

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

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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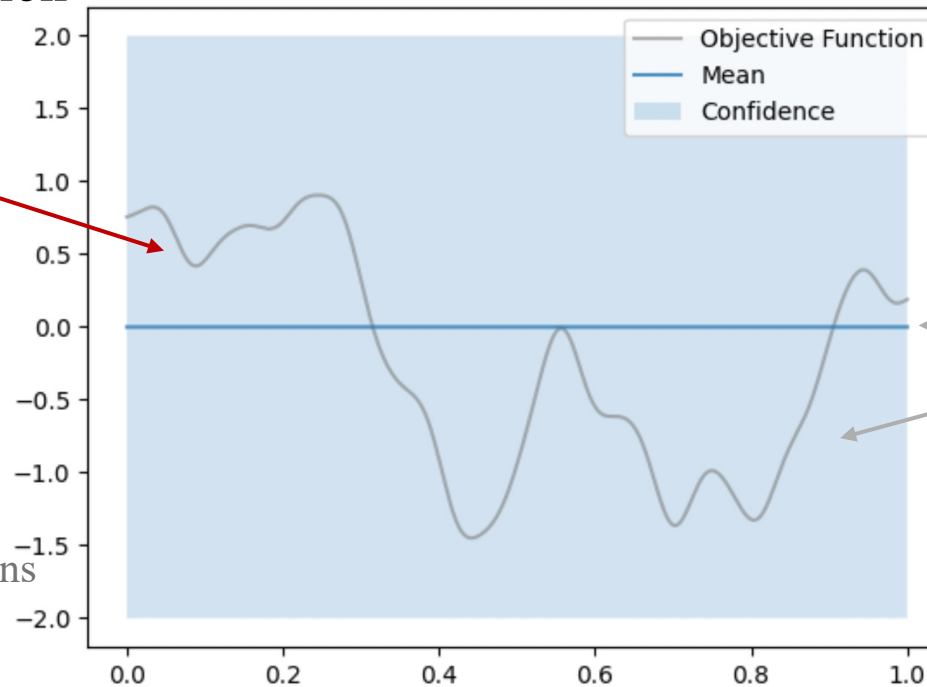
Control design

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

Bayesian Optimization

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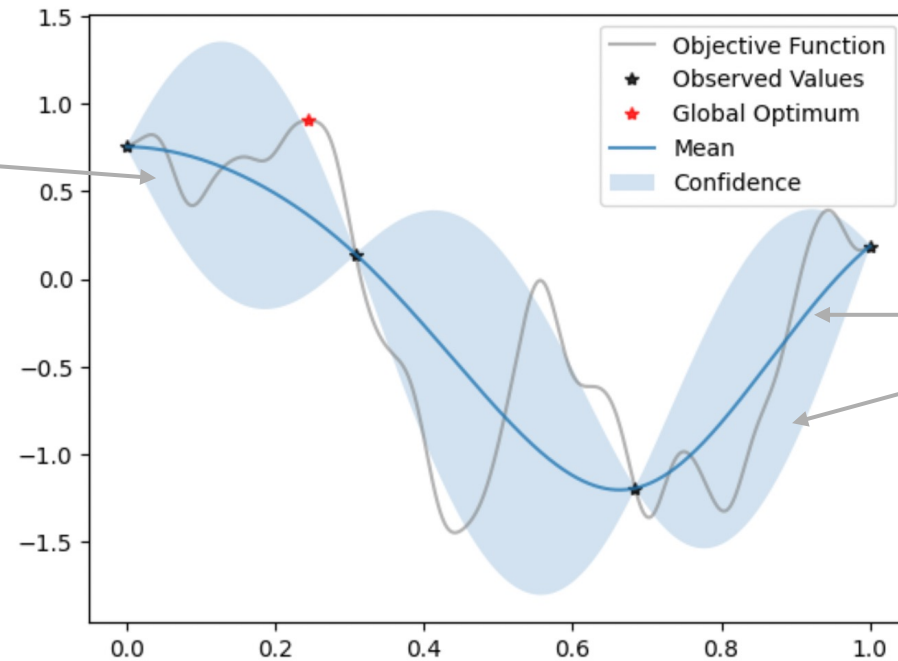
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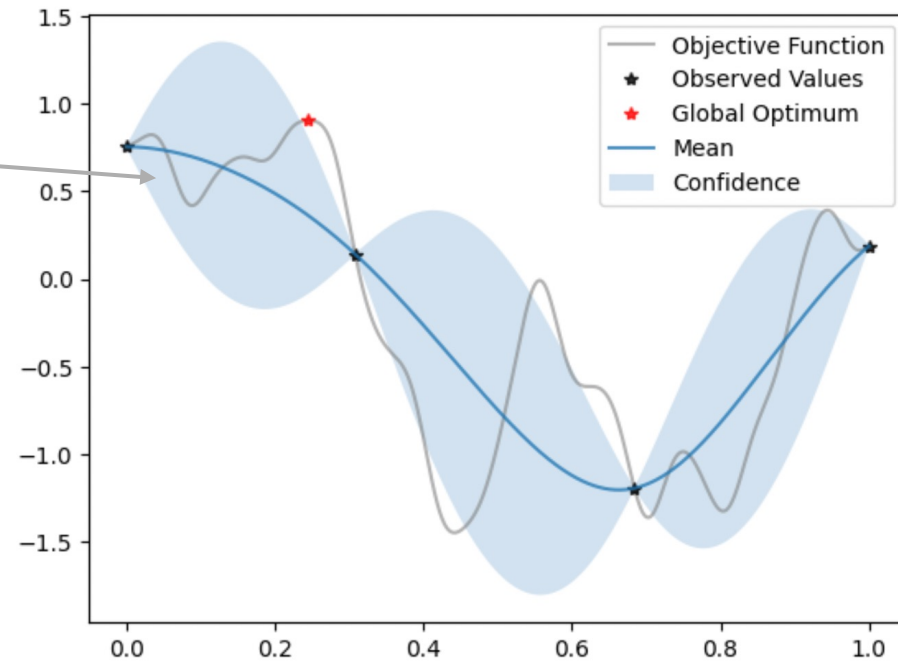
Objective: find global optimum $x^* = \operatorname{argmax}_{x \in \mathcal{X}} f(x)$

