

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

Qian Xie (Cornell ORIE)

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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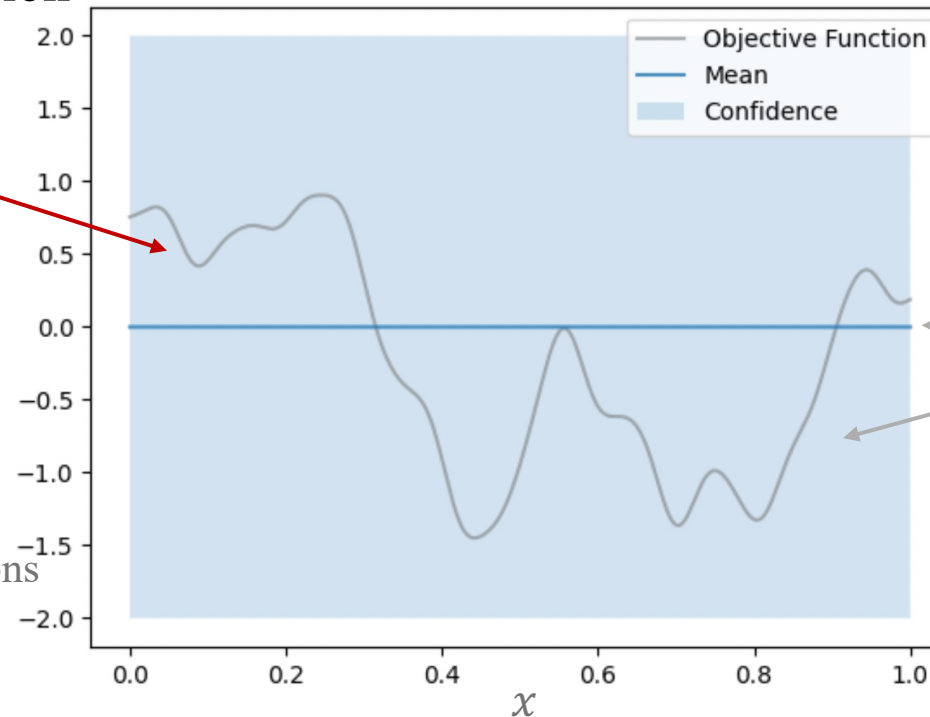
Control design

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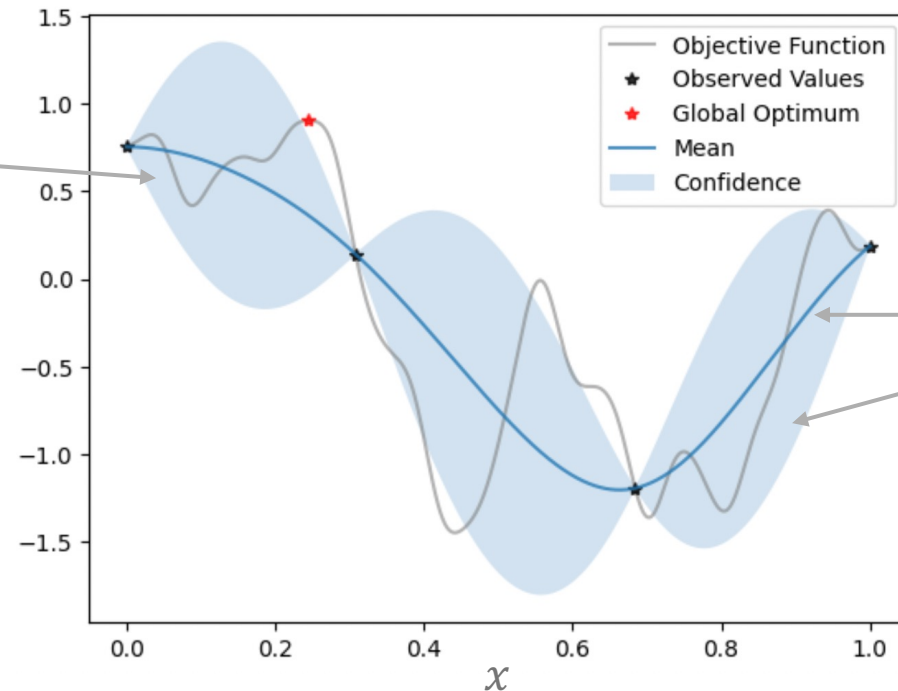
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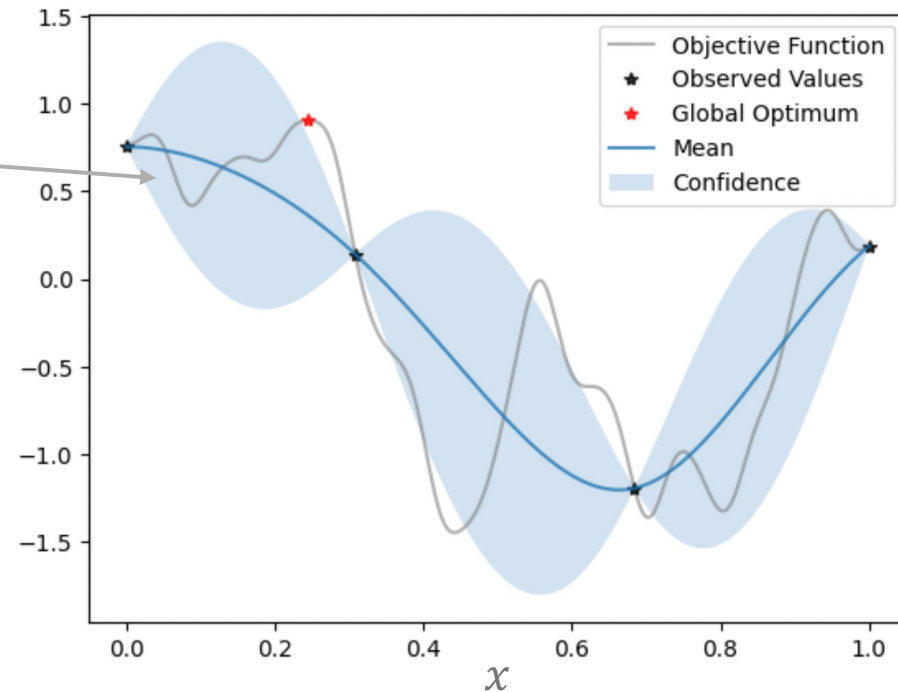
Objective: find global optimum $x^* = \operatorname{argmax}_{x \in \mathcal{X}} f(x)$

Decision: evaluate a set of points

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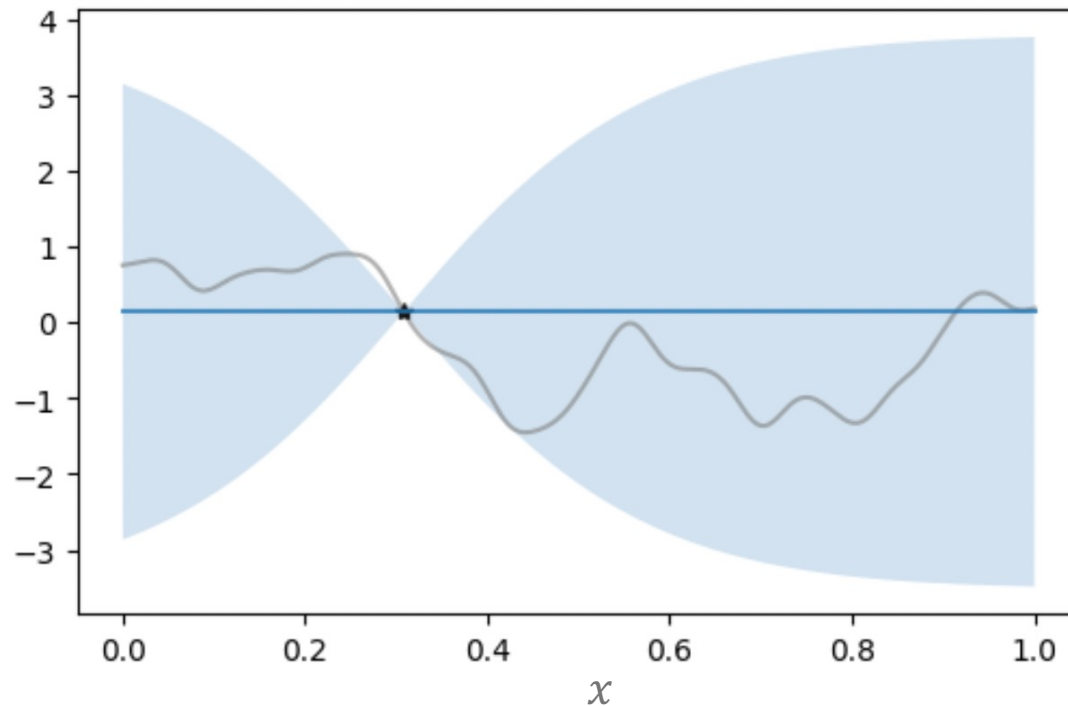
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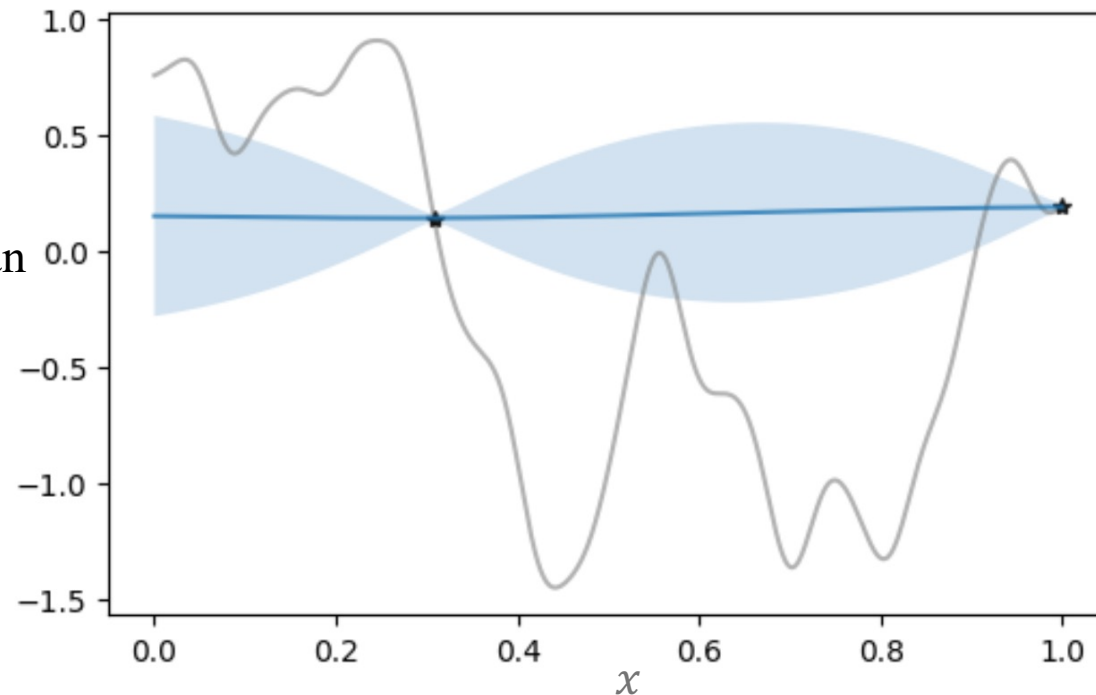
adaptively

