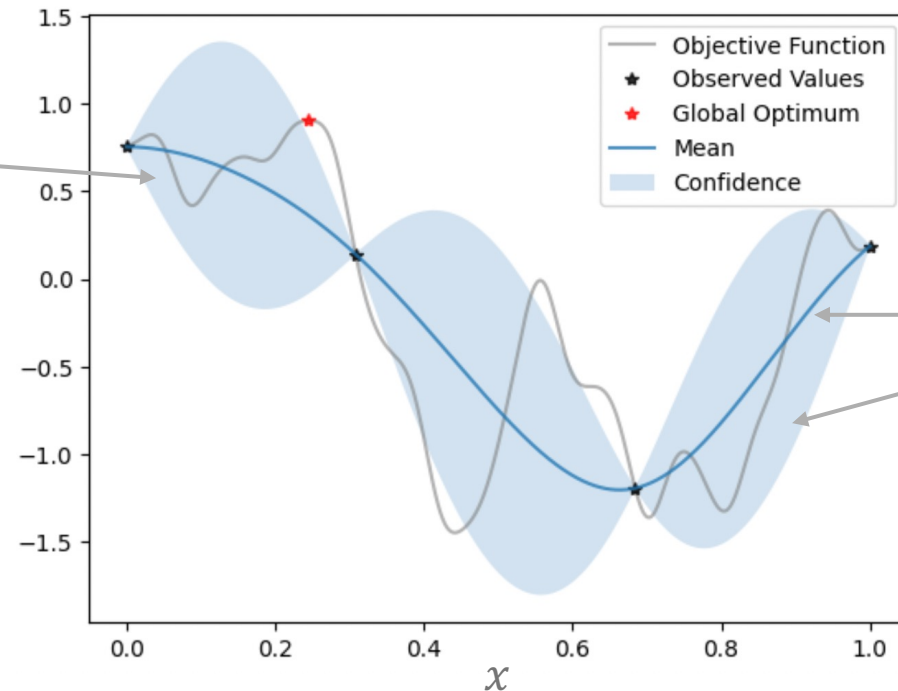
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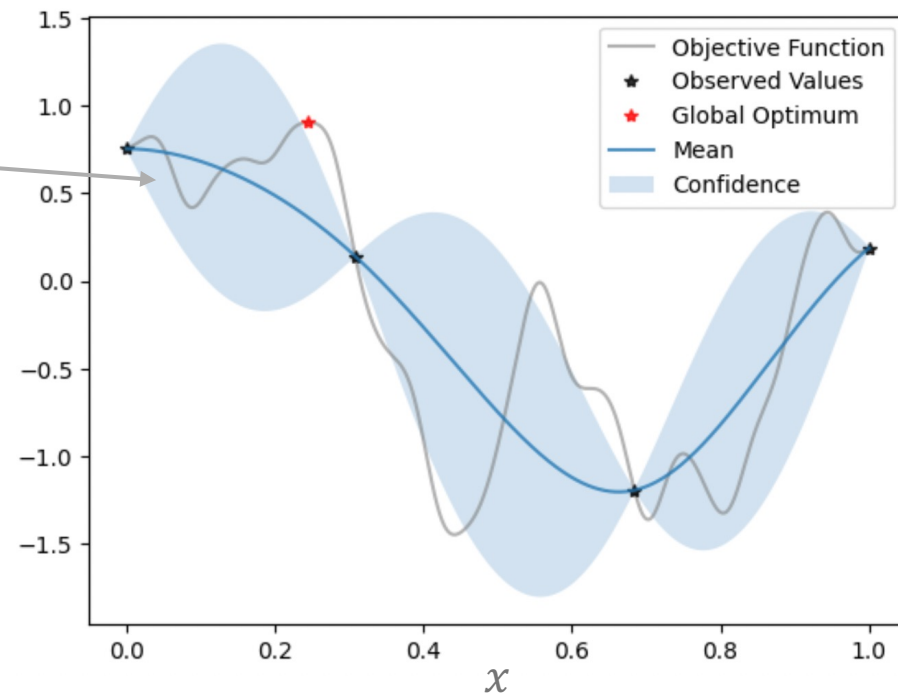
Objective: find global optimum $x^* = \operatorname{argmax}_{x \in \mathcal{X}} f(x)$

Decision: evaluate a set of points

Bayesian Optimization

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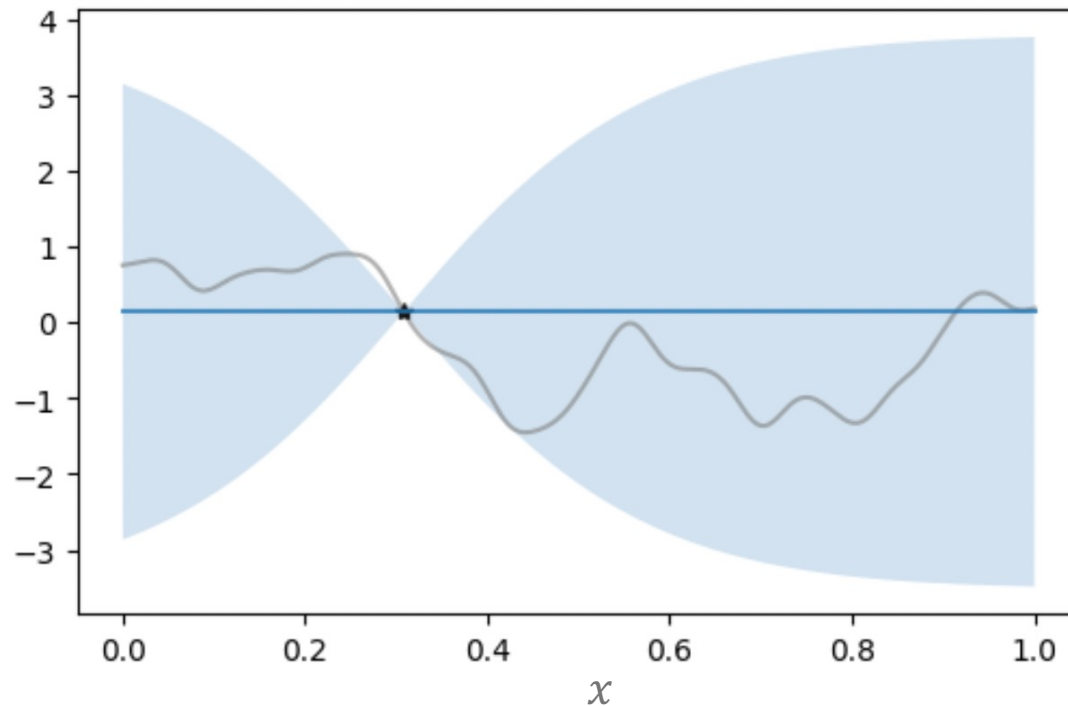
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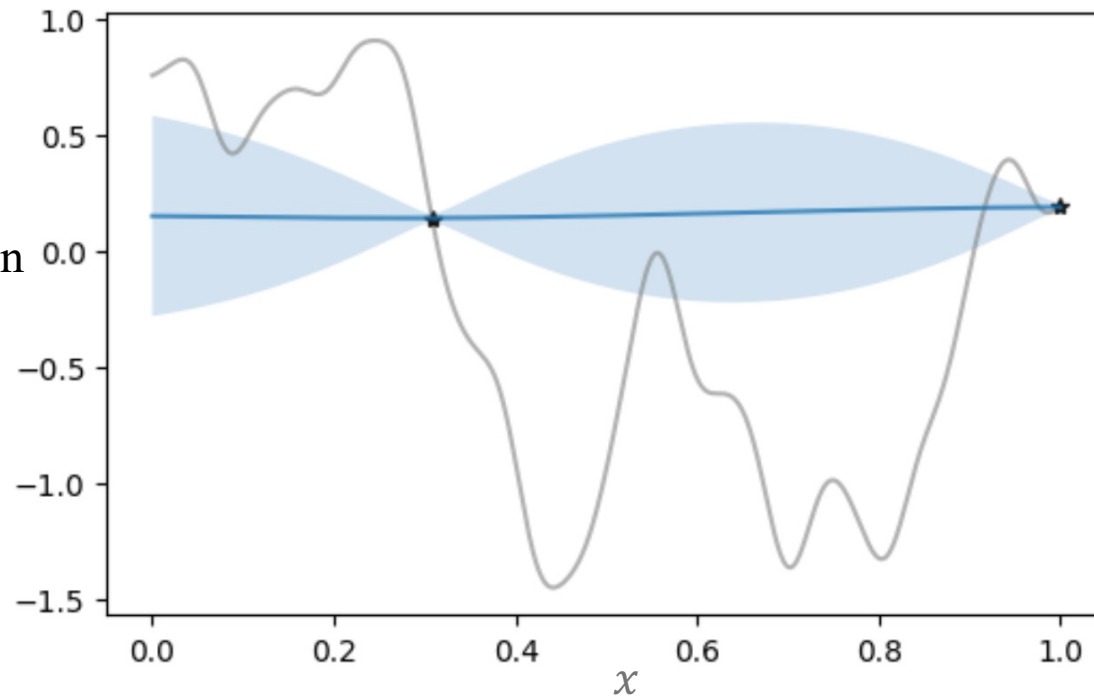
adaptively

Decision: evaluate a set of points

Bayesian Optimization

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Applications:

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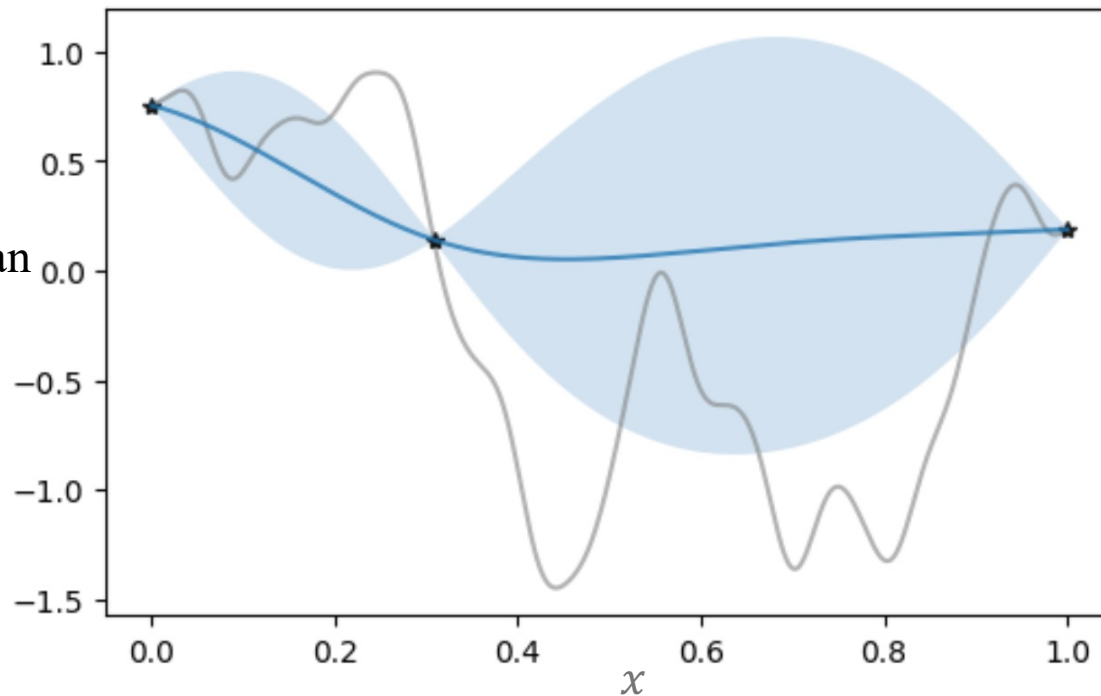
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Bayesian Optimization