Decision: evaluate a set of points

Bayesian Optimization

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

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Applications:

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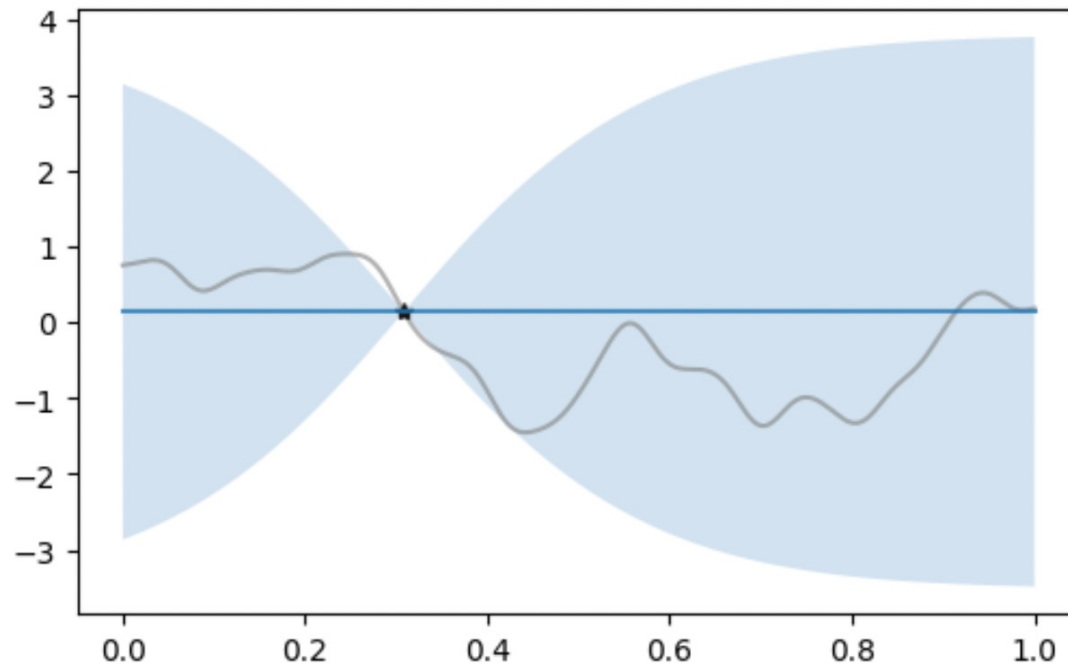