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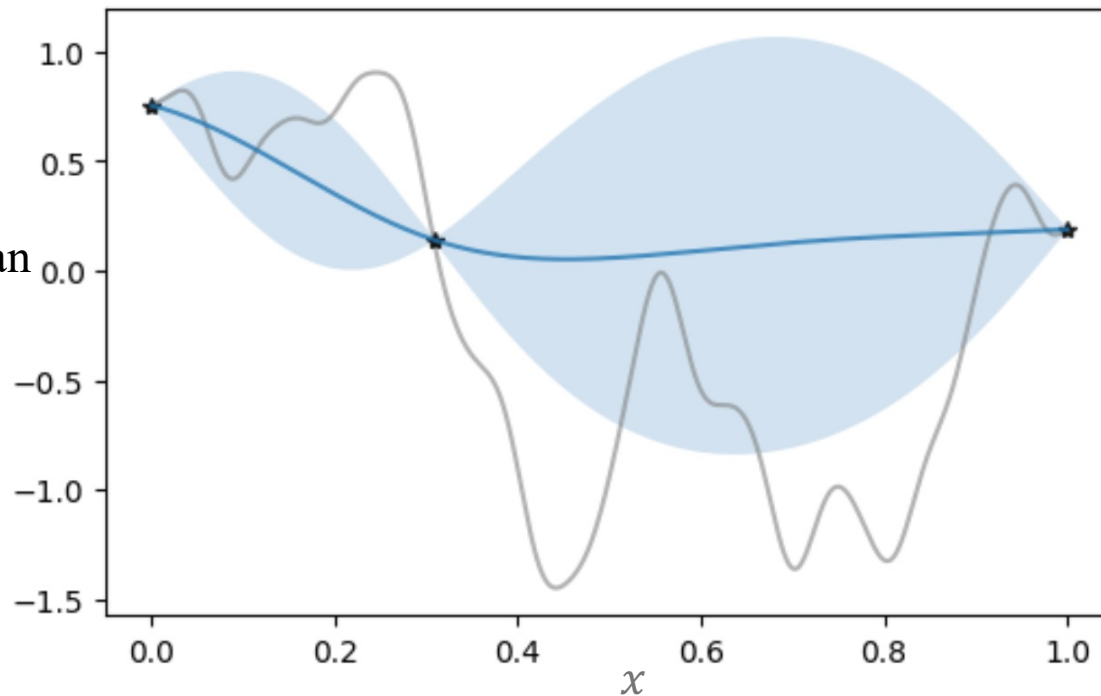
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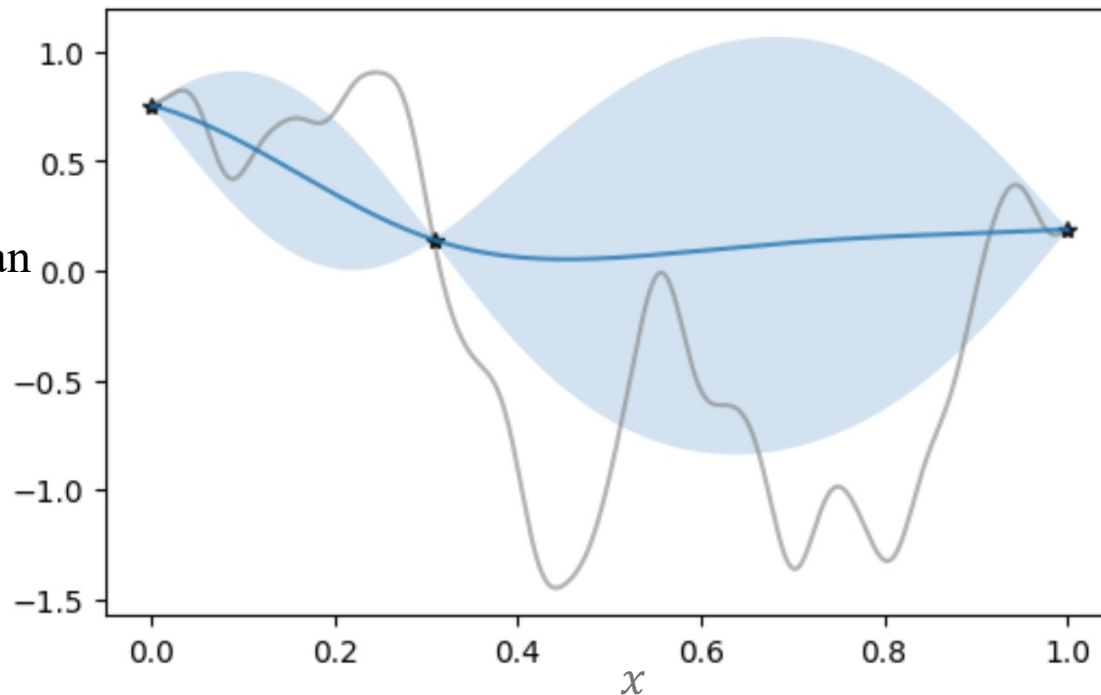
x : hyperparameter/configuration

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

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

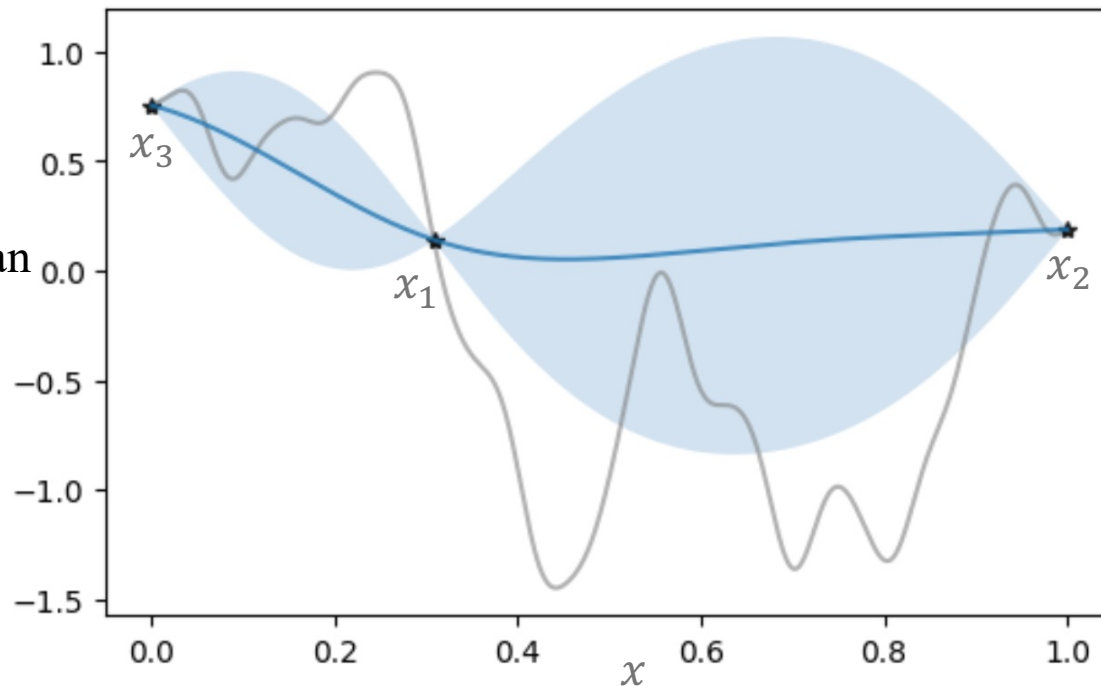
$x_1, x_2, \dots, x_T \in \mathcal{X}$

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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Objective: optimize best observed value at time T

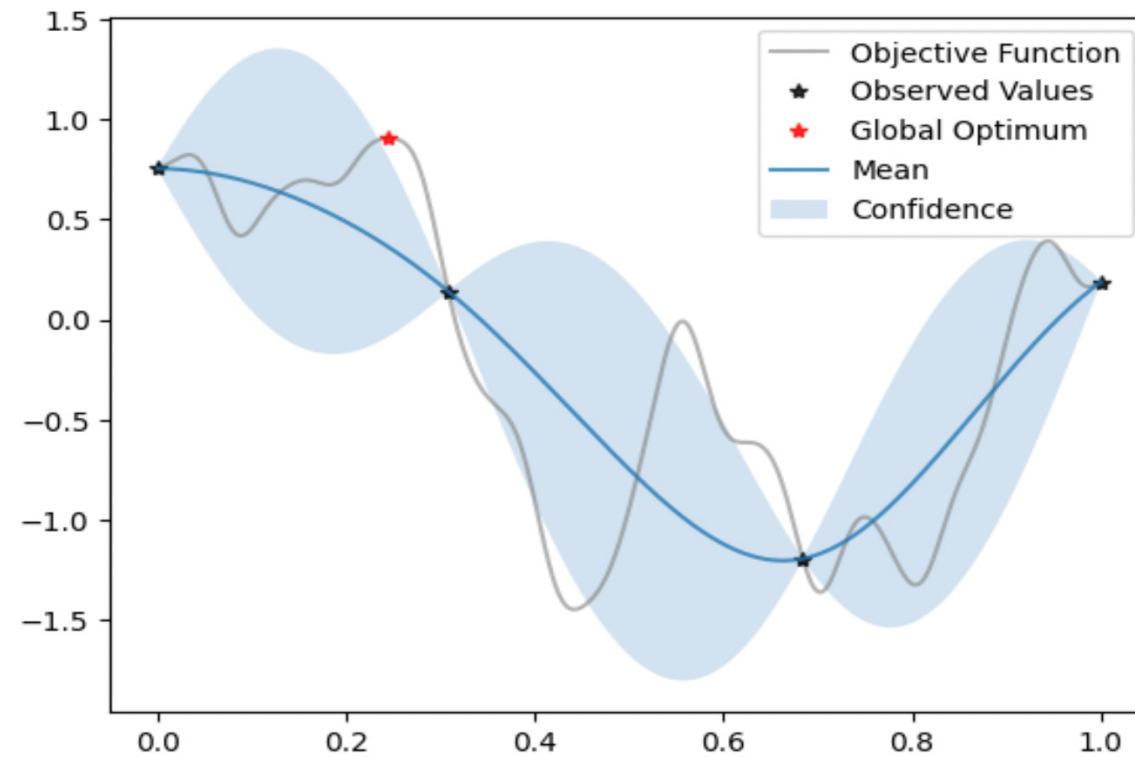
$$\max_{\text{policy}} \mathbb{E} \max_{t=1,2,\dots,T} f(x_t)$$