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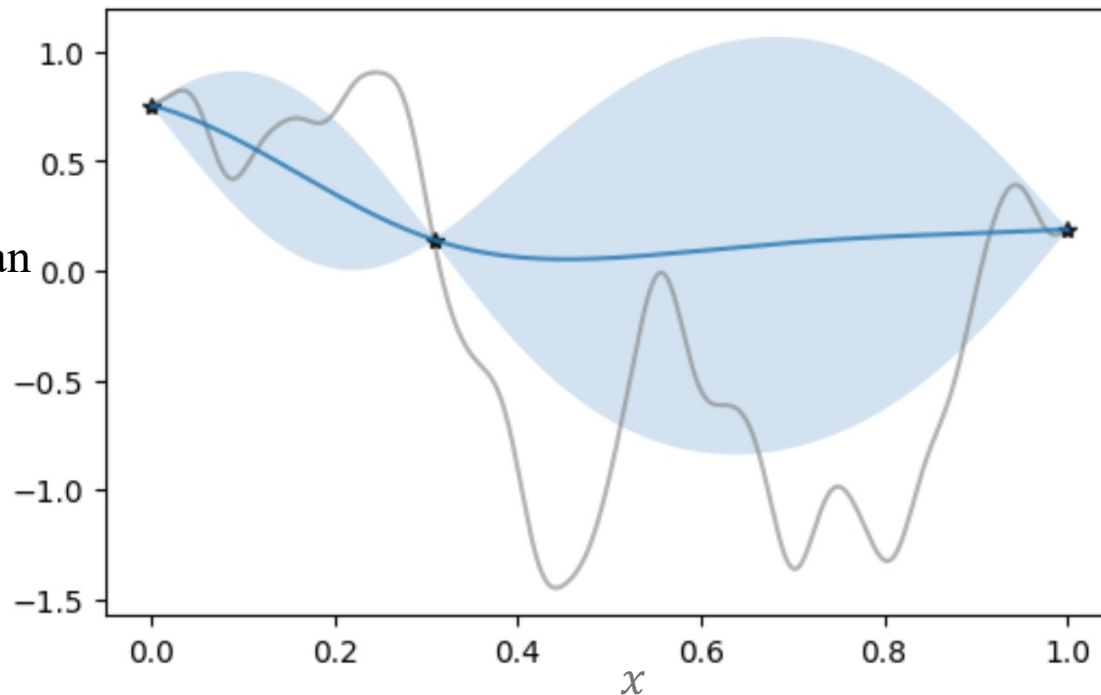
x : hyperparameter/configuration

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

Bayesian Optimization

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x : hyperparameter/configuration

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

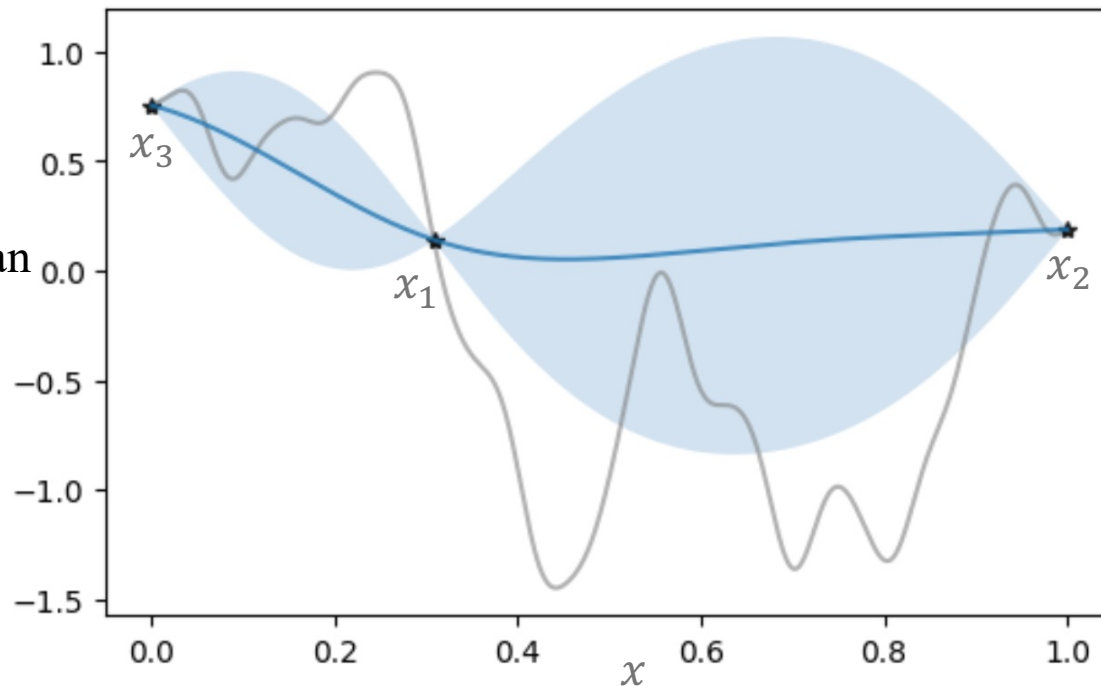
$x_1, x_2, \dots, x_T \in \mathcal{X}$

T : time budget

Bayesian Optimization

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

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



Applications:

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x : hyperparameter/configuration

Objective: optimize best observed value at time T

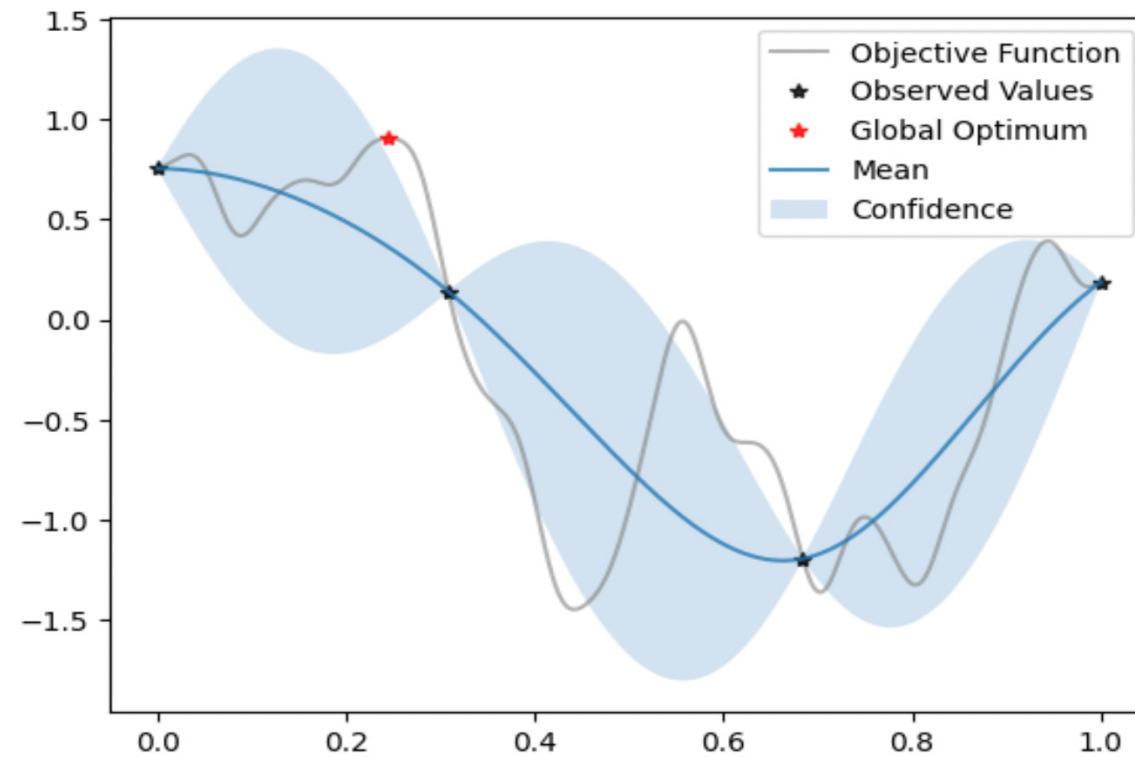
$$\max_{\text{policy}} \mathbb{E} \max_{t=1,2,\dots,T} f(x_t)$$