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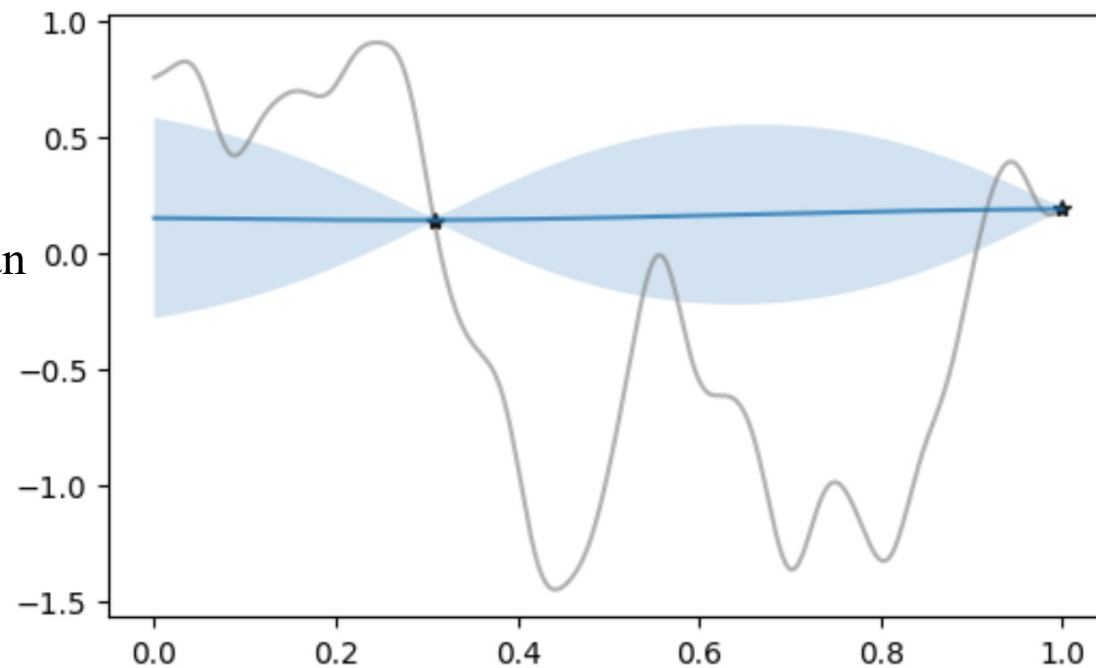
adaptively

Decision: evaluate a set of points

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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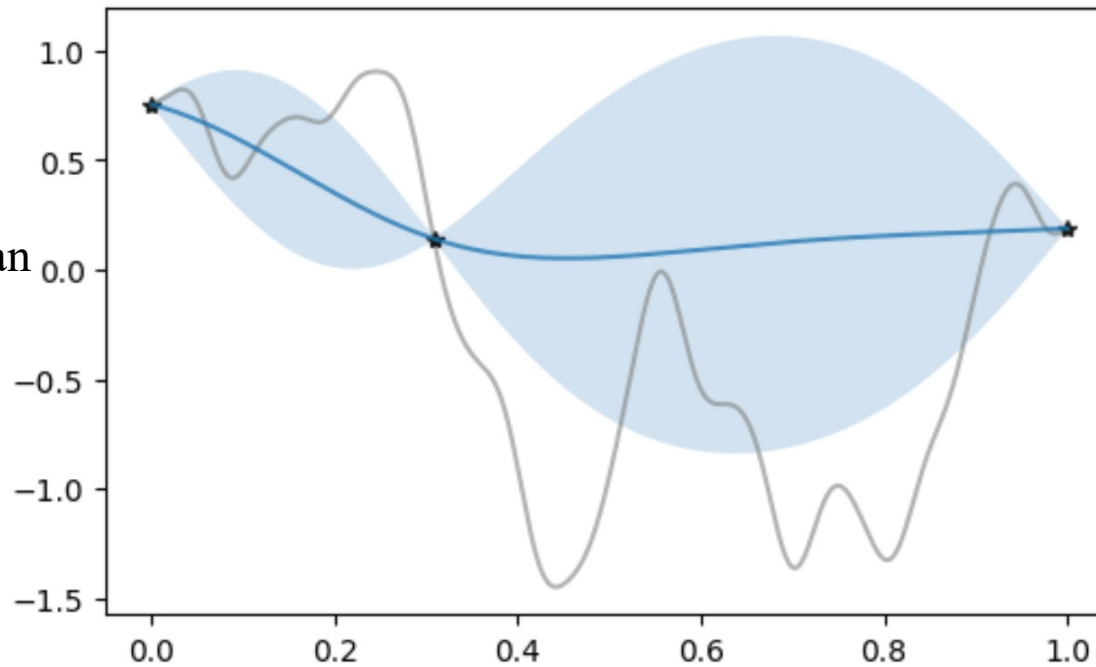
x : hyperparameter/configuration