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

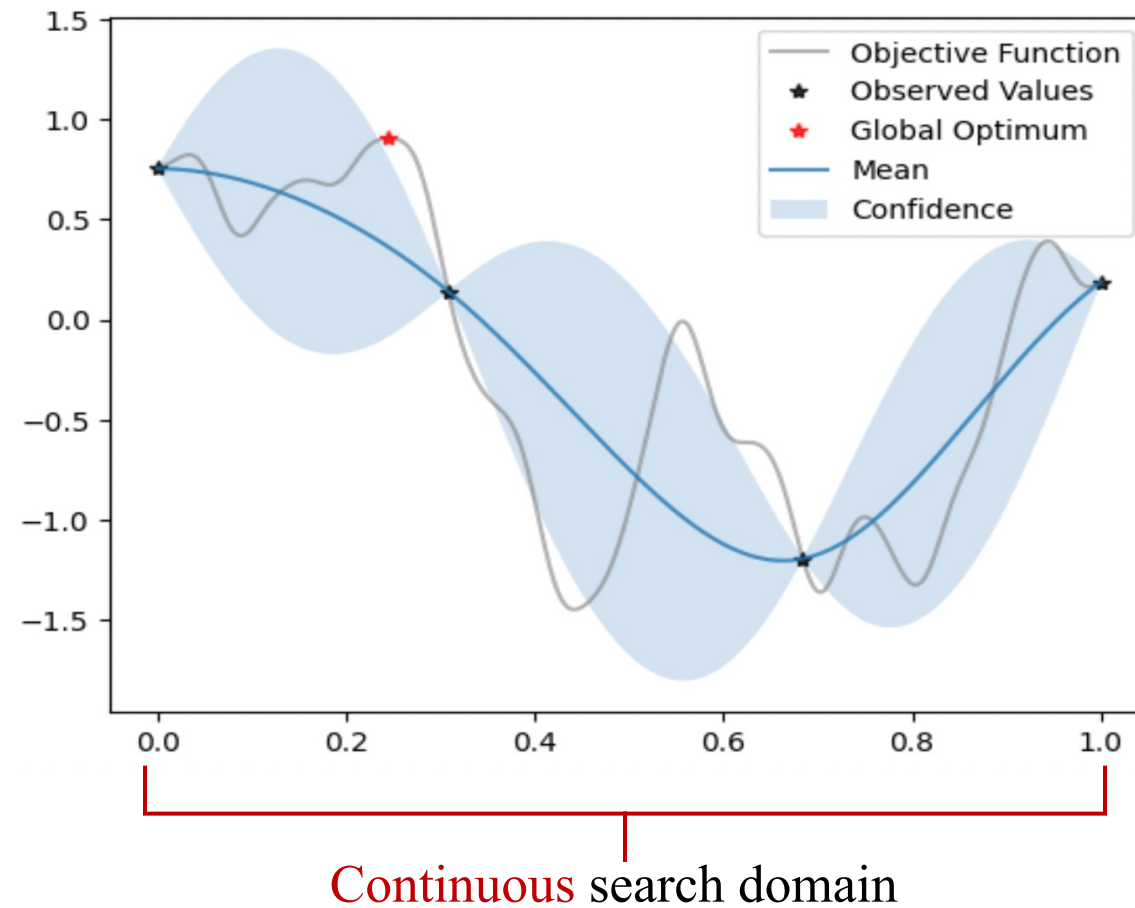
$$x_1, x_2, \dots, x_T \in \mathcal{X}$$

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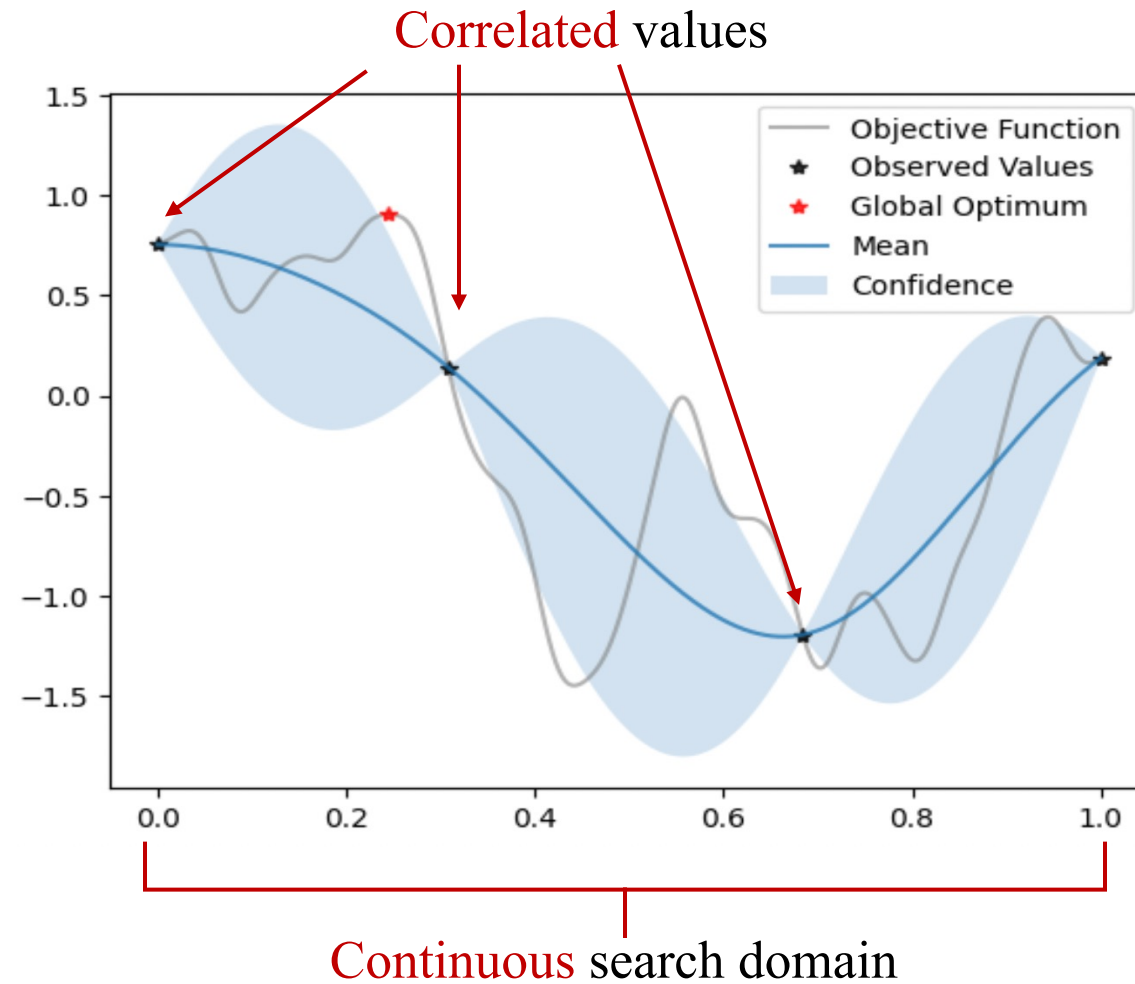
Why is it hard?



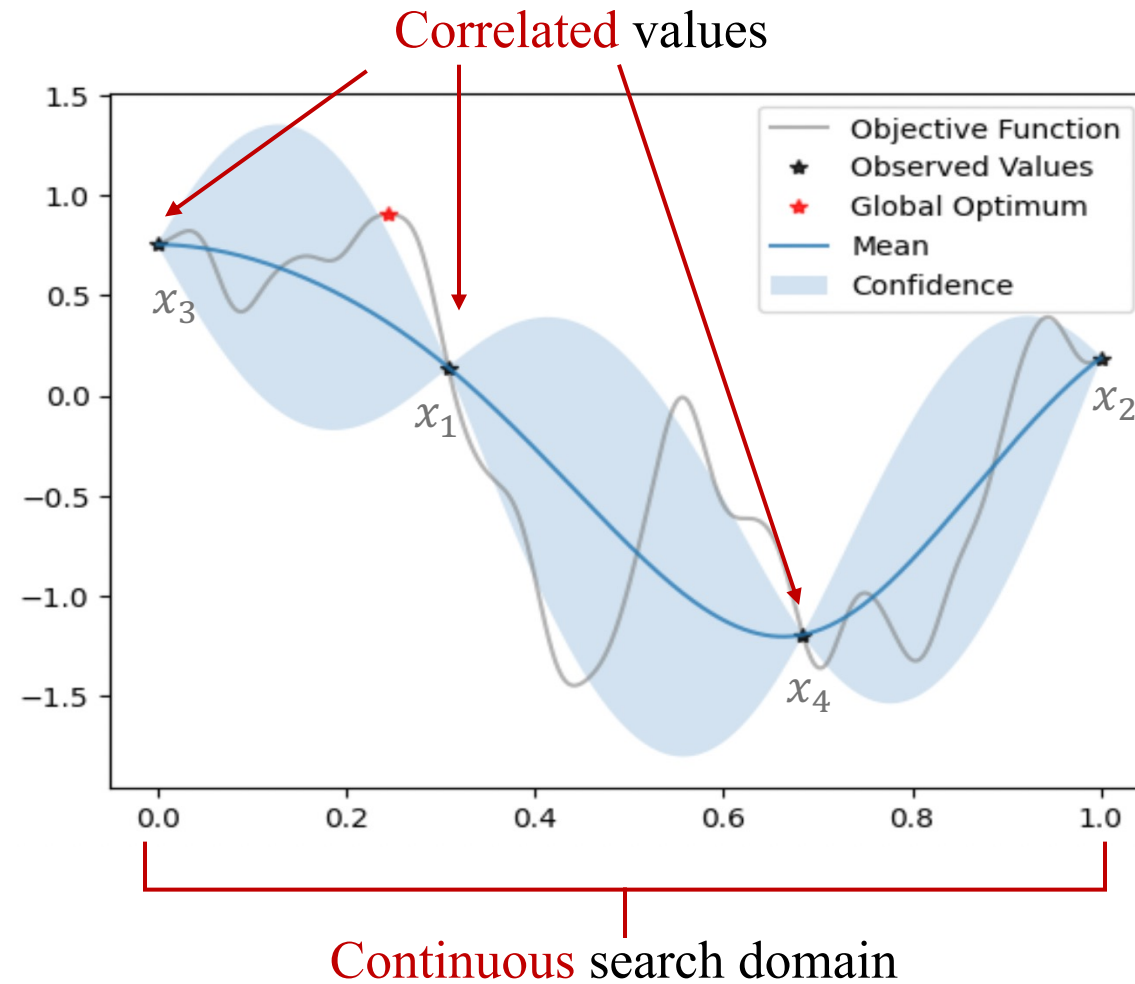
Why is it hard?



Why is it hard?



Why is it hard?