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

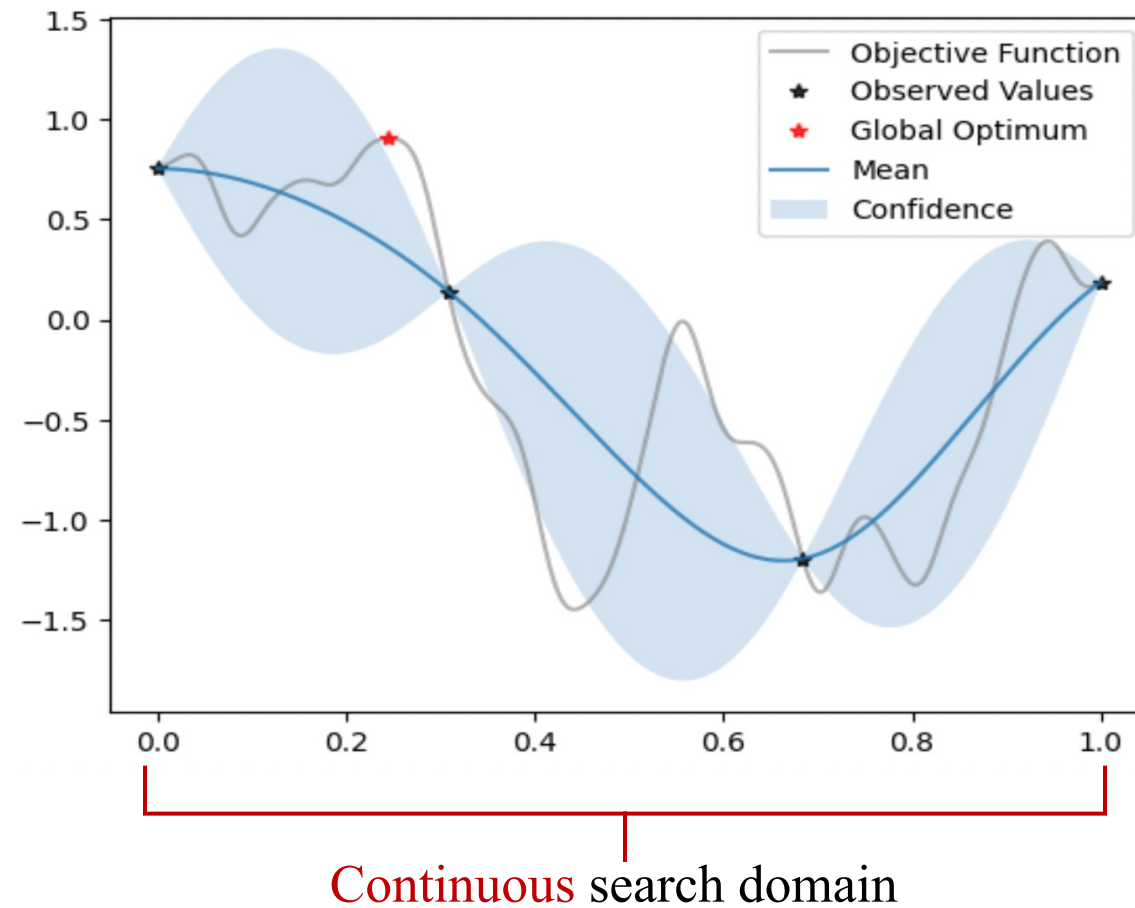
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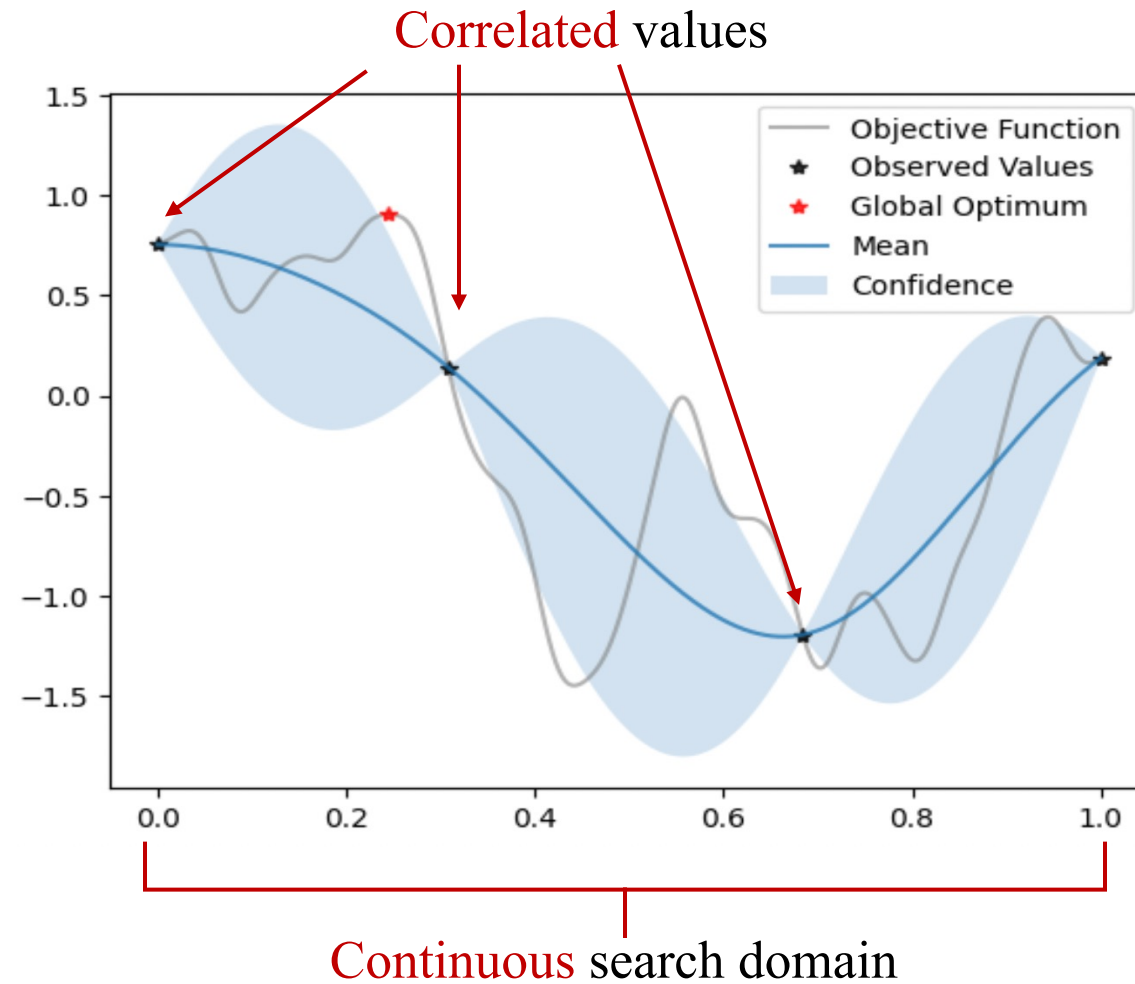
Why is it hard?



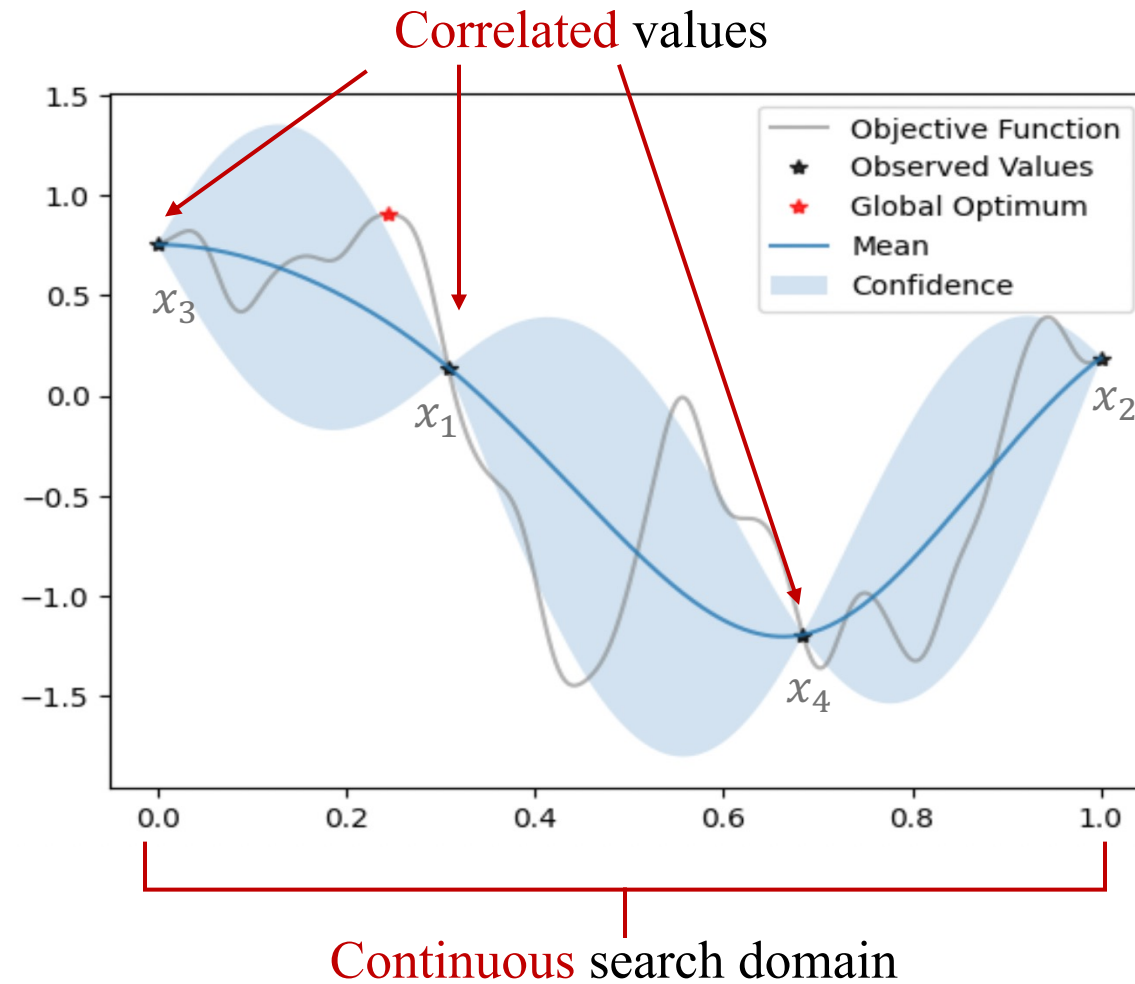
Why is it hard?



Why is it hard?



Why is it hard?



Hard budget constraint

~~$t=1$~~



~~$t=2$~~



~~$t=3$~~



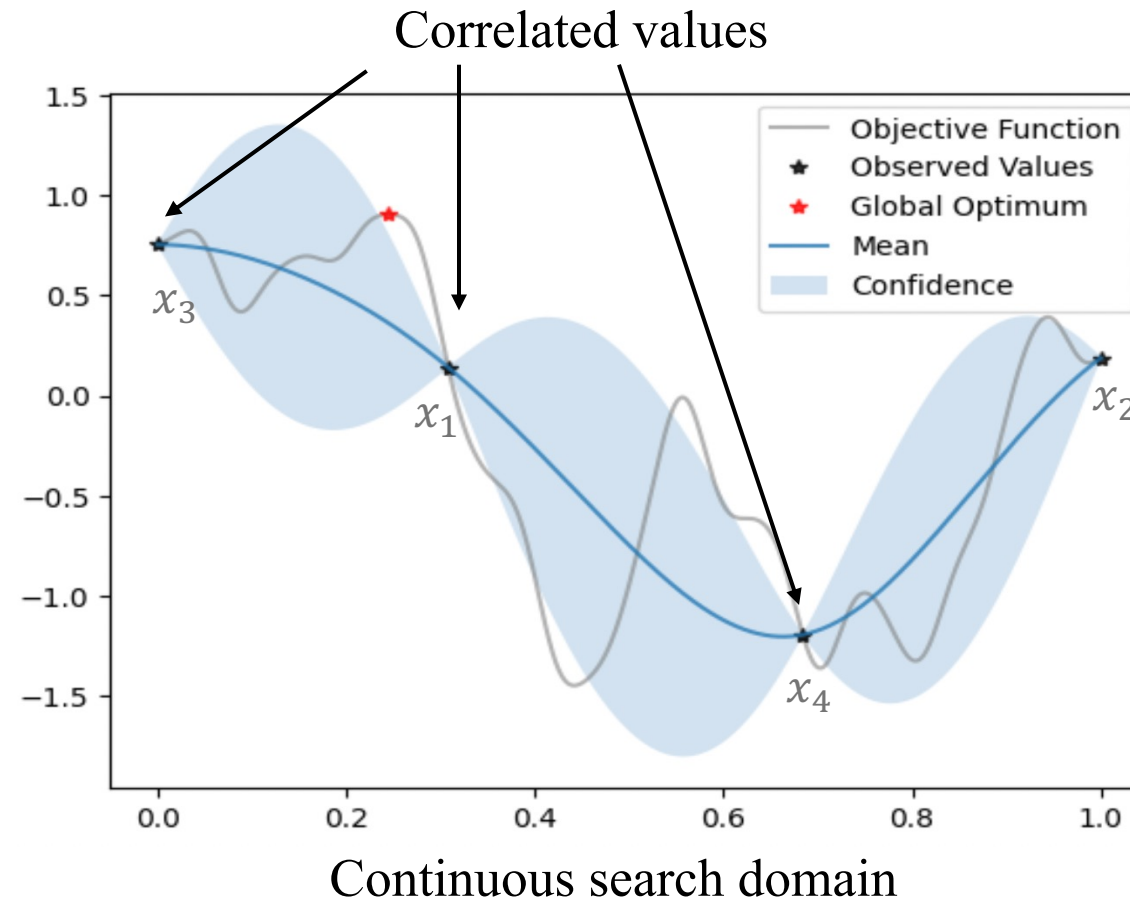
~~$t=4$~~







\vdots

~~$t=T$~~

Why is it hard?