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

Bayesian Optimization

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Applications:

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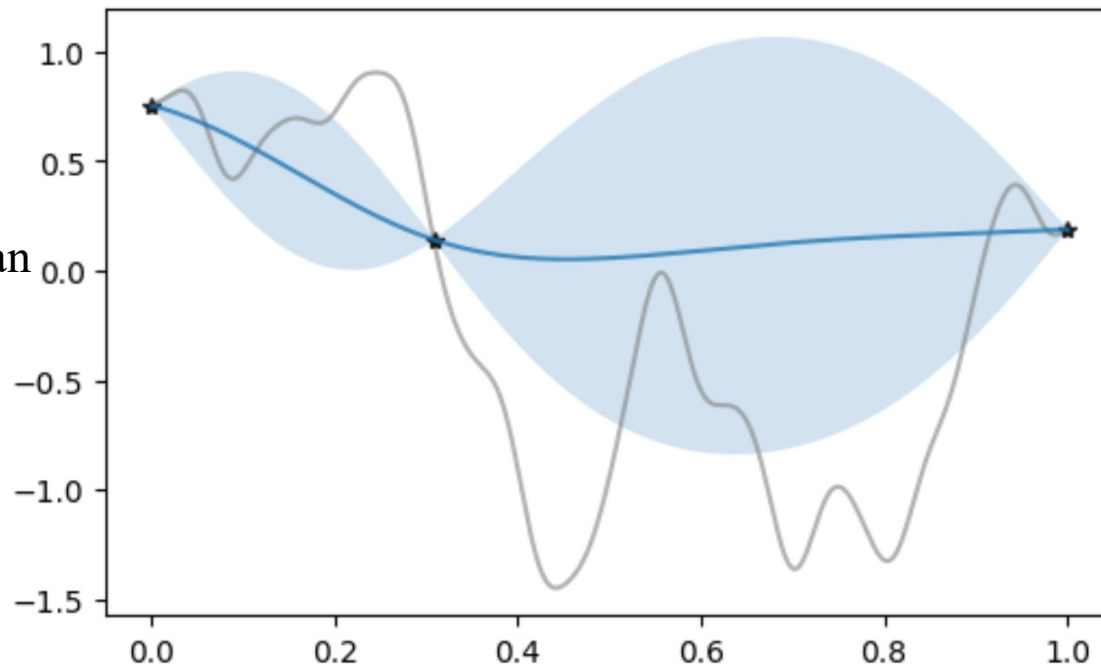
adaptively

Decision: evaluate a set of points

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:

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

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:

Hyperparameter tuning

Drug discovery

Control design

x : hyperparameter/configuration

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

Objective: optimize best observed value at time T

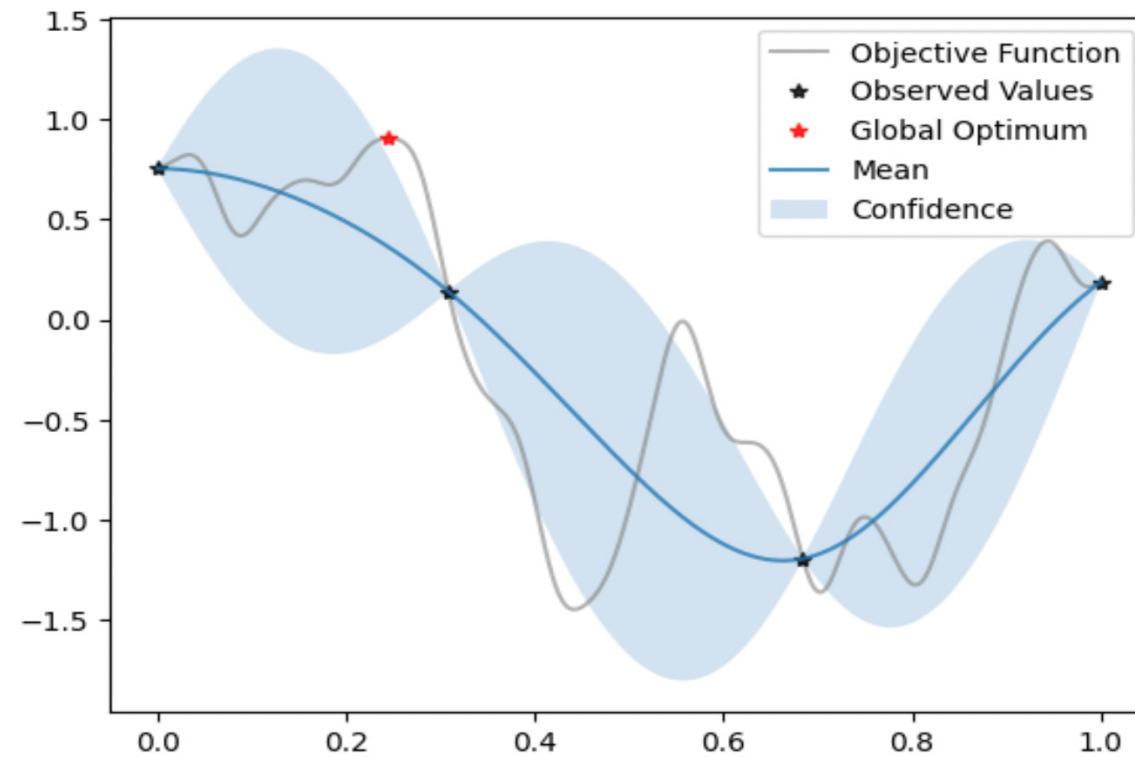
$$\max_{\text{policy}} \mathbb{E} \max_{t=1,2,\dots,T} f(x_t)$$

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

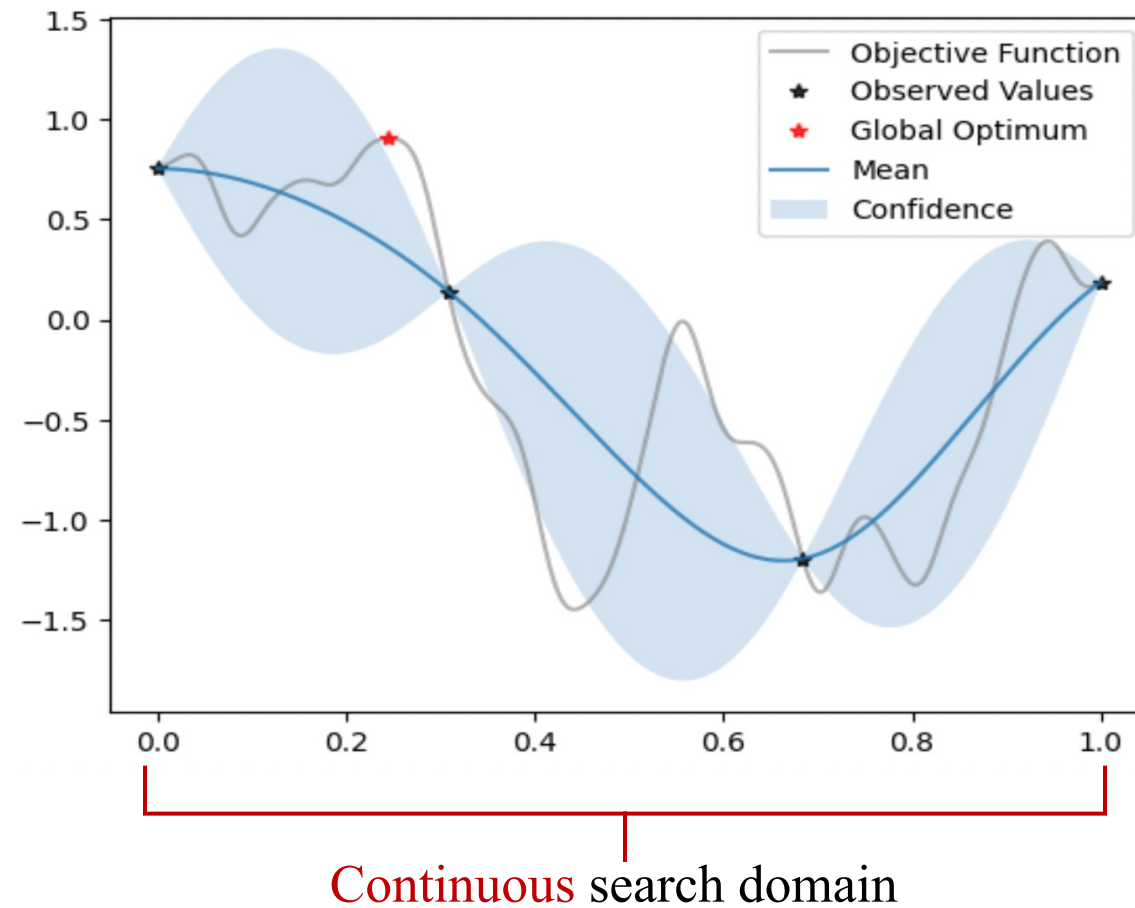
$$x_1, x_2, \dots, x_T \in \mathcal{X}$$