Hard budget constraint

~~$t=1$~~



~~$t=2$~~



~~$t=3$~~



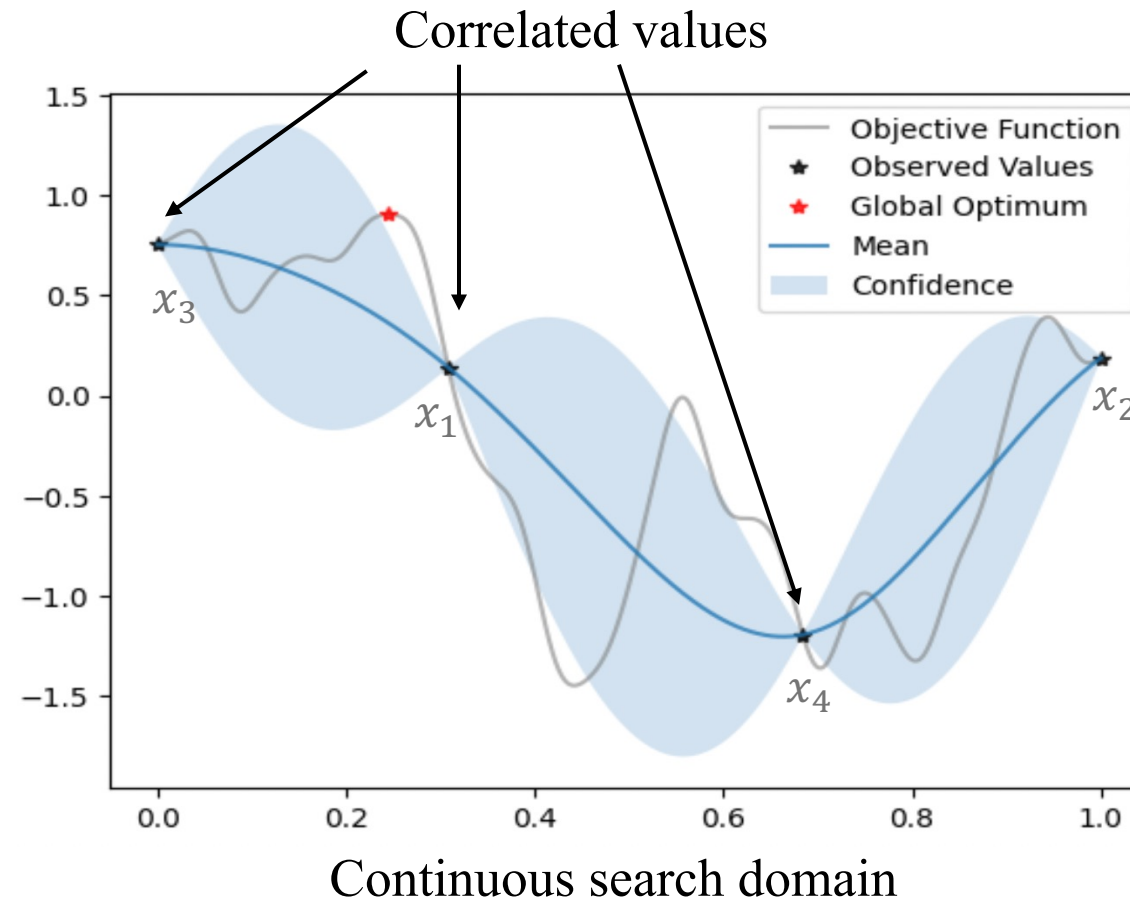
~~$t=4$~~







\vdots

~~$t=T$~~

Why is it hard?

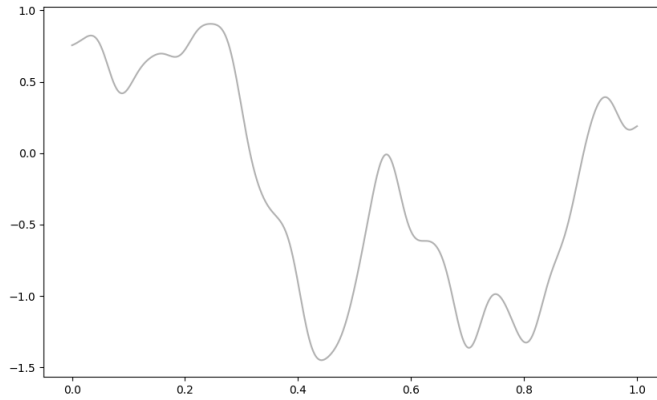


Hard budget constraint

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

\Rightarrow Optimal policy unknown!