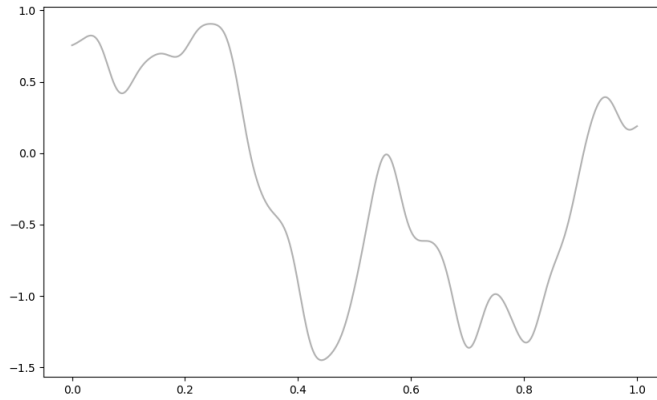


Hard budget constraint

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

\Rightarrow Optimal policy unknown!

Bayesian Optimization

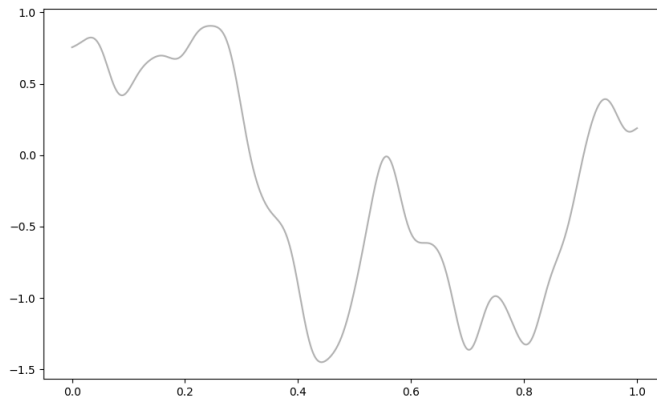


Continuous

Correlated

Hard budget constraint

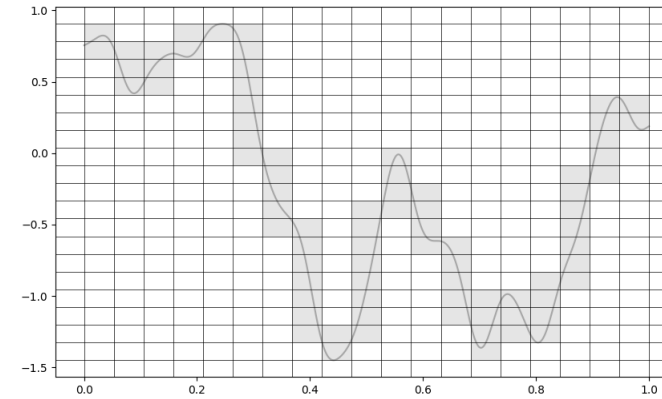
Bayesian Optimization



Continuous

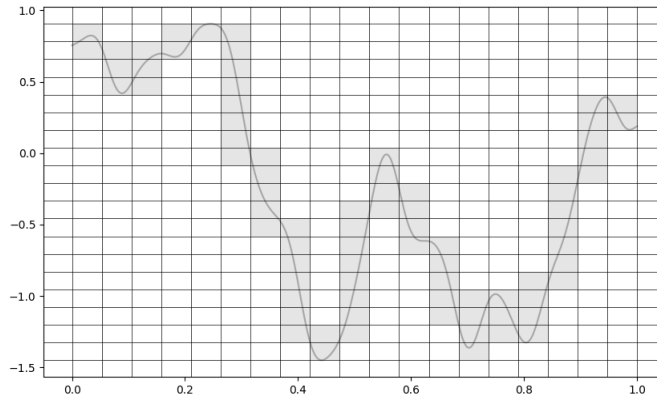
Correlated

Hard budget constraint



Discrete

Bayesian Optimization



Continuous

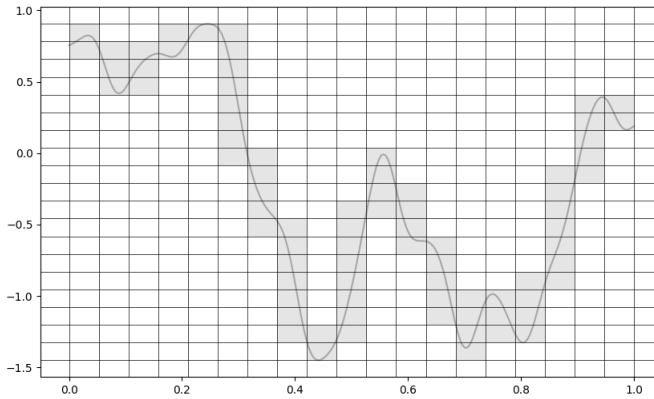


Discrete

Correlated

Hard budget constraint

Bayesian Optimization



Continuous



Discrete

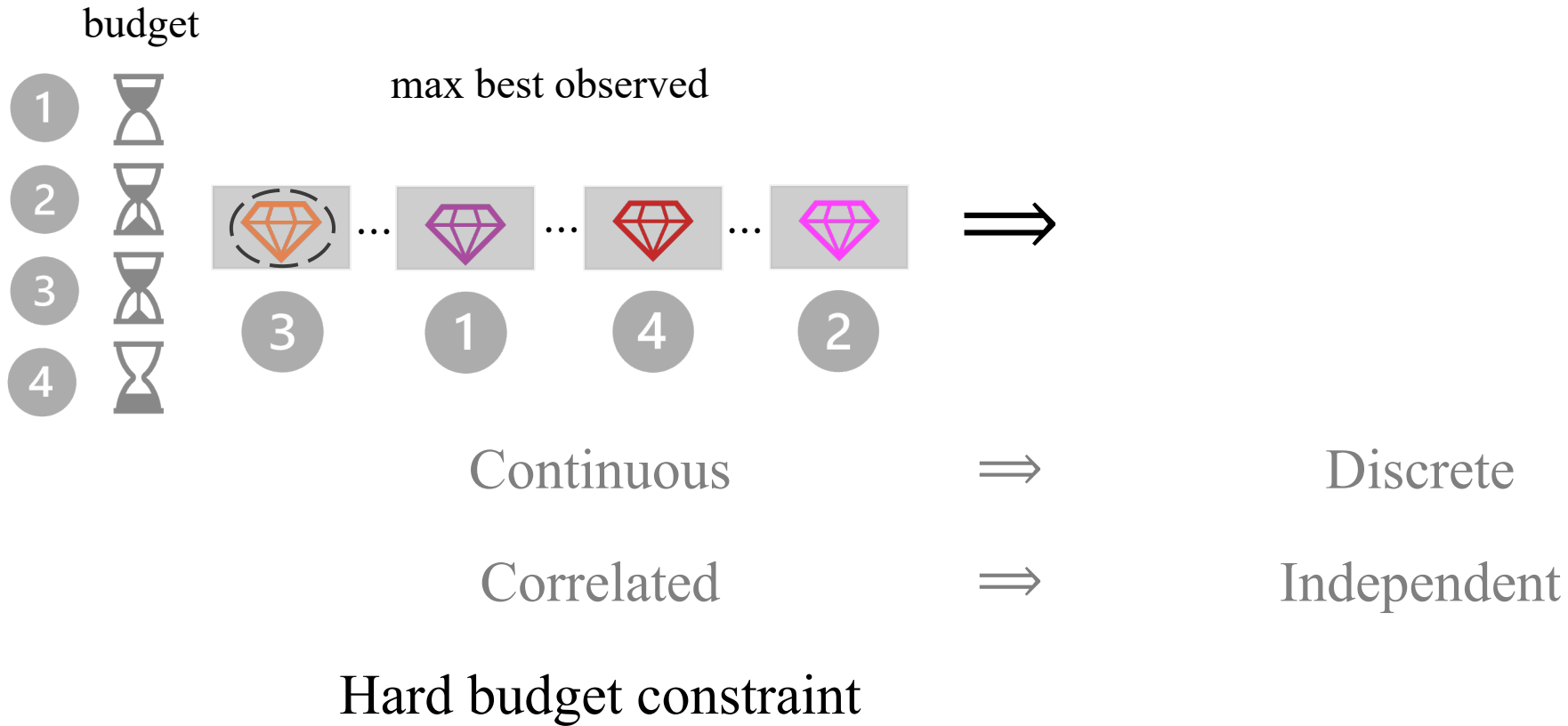
Correlated



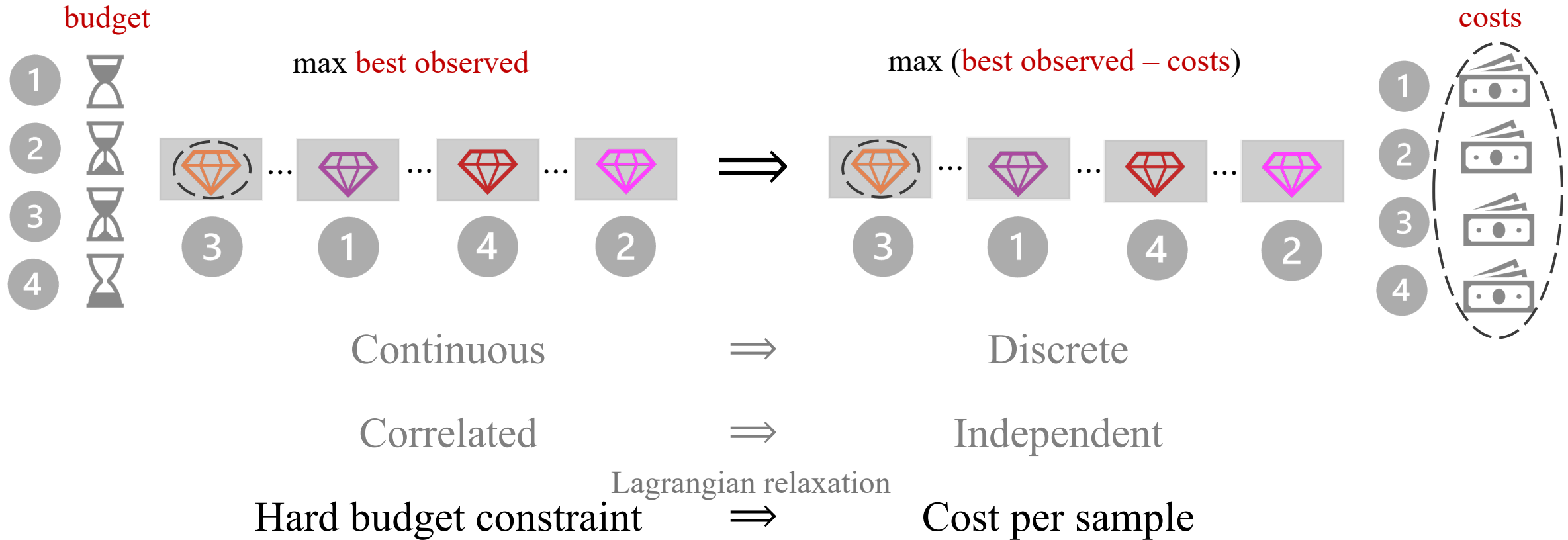
Independent

Hard budget constraint

Bayesian Optimization

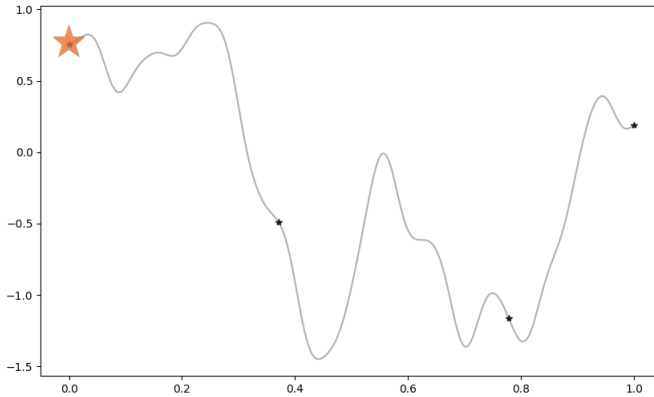


Bayesian Optimization



Bayesian Optimization \Rightarrow Pandora's Box

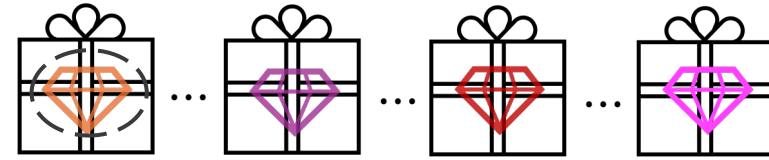
Special case of Markovian/