T : time budget

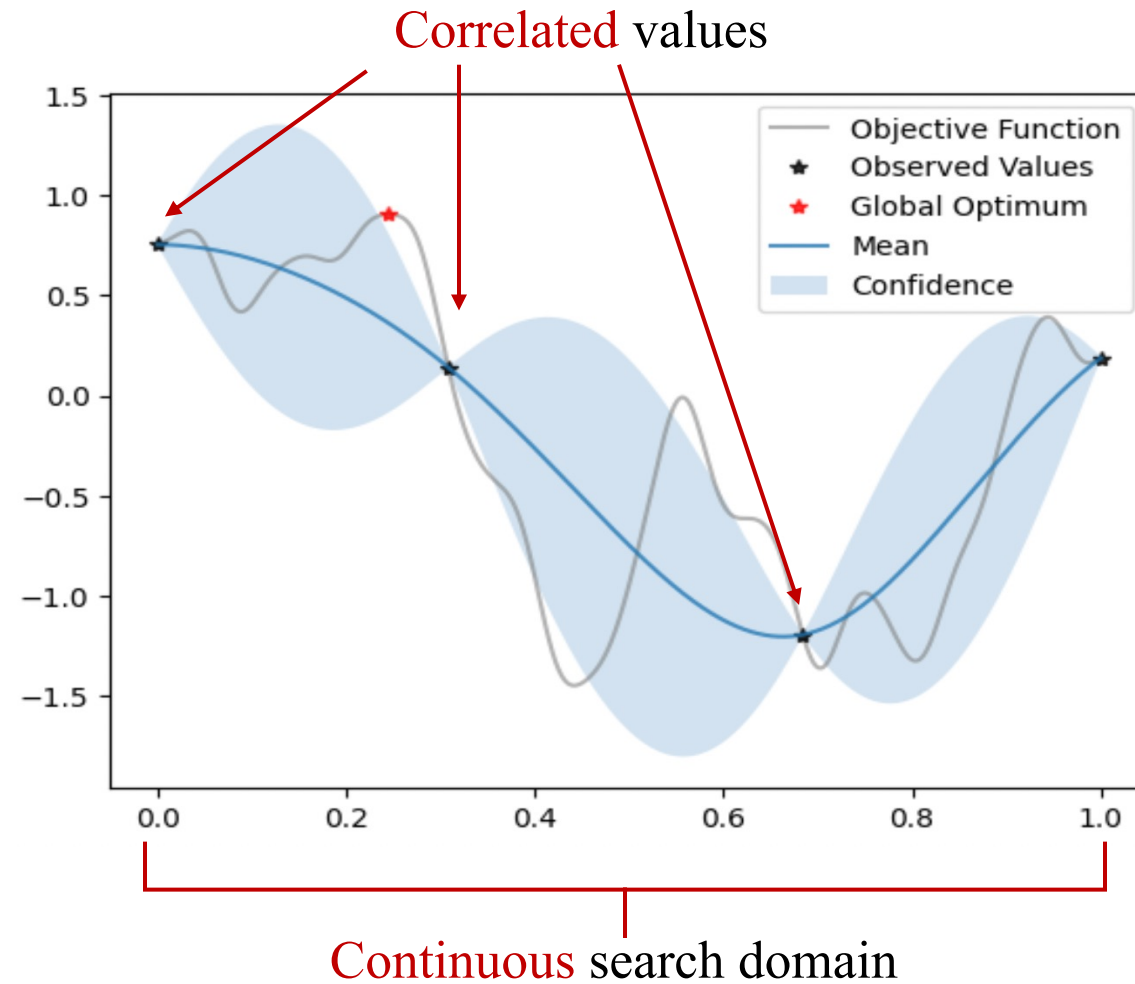
Why is it hard?