Bayesian Optimization

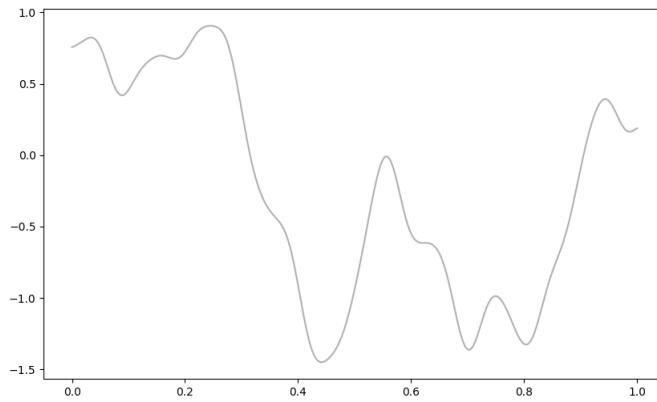


Continuous

Correlated

Hard budget constraint

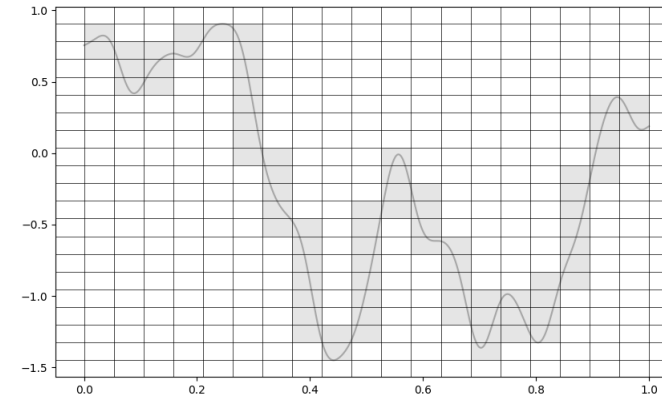
Bayesian Optimization



Continuous

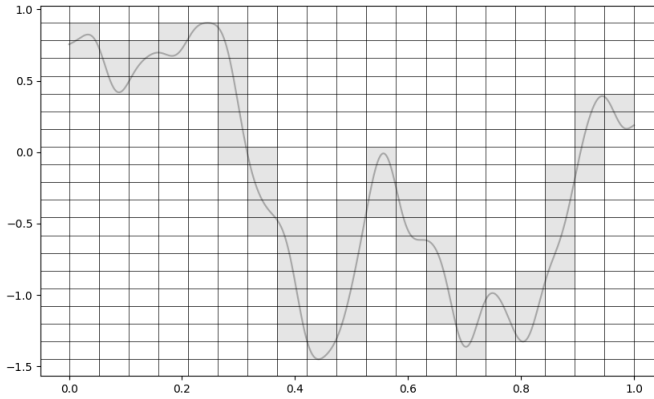
Correlated

Hard budget constraint



Discrete

Bayesian Optimization



Continuous

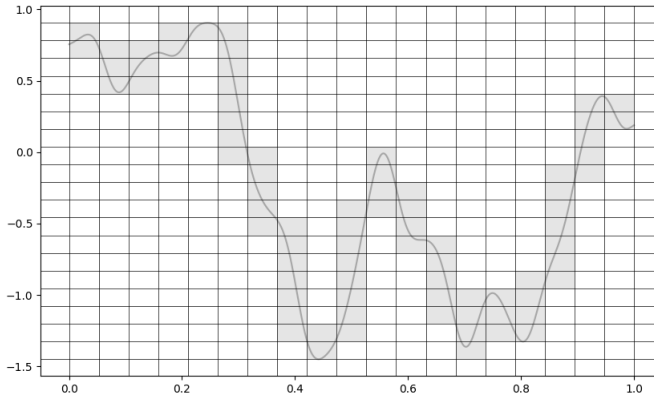


Discrete

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Hard budget constraint

Bayesian Optimization



Continuous



Discrete

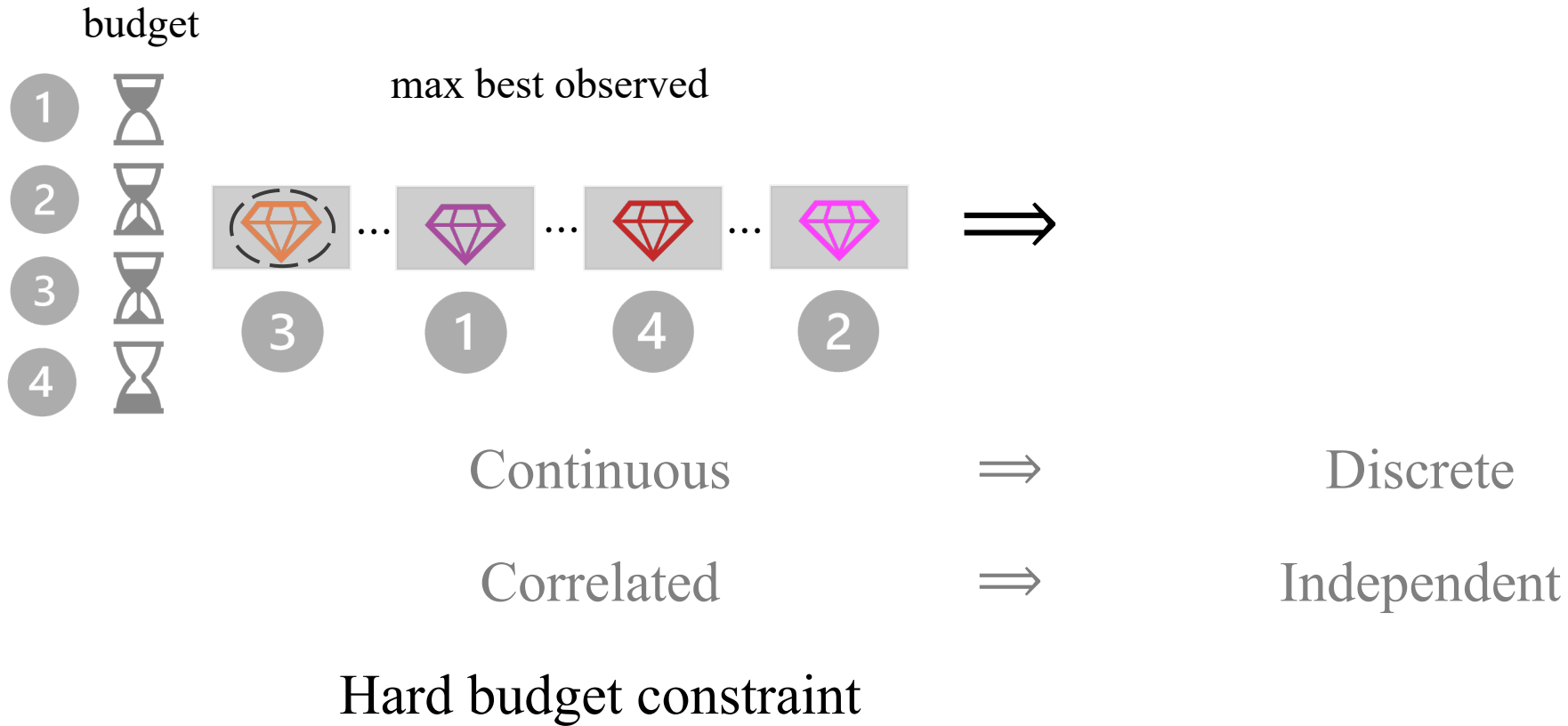
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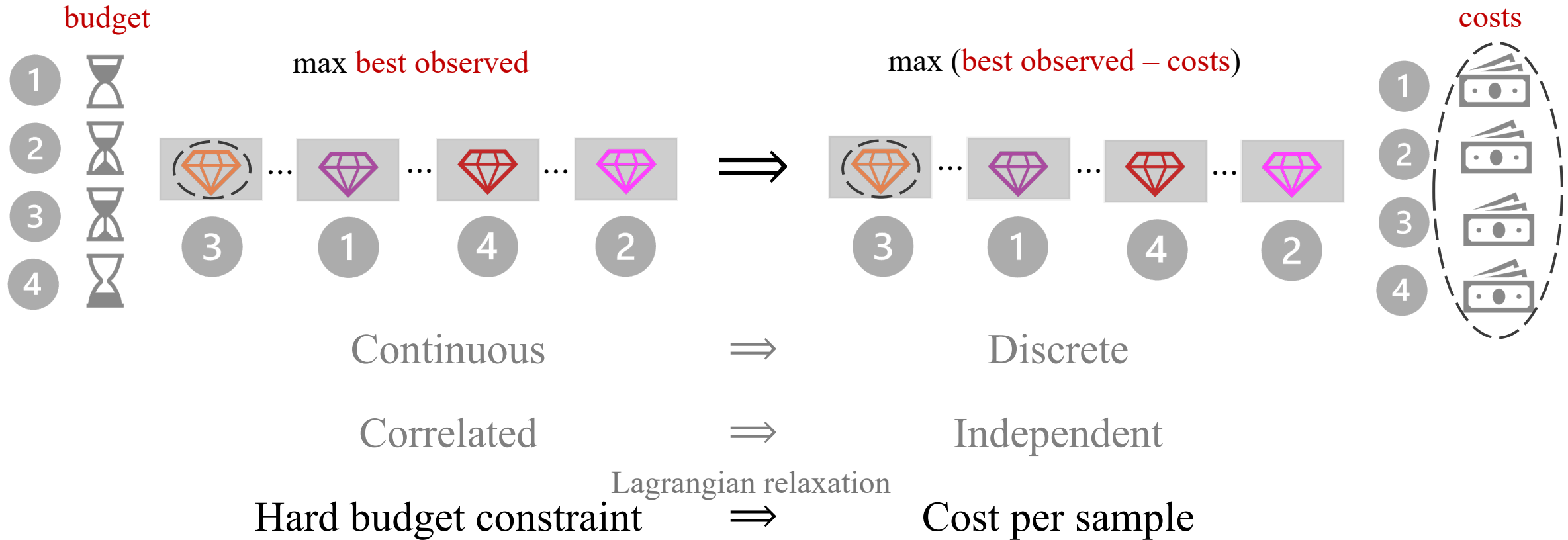
Independent

Hard budget constraint

Bayesian Optimization

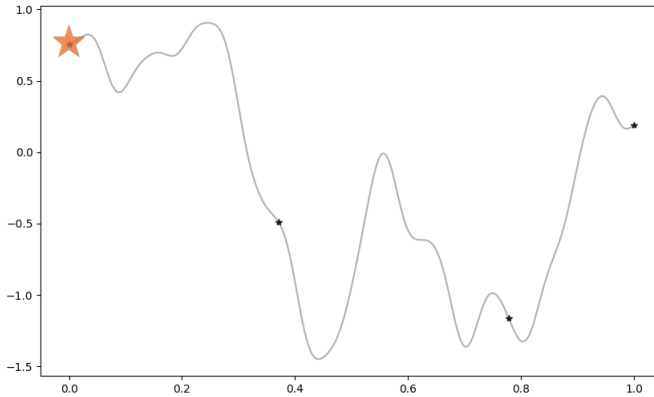


Bayesian Optimization



Bayesian Optimization \Rightarrow Pandora's Box

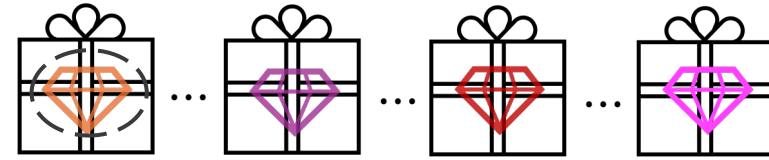
Special case of Markovian/
Bayesian multi-armed bandits



Continuous

Correlated

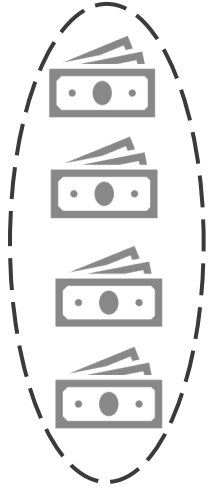
Hard budget constraint



Discrete

Independent

Cost per sample



Bayesian Optimization \Rightarrow Pandora's Box

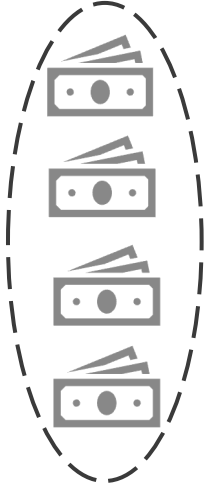
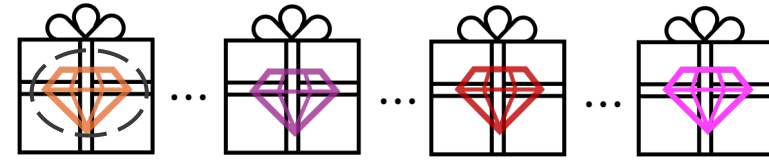
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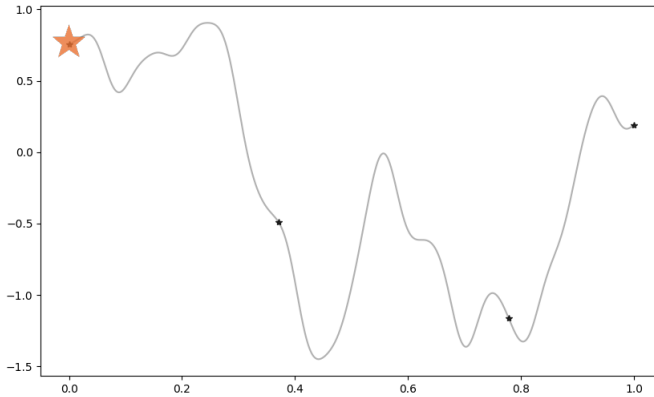
Independent



Cost per sample

Optimal policy: Gittins index [Weitzman'79]

Bayesian Optimization \Rightarrow Pandora's Box

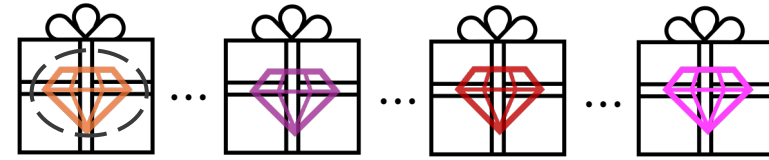


Continuous

Correlated

Hard budget constraint

Is Gittins index good?

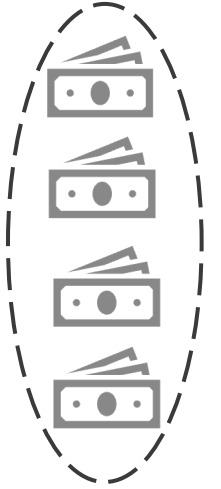


Discrete

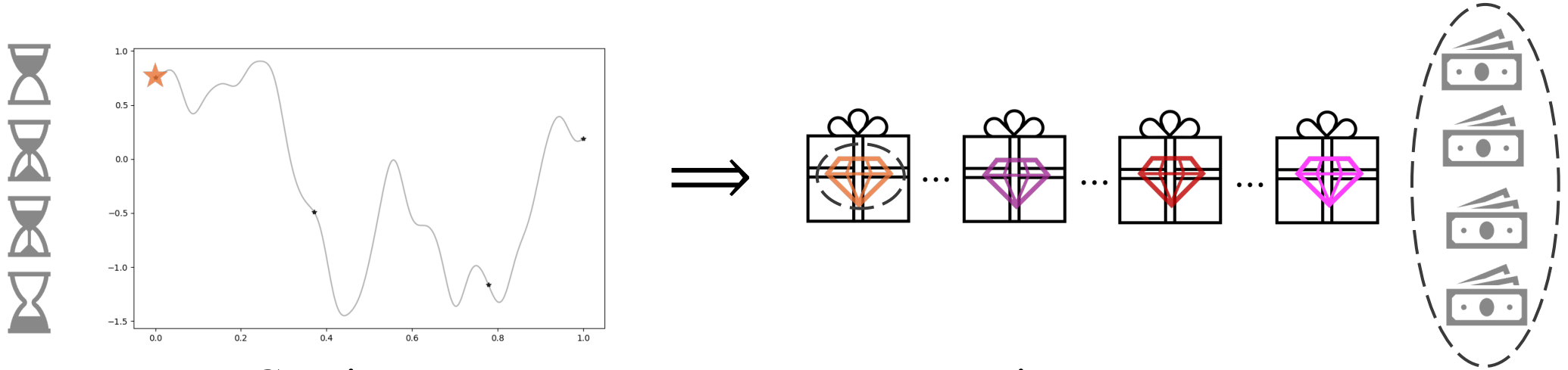
Independent

Cost per sample

Optimal policy: Gittins index



Bayesian Optimization \Rightarrow Pandora's Box



Continuous

\Rightarrow

Discrete

Correlated

\Rightarrow

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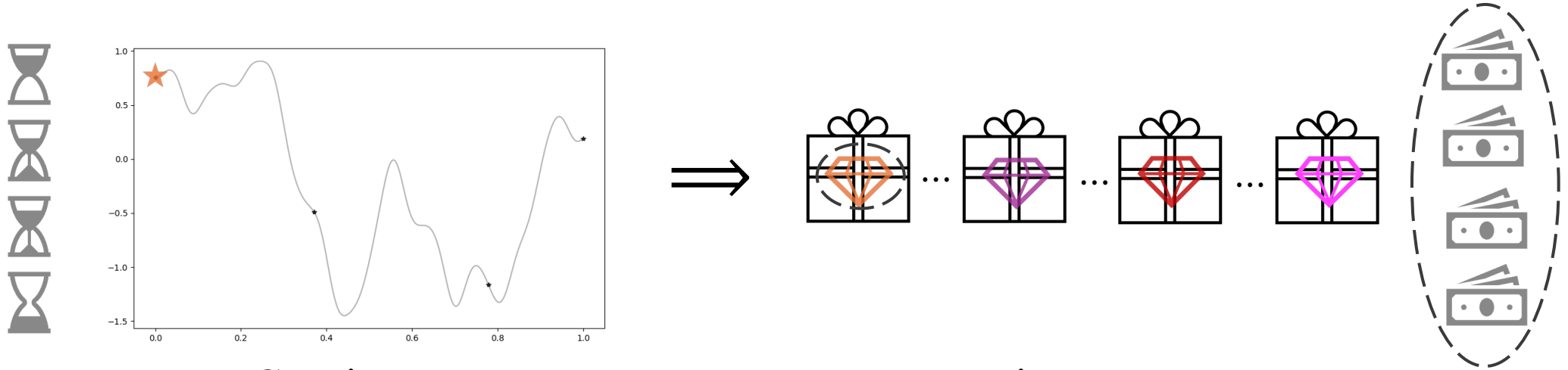
Hard budget constraint

\Rightarrow

Cost per sample

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?