Bayesian multi-armed bandits



Continuous

Correlated

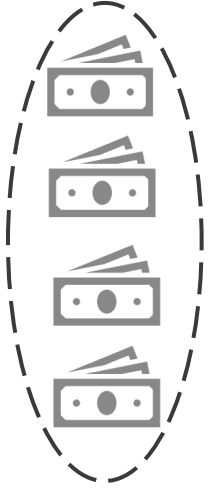
Hard budget constraint



Discrete

Independent

Cost per sample



Bayesian Optimization \Rightarrow Pandora's Box

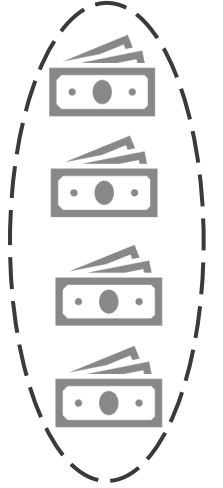
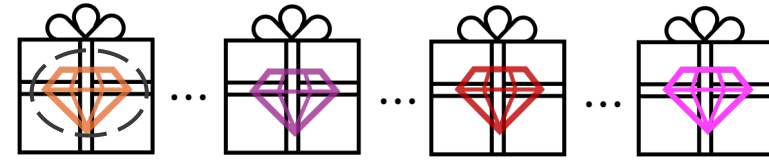
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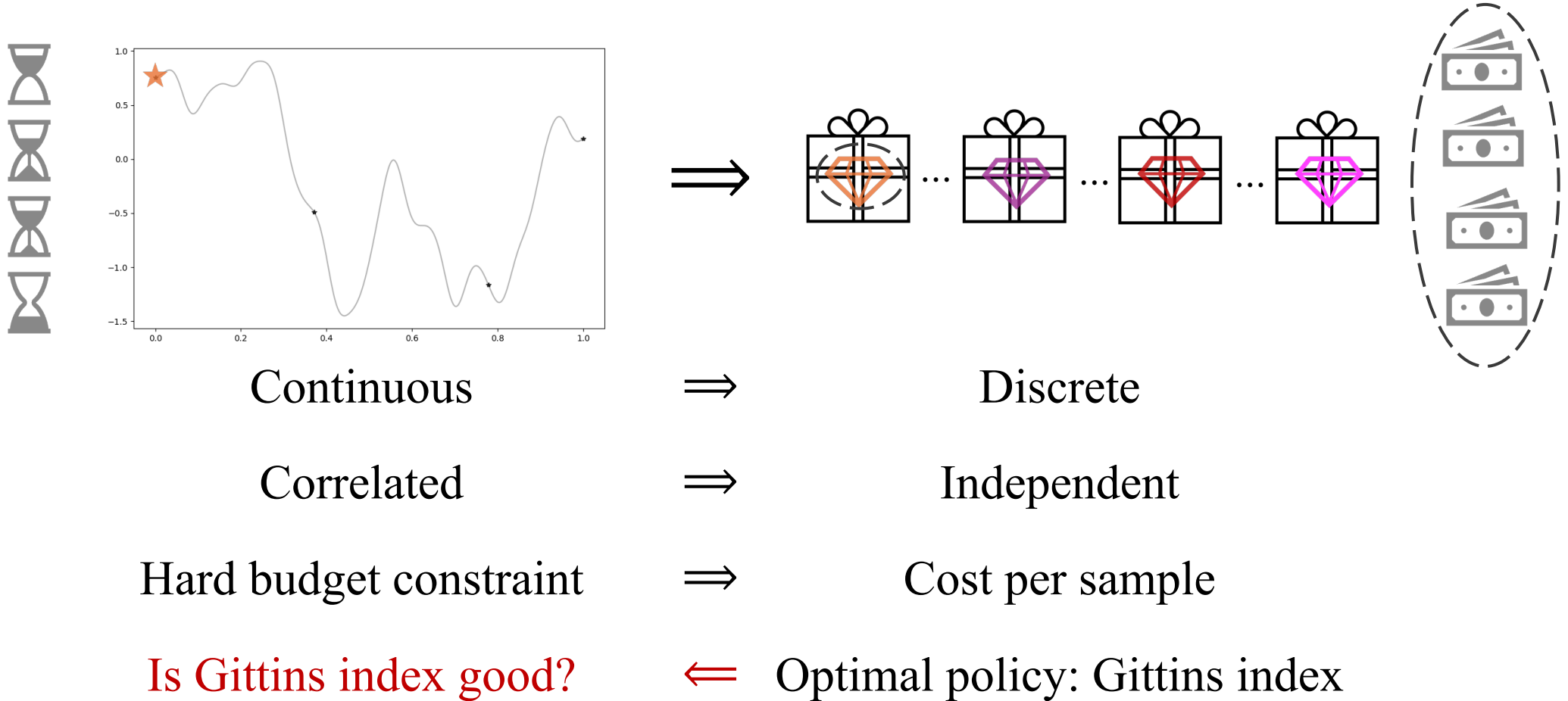
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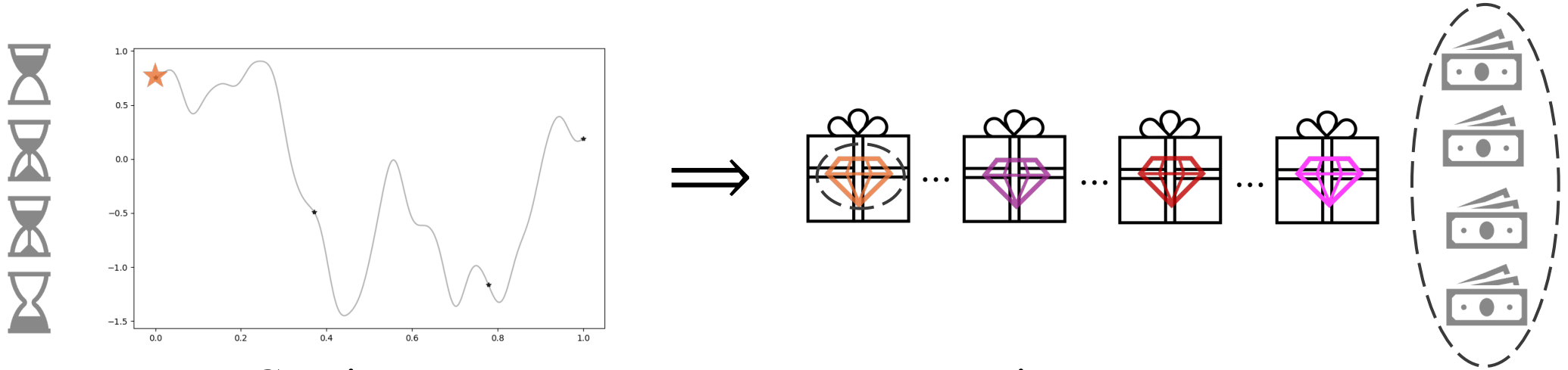
Cost per sample

Optimal policy: Gittins index [Weitzman'79]

Bayesian Optimization \Rightarrow Pandora's Box

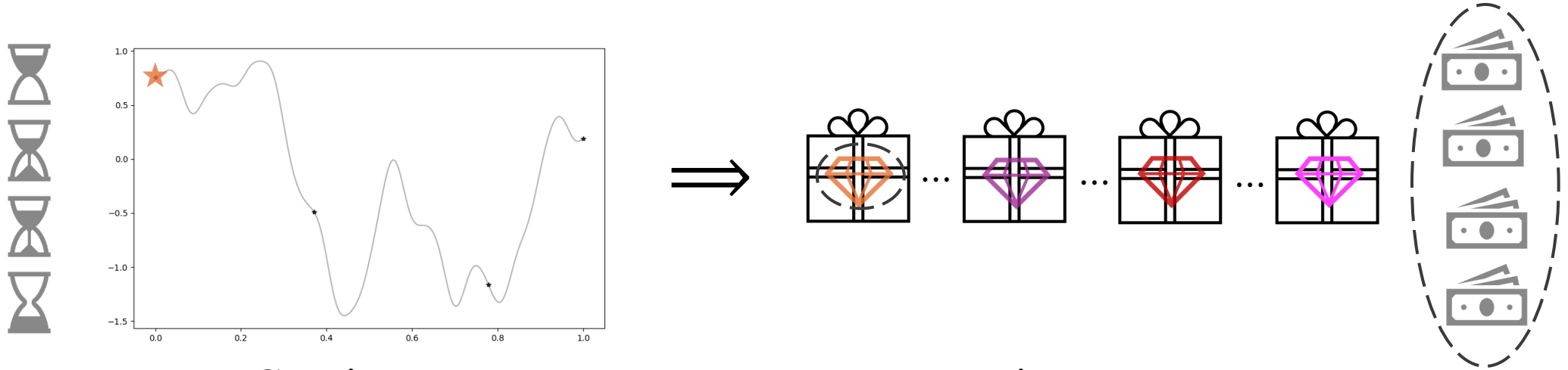


Bayesian Optimization \Rightarrow Pandora's Box



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

Bayesian Optimization \Rightarrow Pandora's Box



Continuous

\Rightarrow

Discrete

Correlated

\Rightarrow

Independent

Hard budget constraint

\Rightarrow

Cost per sample

Is Gittins index good?