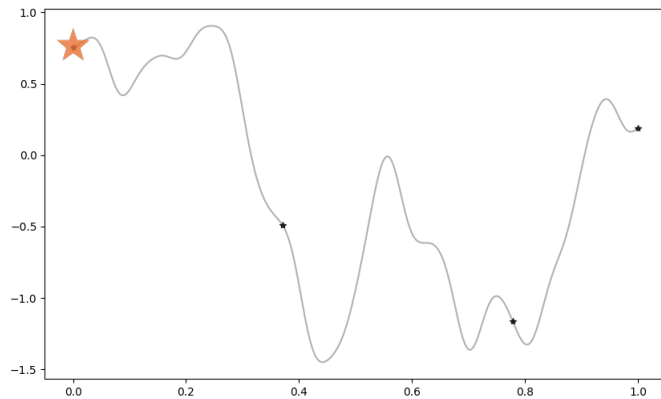
\Leftarrow

Optimal policy: Gittins index

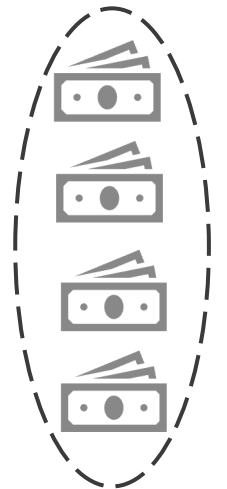
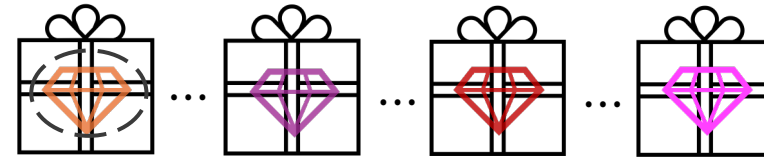
Our contributions!

Our Contributions

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



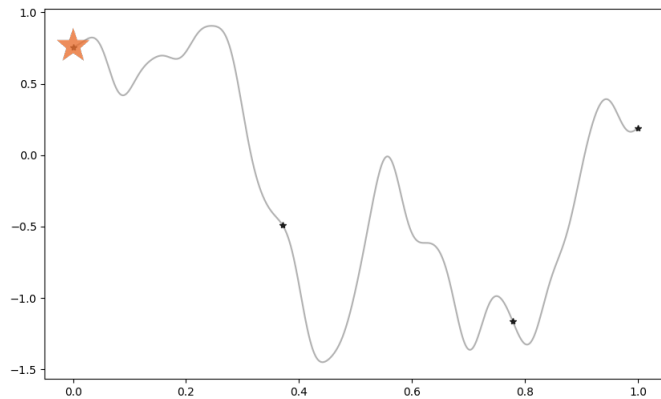
?



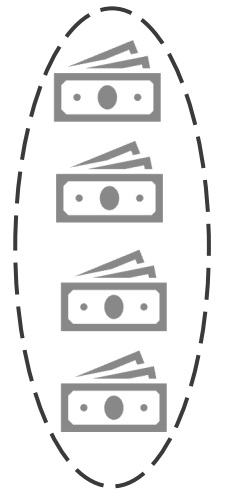
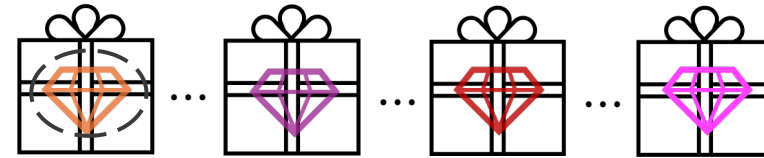
Pandora's Box Gittins index

Our Contributions

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



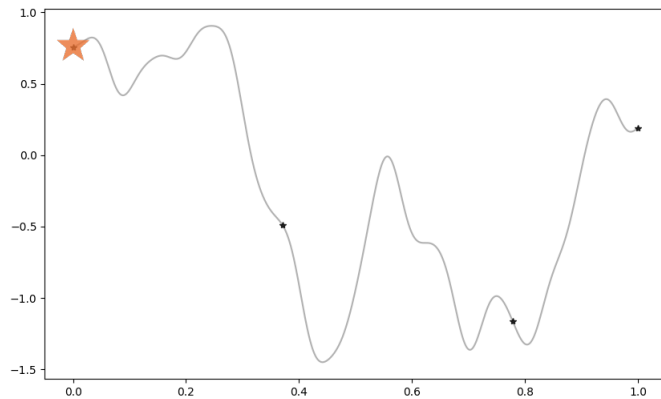
Our work



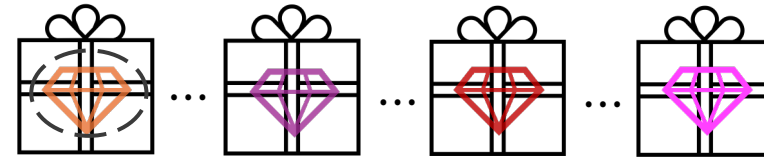
Pandora's Box Gittins index

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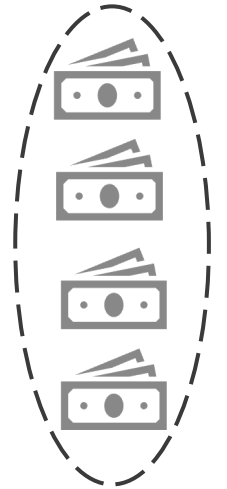
- Develop PBGI policy for Bayesian optimization
- Show **performance** against baselines on synthetic & empirical experiments



Our work

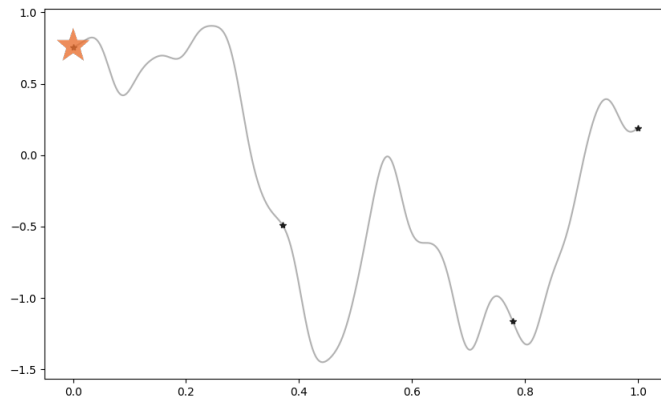


Pandora's Box Gittins index

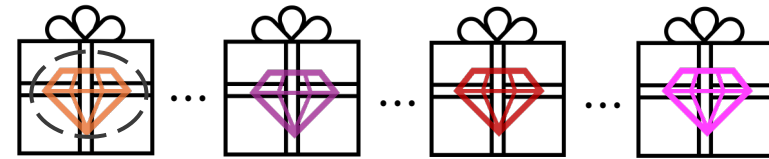


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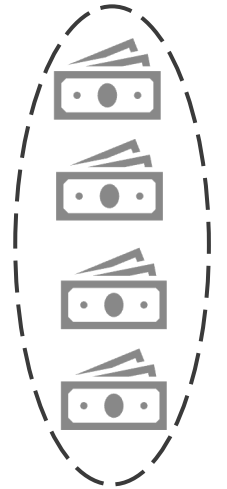
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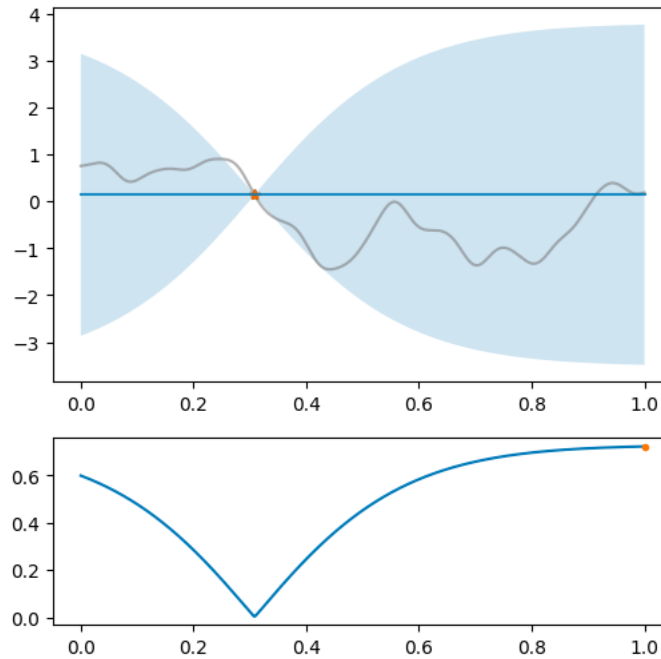


Pandora's Box Gittins index



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

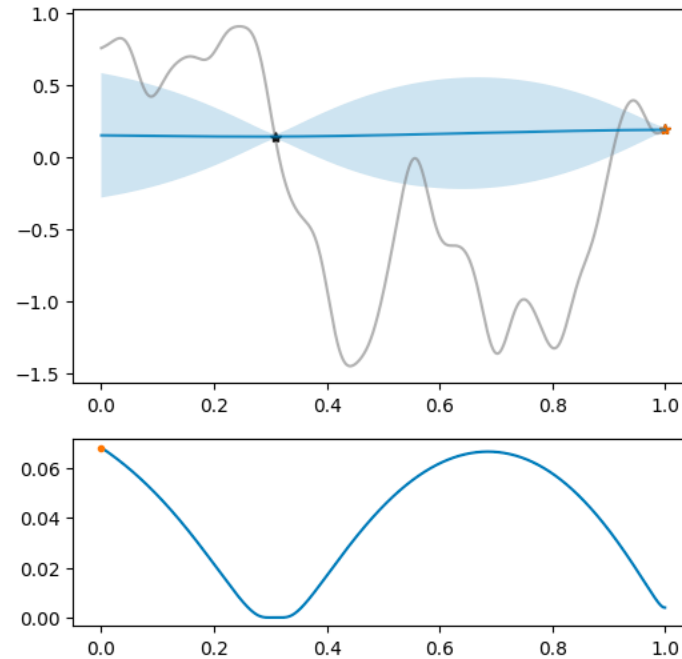
$$\text{EI}_{f|D}(x; y) = \mathbb{E}[(f|D)(x) - y]^+$$

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

D : observed data

y_{best} : current best observed value

Popular One-step Heuristic: EI



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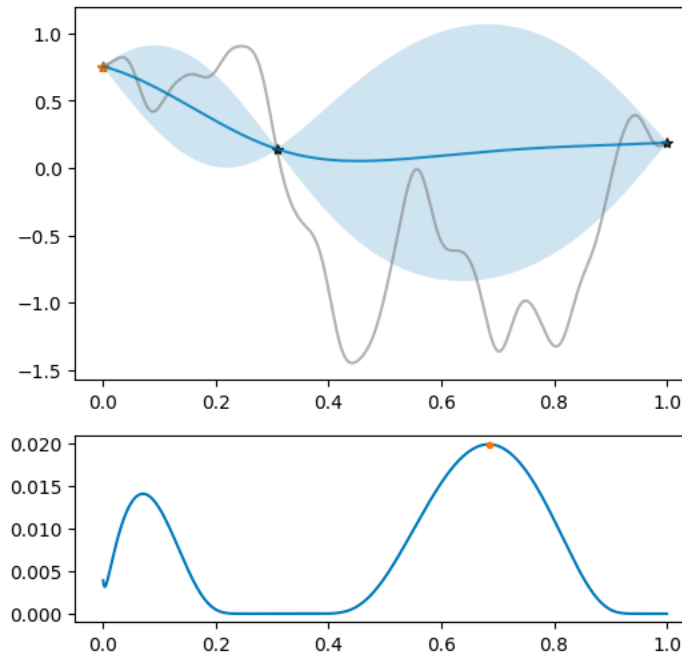
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Popular One-step Heuristic: EI

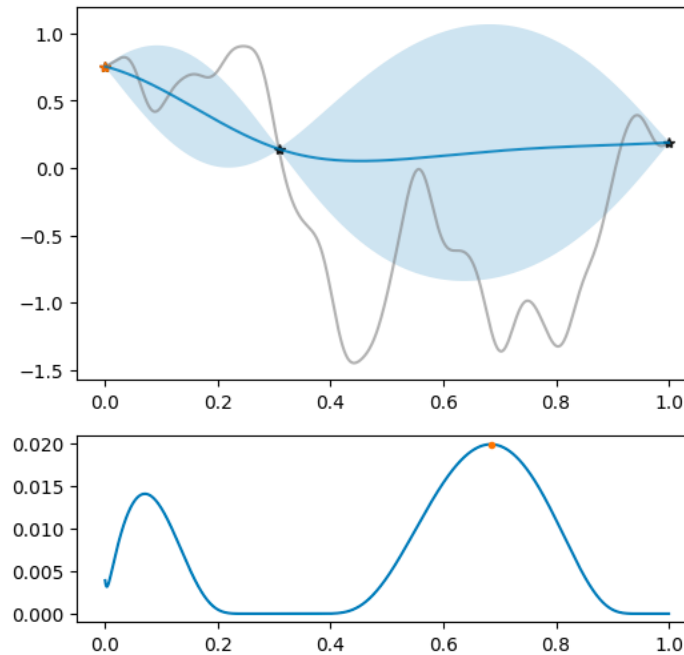
Other heuristics:

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
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Expected improvement

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

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

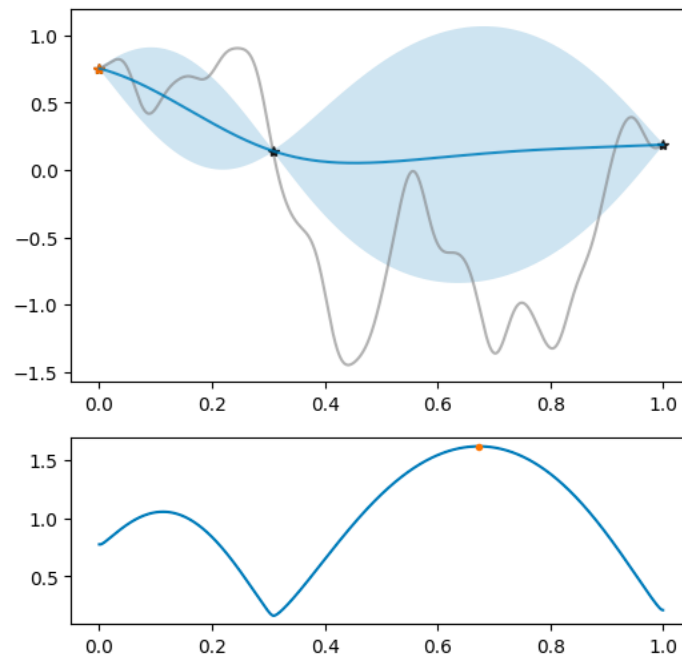
D : observed data

y_{best} : current best observed value

New One-step Heuristic: PBGI

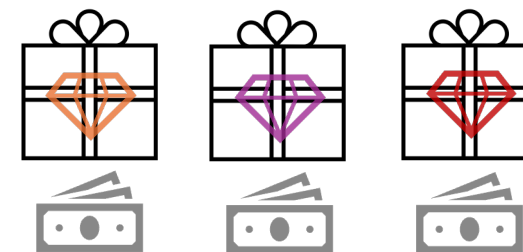
Other heuristics:

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



Pandora's box Gittins index

Pandora's box



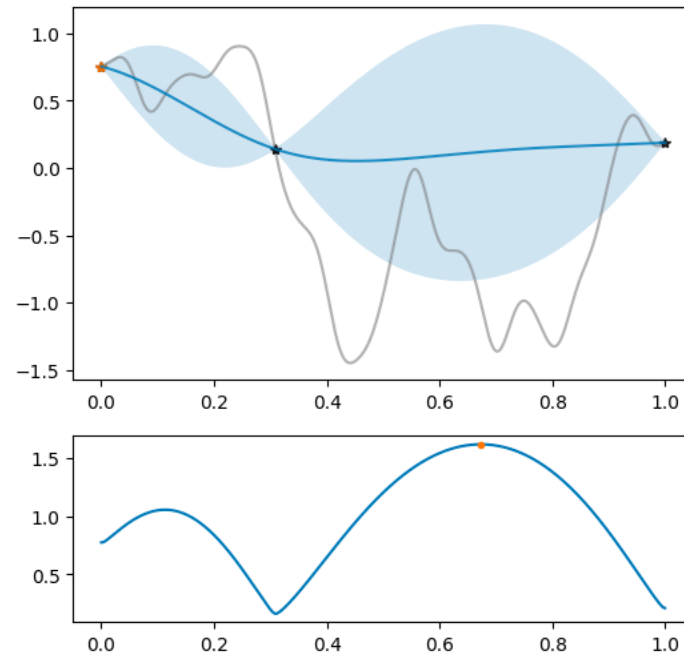
PBGI policy: evaluate $\operatorname{argmax}_x \alpha^*(x)$

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

New One-step Heuristic: PBGI

Other heuristics:

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- Thompson Sampling (TS)
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Pandora's box Gittins index

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

PBGI policy: evaluate $\arg\max_x \alpha^*(x)$

Pandora's box



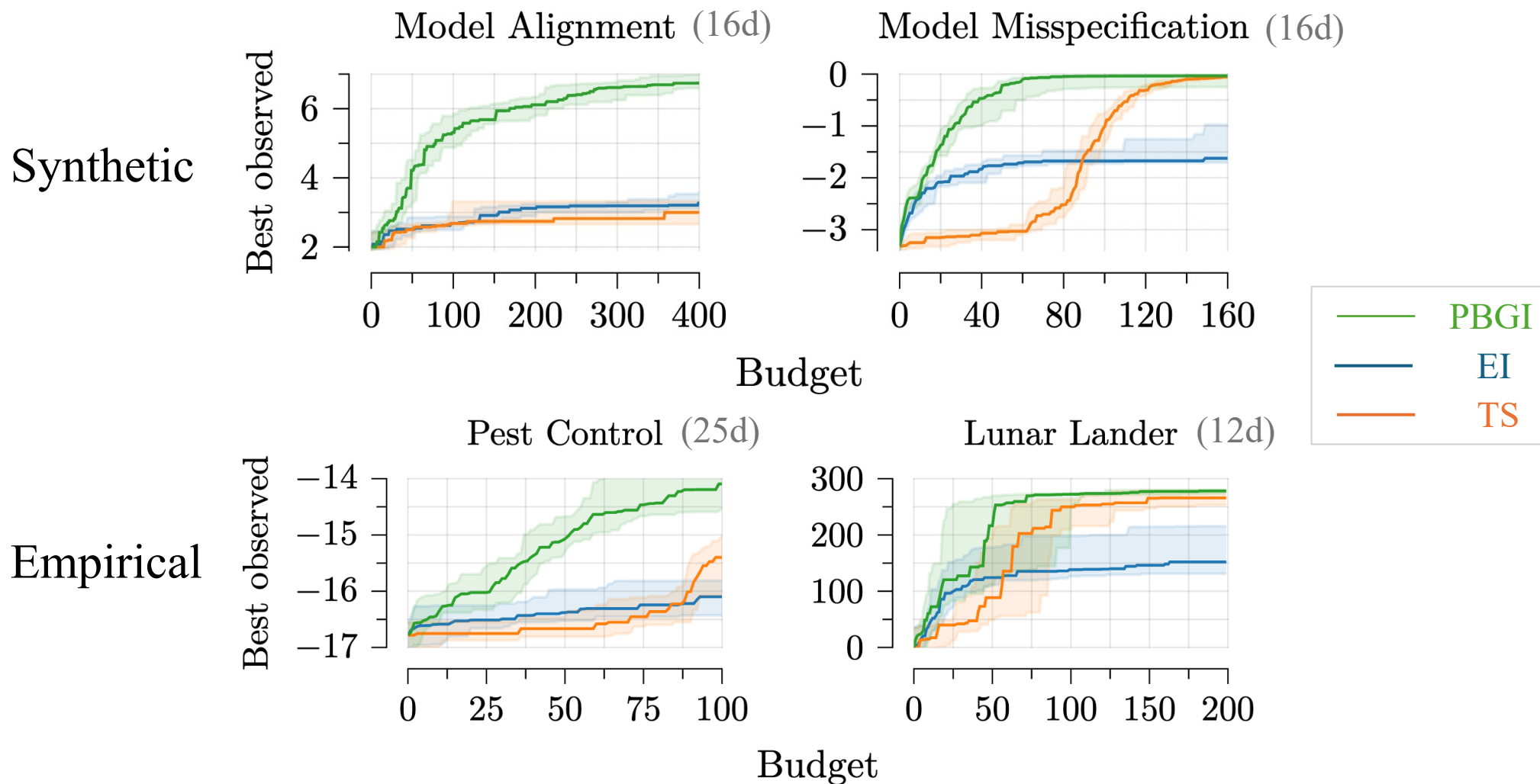
λ λ λ

λ : cost-per-sample
(Lagrange multiplier)