How to translate?

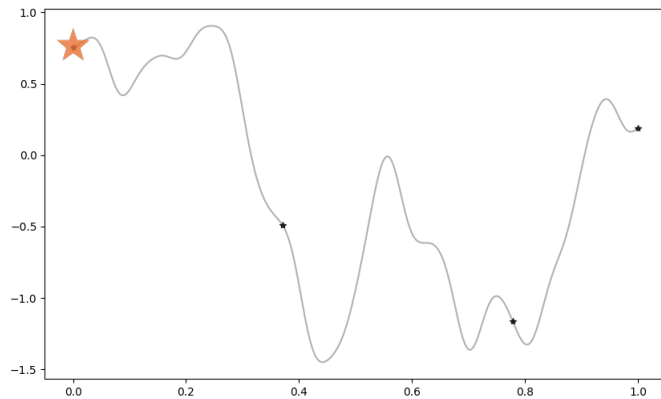
\Leftarrow

Optimal policy: Gittins index

Our contributions!

Our Contributions

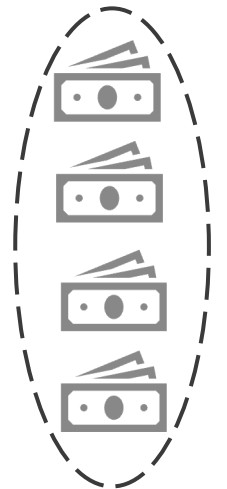
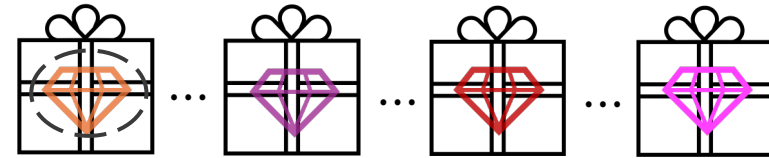
- How to translate?
- Is Pandora's Box Gittins index (PBGI) good?



?

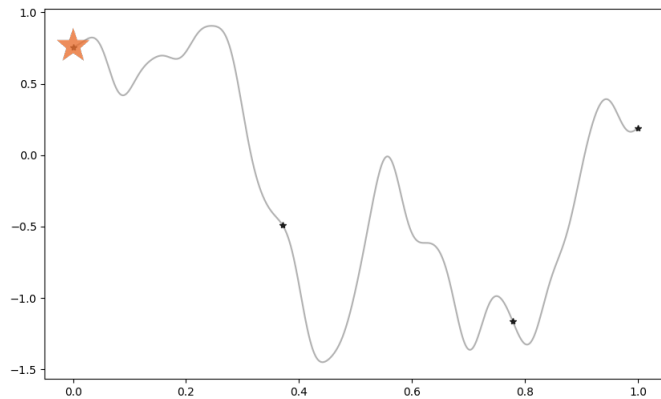


Pandora's Box Gittins index

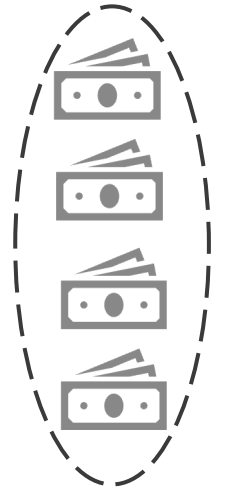
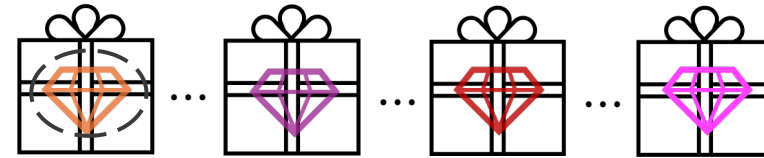


Our Contributions

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



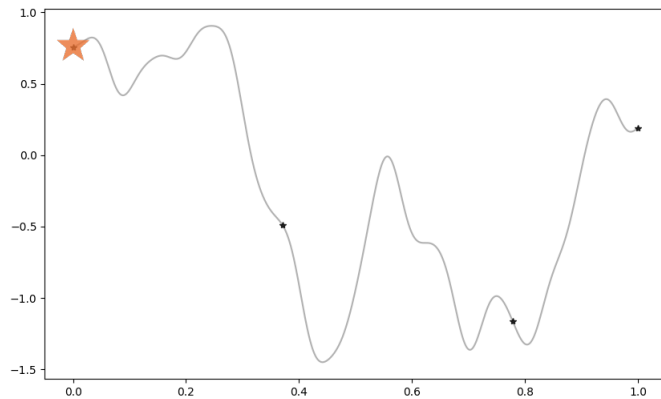
Our work



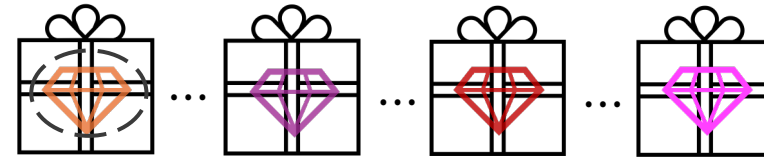
Pandora's Box Gittins index

Our Contributions

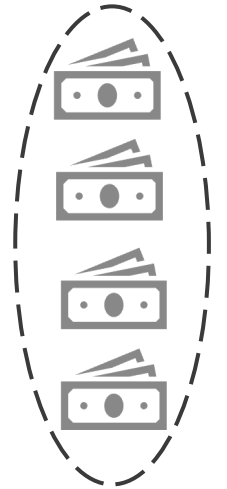
- Develop PBGI policy for Bayesian optimization
- Show **performance** against baselines on synthetic & empirical experiments



Our work

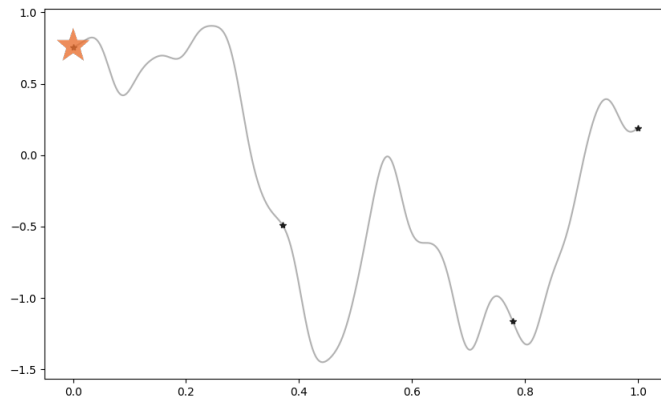


Pandora's Box Gittins index



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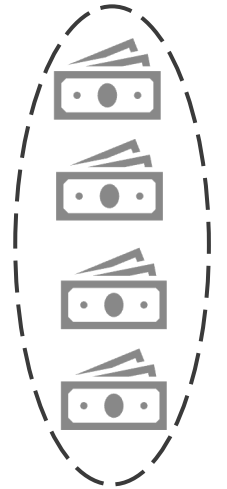
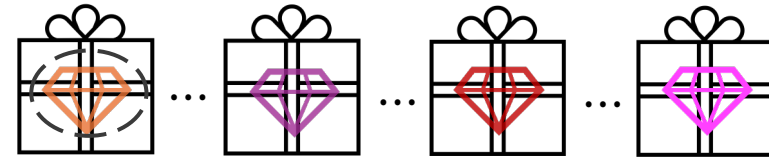
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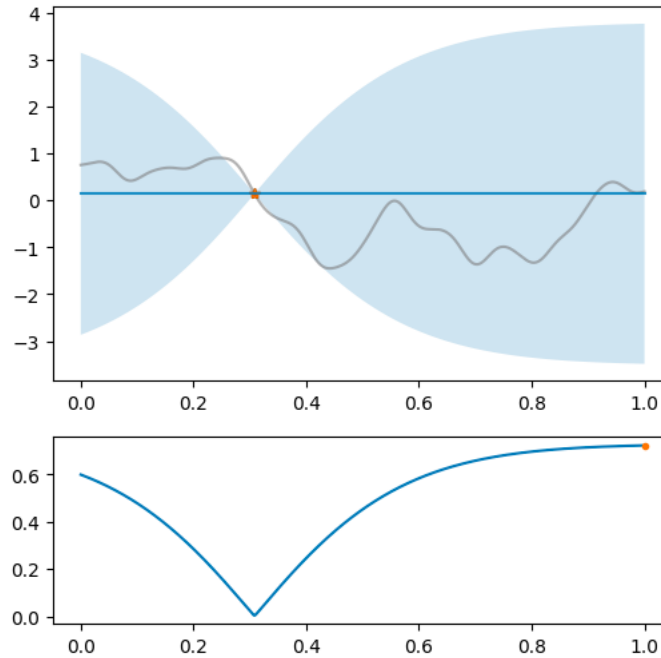


Pandora's Box Gittins index



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

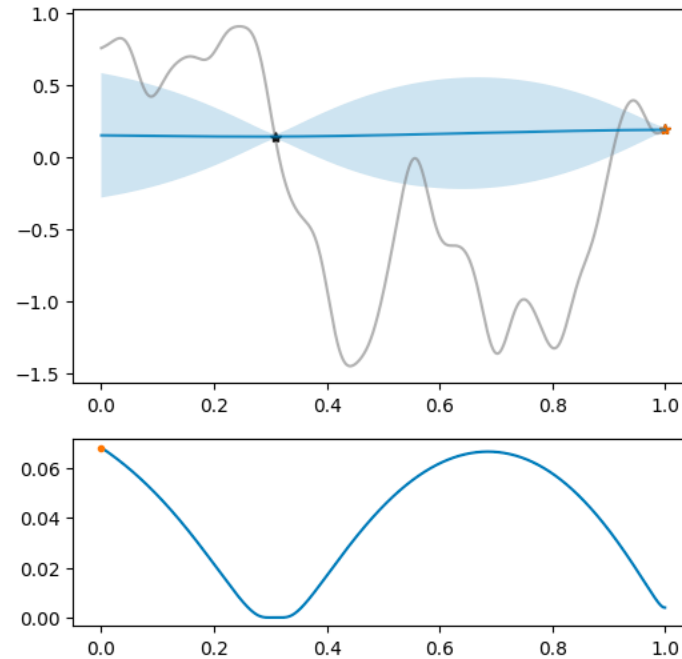
$$\text{EI}_{f|D}(x; y) = \mathbb{E}[(f|D)(x) - y]^+$$

D : observed data

y_{best} : current best observed value

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

Popular One-step Heuristic: EI



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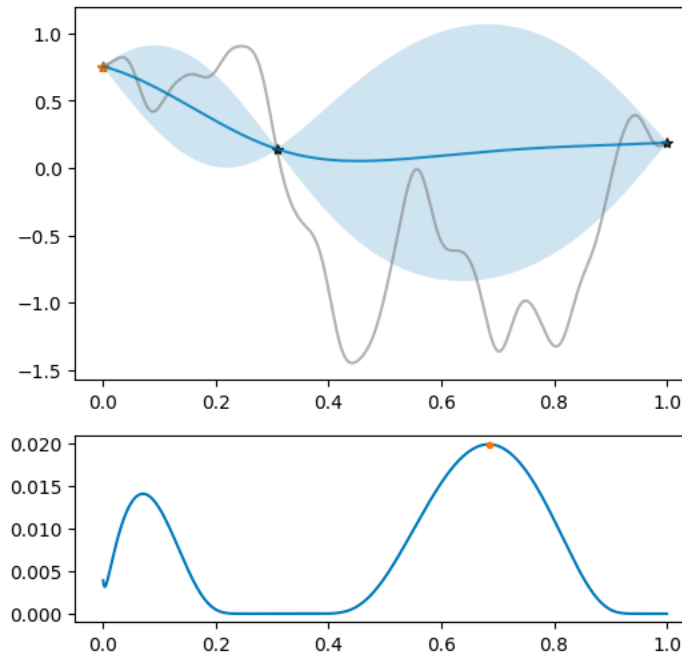
$$\text{EI}_{f|D}(x; y) = \mathbb{E}[(f(x) - y)^+]$$

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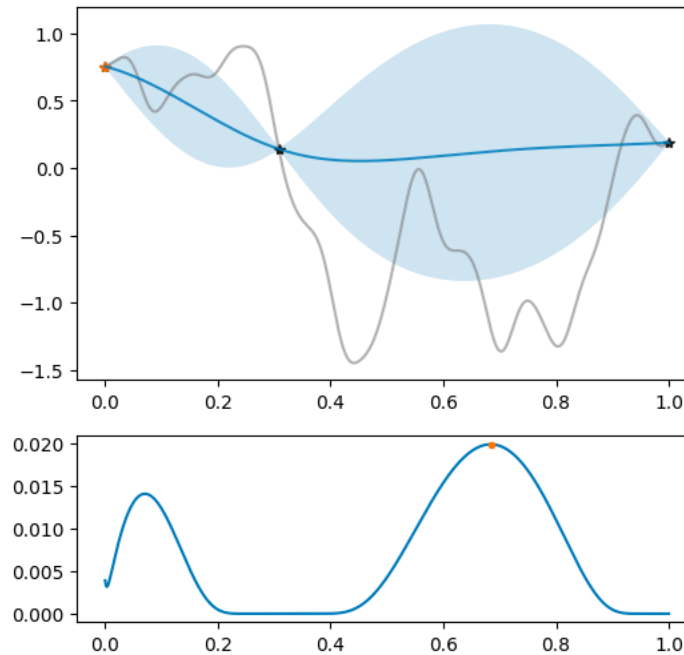
Popular One-step Heuristic: EI

Other heuristics:

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

simple

slow



mean: prediction

variance: confidence/uncertainty

Trade-off between

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

Expected improvement

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

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

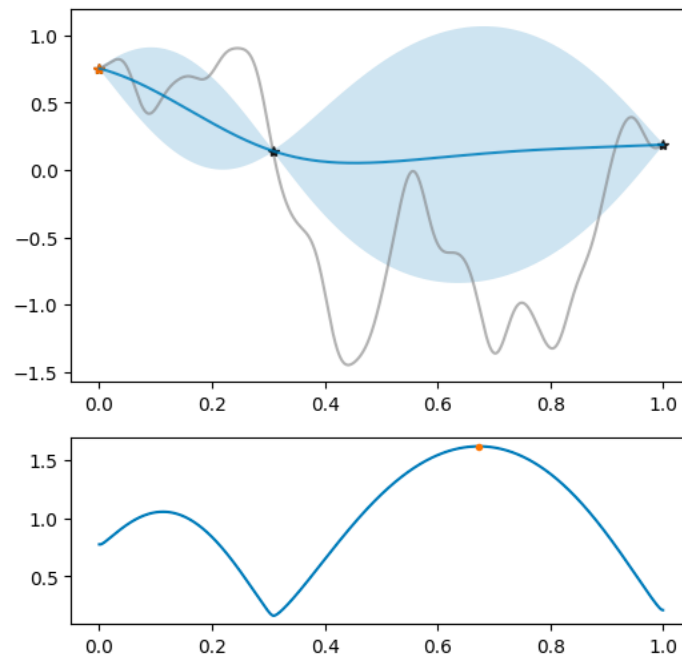
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New One-step Heuristic: PBGI

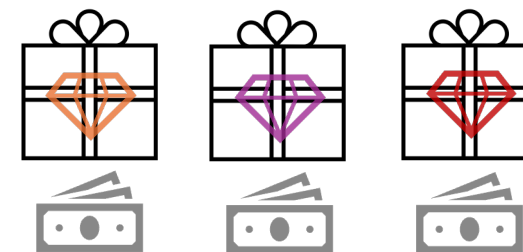
Other heuristics:

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- Multi-step Lookahead EI



Pandora's box Gittins index

Pandora's box



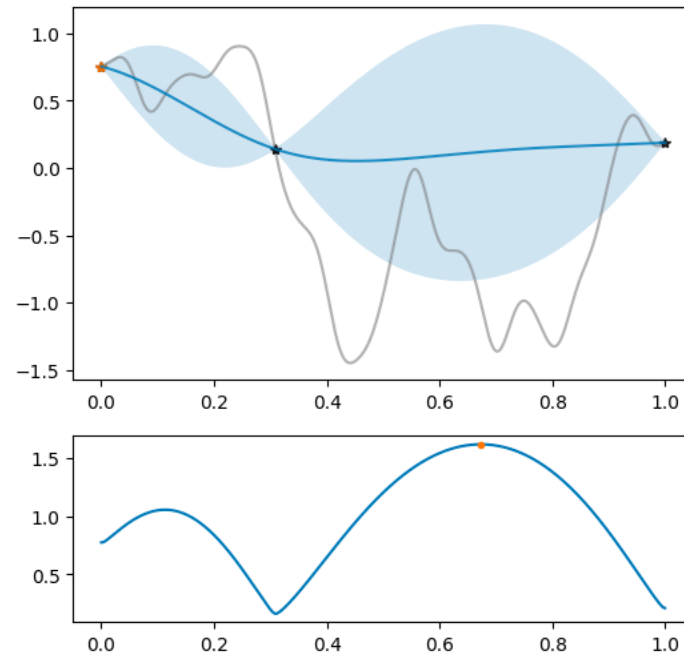
PBGI policy: evaluate $\operatorname{argmax}_x \alpha^*(x)$

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

New One-step Heuristic: PBGI

Other heuristics:

- Upper Confidence Bound
- Thompson Sampling (TS)
- Knowledge Gradient
- Predictive Entropy Search
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Pandora's box Gittins index

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

PBGI policy: evaluate $\arg\max_x \alpha^*(x)$ $\alpha^*(x)$: solution to $\text{EI}_{f|D}(x; \alpha^*(x)) = \lambda$

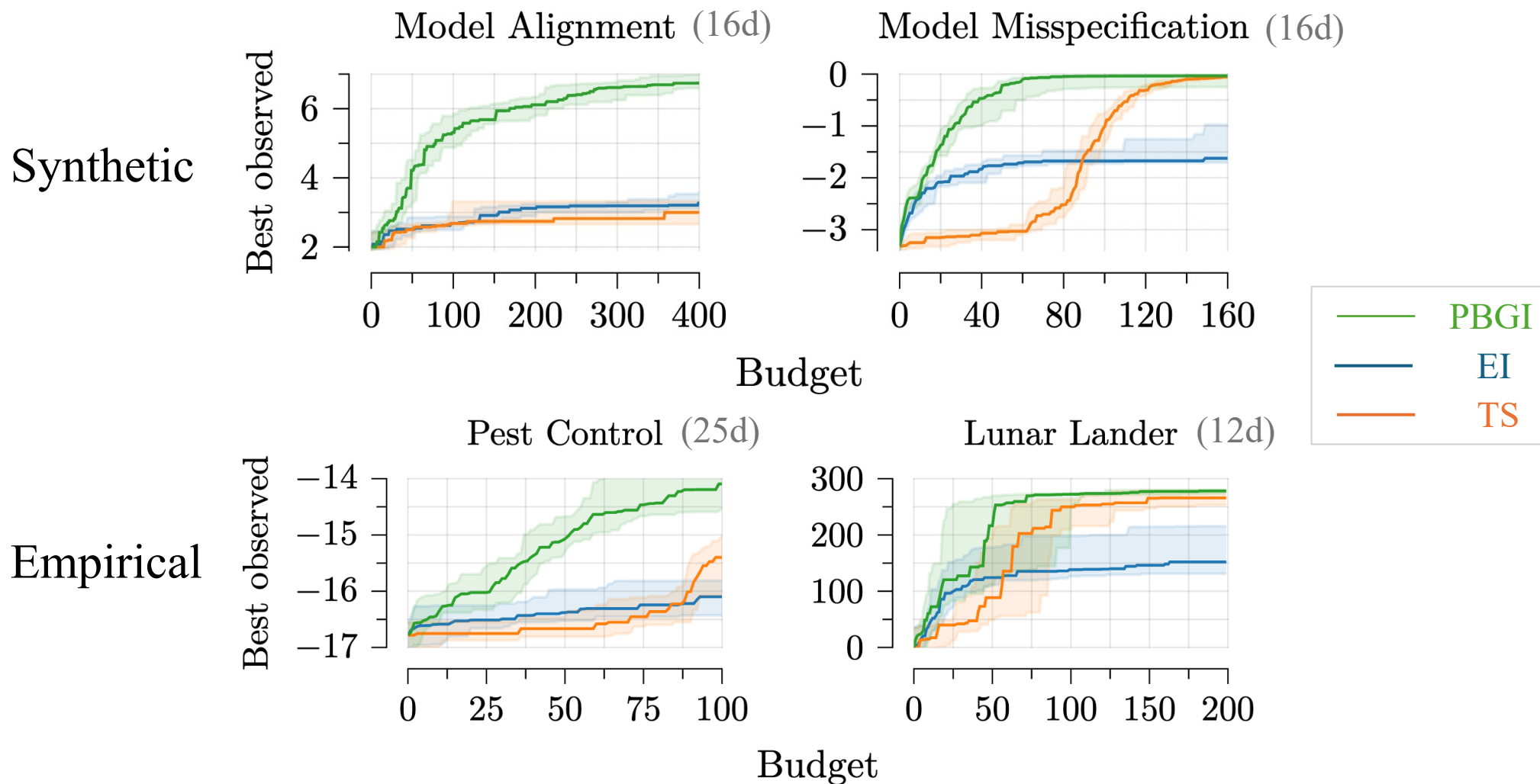
Pandora's box



λ λ λ

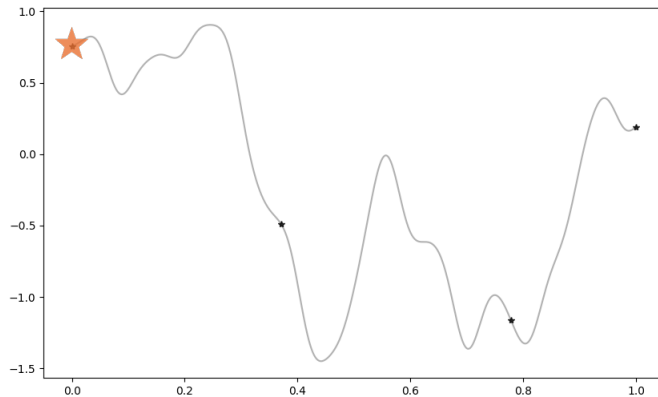
λ : cost-per-sample
(Lagrange multiplier)