D : observed data

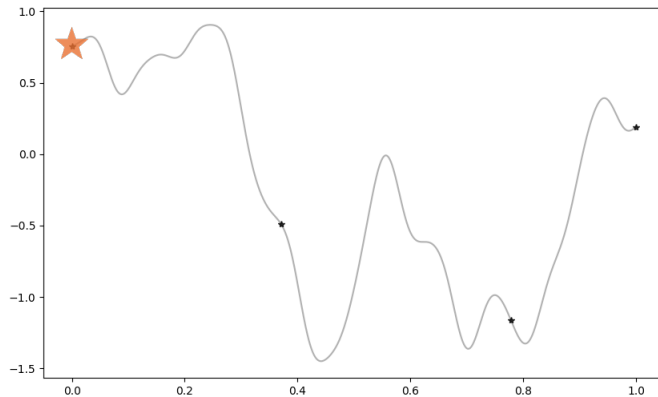
$\alpha^*(x)$: solution to $\text{EI}_{f|D}(x; \alpha^*(x)) = \lambda$

Experiment Results: PBGI vs EI vs TS

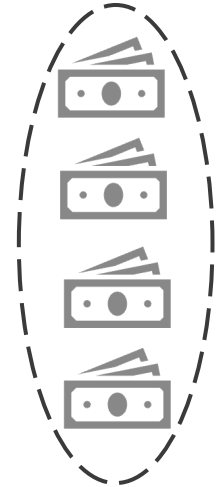
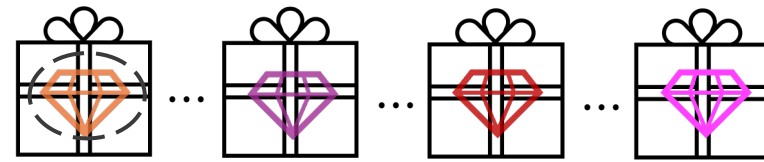


Conclusions

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



Our work

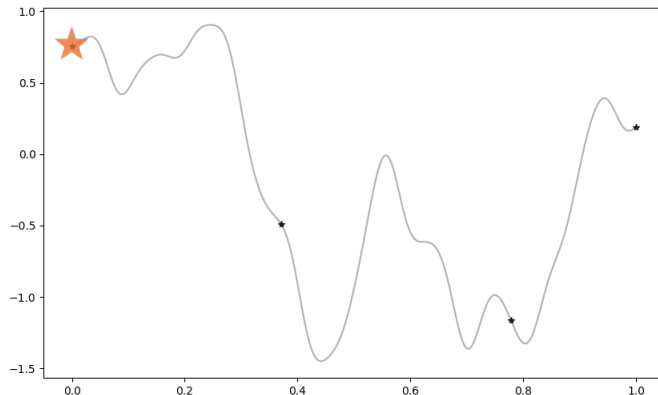


Pandora's box Gittins index

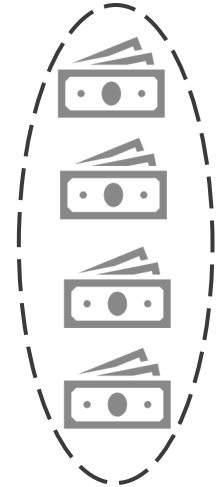
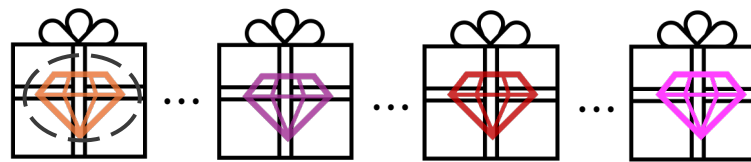
Check our preprint on arXiv!

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

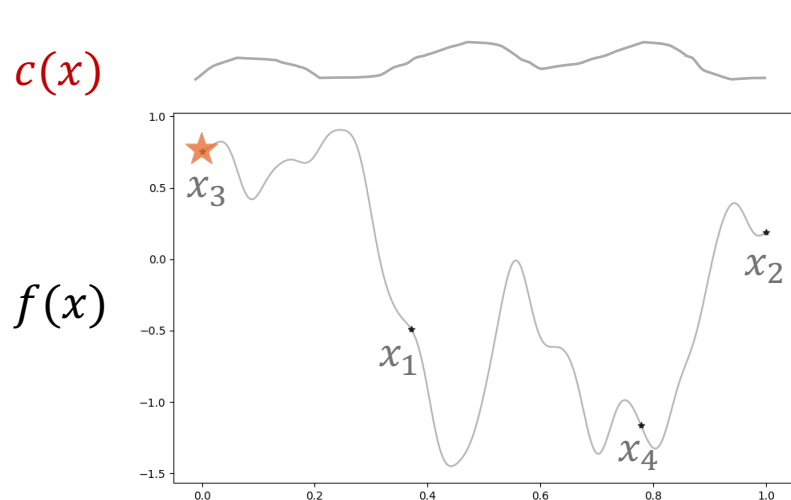


Pandora's box Gittins index

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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**

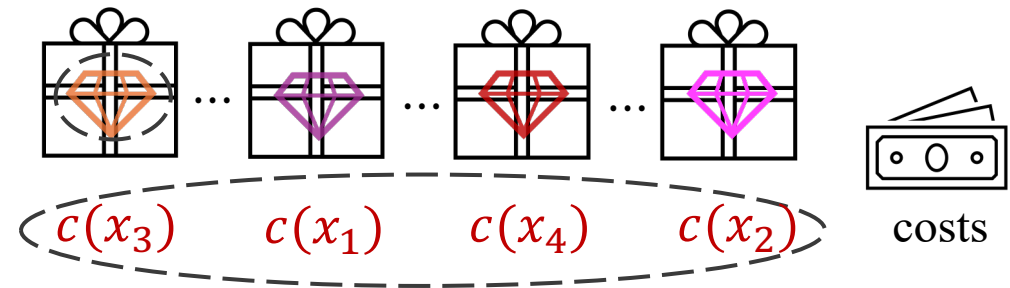


Our work



budget

max (best observed – costs)

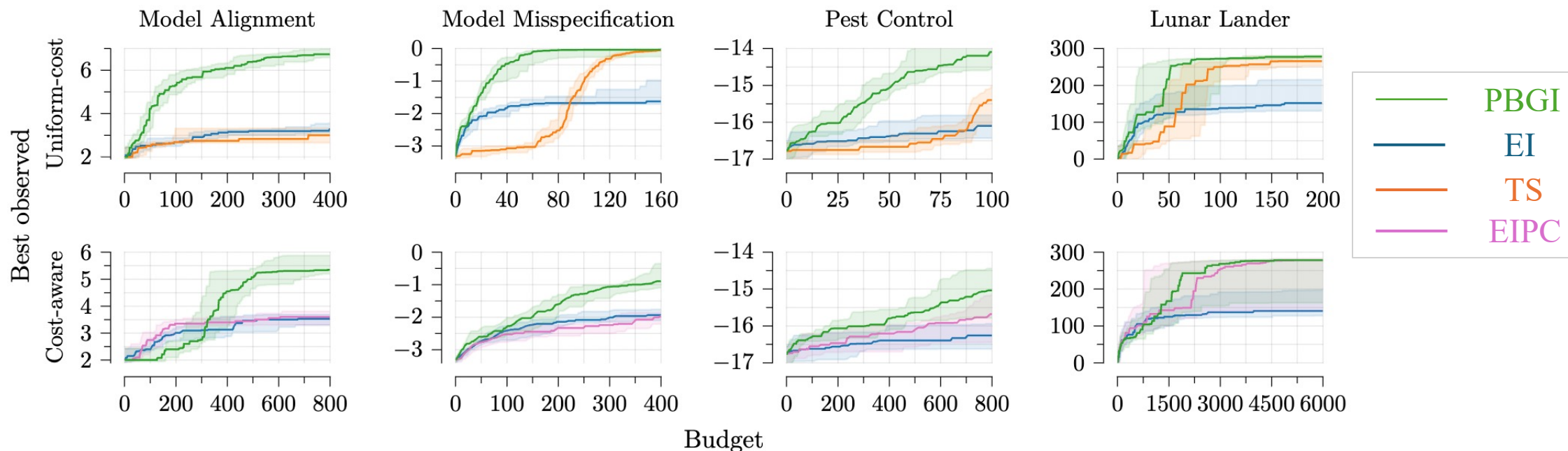


Pandora's Box Gittins index

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Heterogeneous-cost Experiment Results

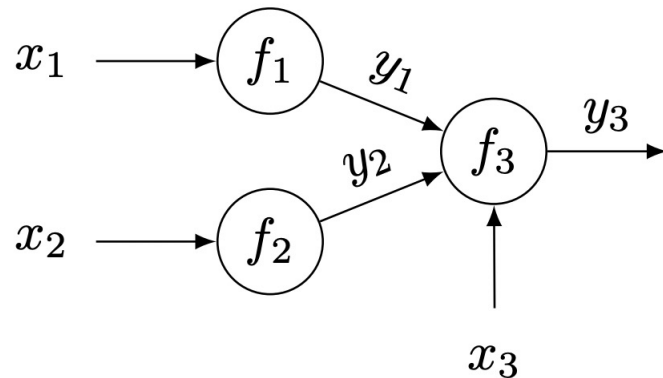
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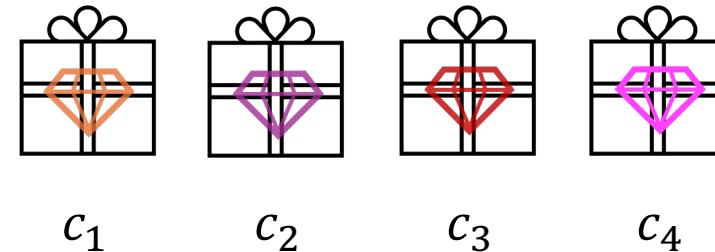
- Propose easy-to-compute PBGI policy for Bayesian optimization
- Show the effectiveness of PBGI on synthetic & empirical experiments
- Extend to Bayesian optimization with heterogeneous evaluation costs
- Open door for **complex BO** (freeze-thaw, multi-fidelity, function network, etc.)



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Pandora's Box Gittins index



Check our preprint on arXiv!