Experiment Results: PBGI vs EI vs TS

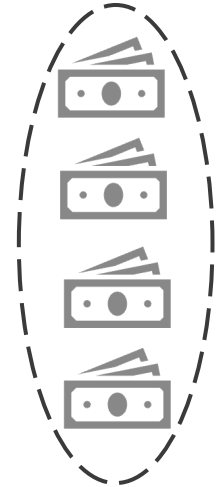
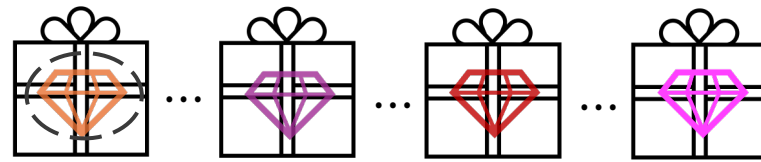


Conclusions

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



Our work

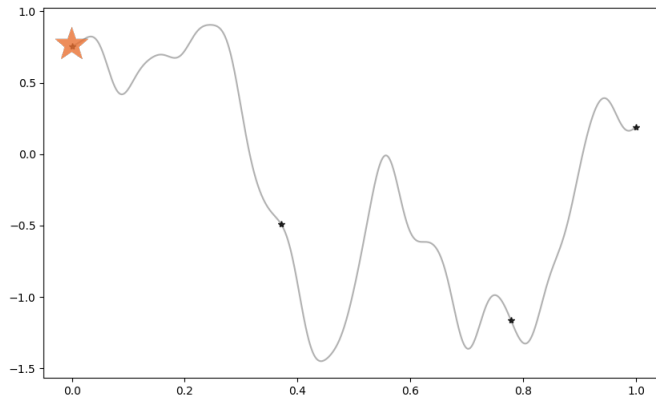


Pandora's box Gittins index

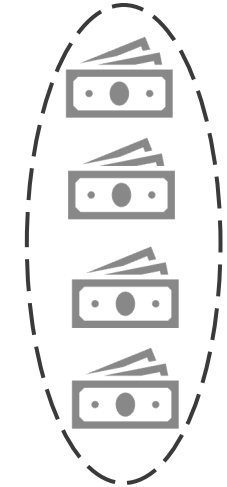
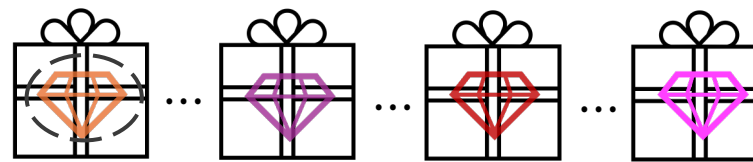
Check our preprint on arXiv!

Conclusions

- Propose easy-to-compute PBGI policy for Bayesian optimization
- Show the **effectiveness of PBGI** on synthetic & empirical experiments particularly on medium-high dimensions and relatively-large domains!



Our work

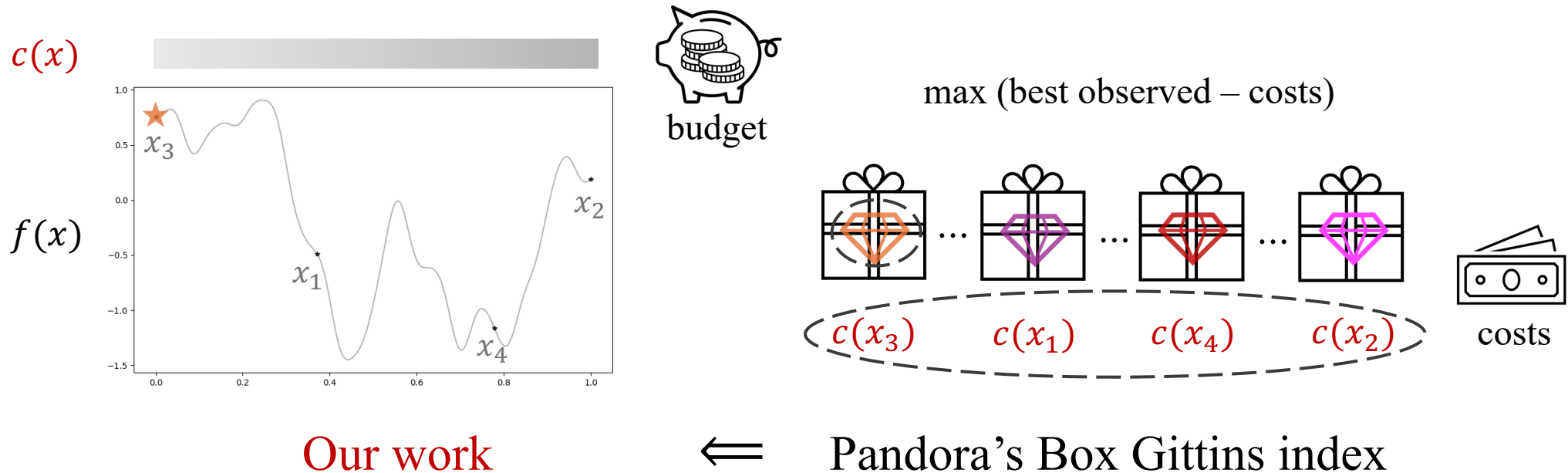


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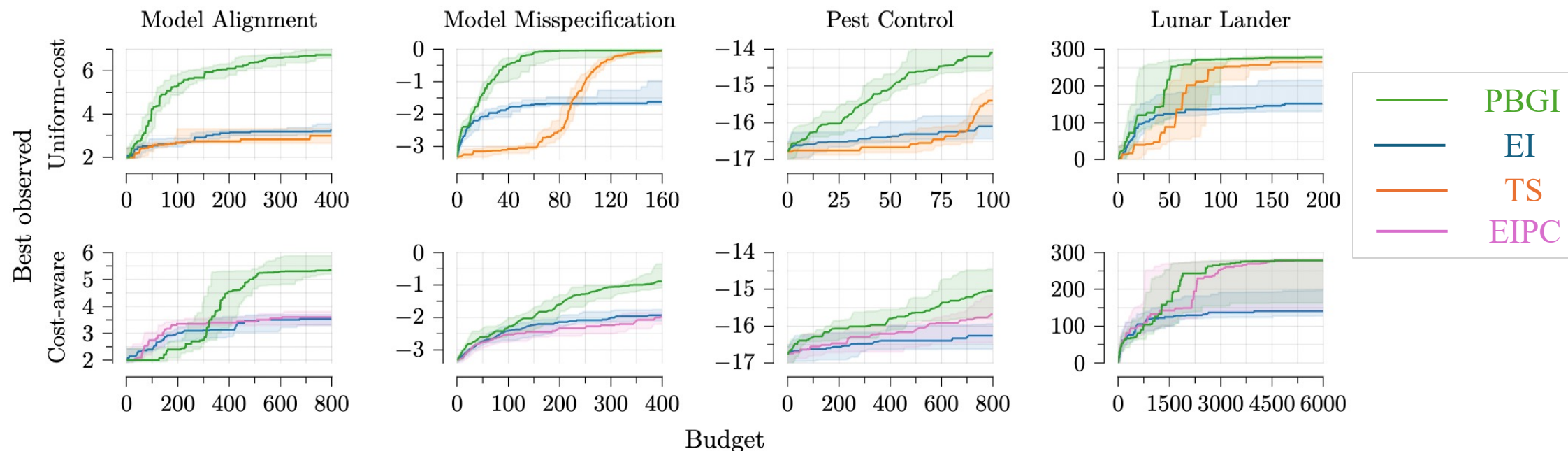
- Propose easy-to-compute PBGI policy for Bayesian optimization
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- Extend to Bayesian optimization with **heterogeneous evaluation costs**



Check our preprint on arXiv!

Heterogeneous-cost Experiment Results

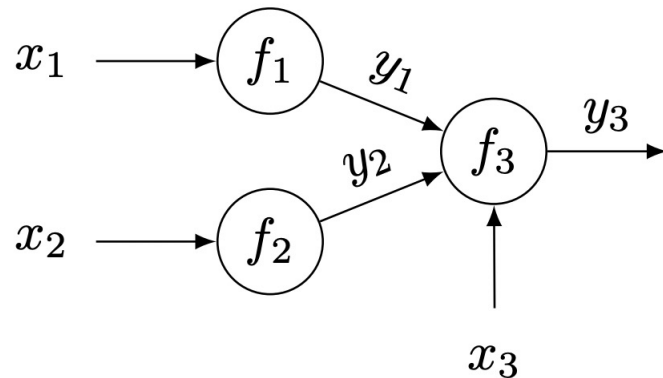
- Show the effectiveness of PBGI on synthetic & empirical experiments
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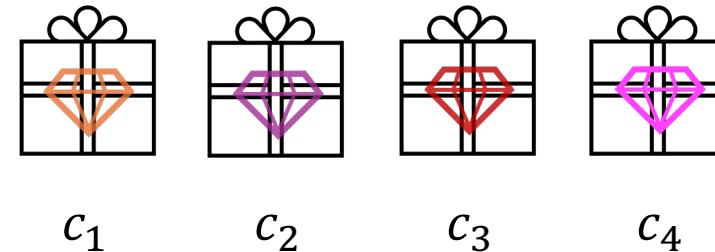
- Propose easy-to-compute PBGI policy for Bayesian optimization
- Show the effectiveness of PBGI on synthetic & empirical experiments
- Extend to Bayesian optimization with heterogeneous evaluation costs
- Open door for **complex BO** (freeze-thaw, multi-fidelity, function network, etc.)



?



Pandora's Box Gittins index



Check our preprint on arXiv!