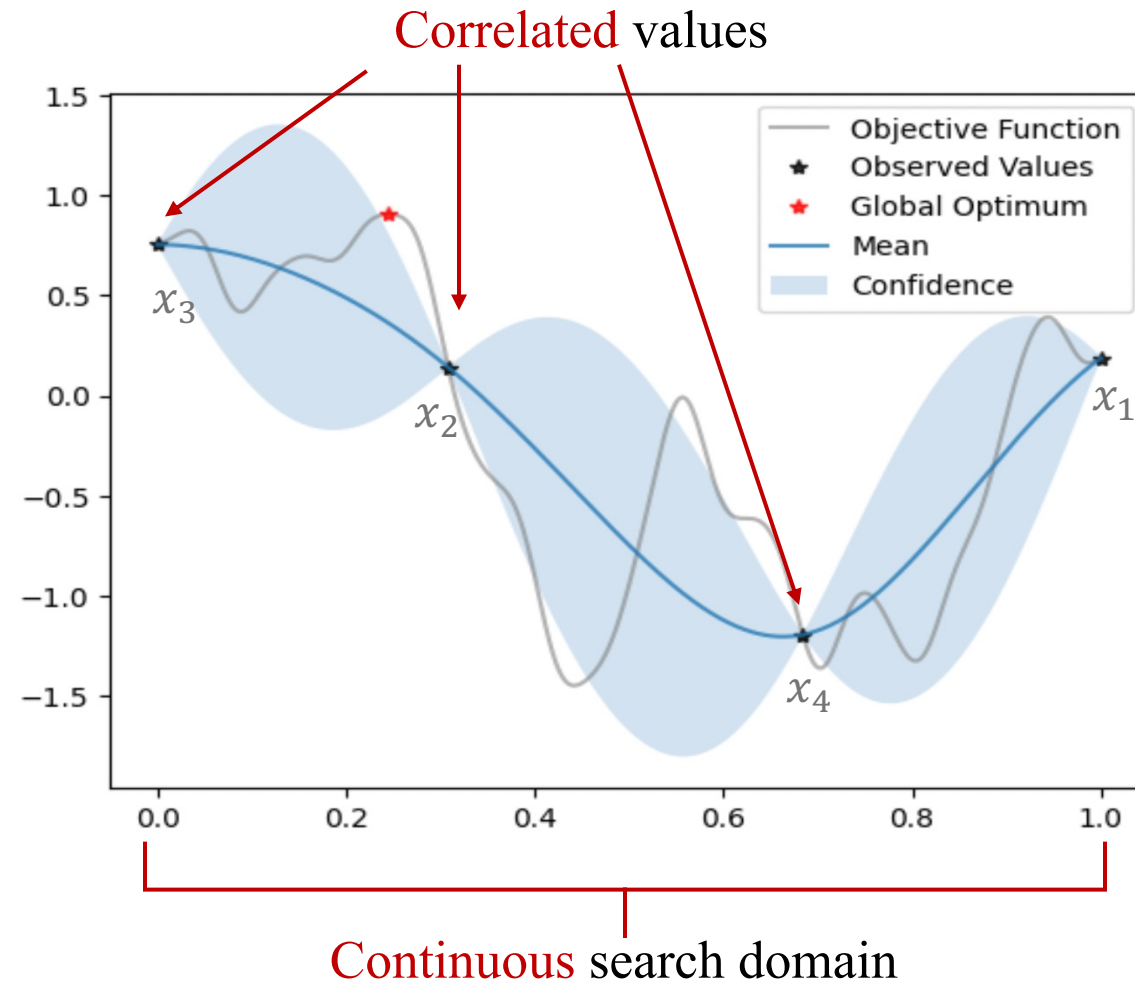
Why is it hard?



Why is it hard?



Why is it hard?



Hard budget **constraint**

~~$t=1$~~



~~$t=2$~~



~~$t=3$~~



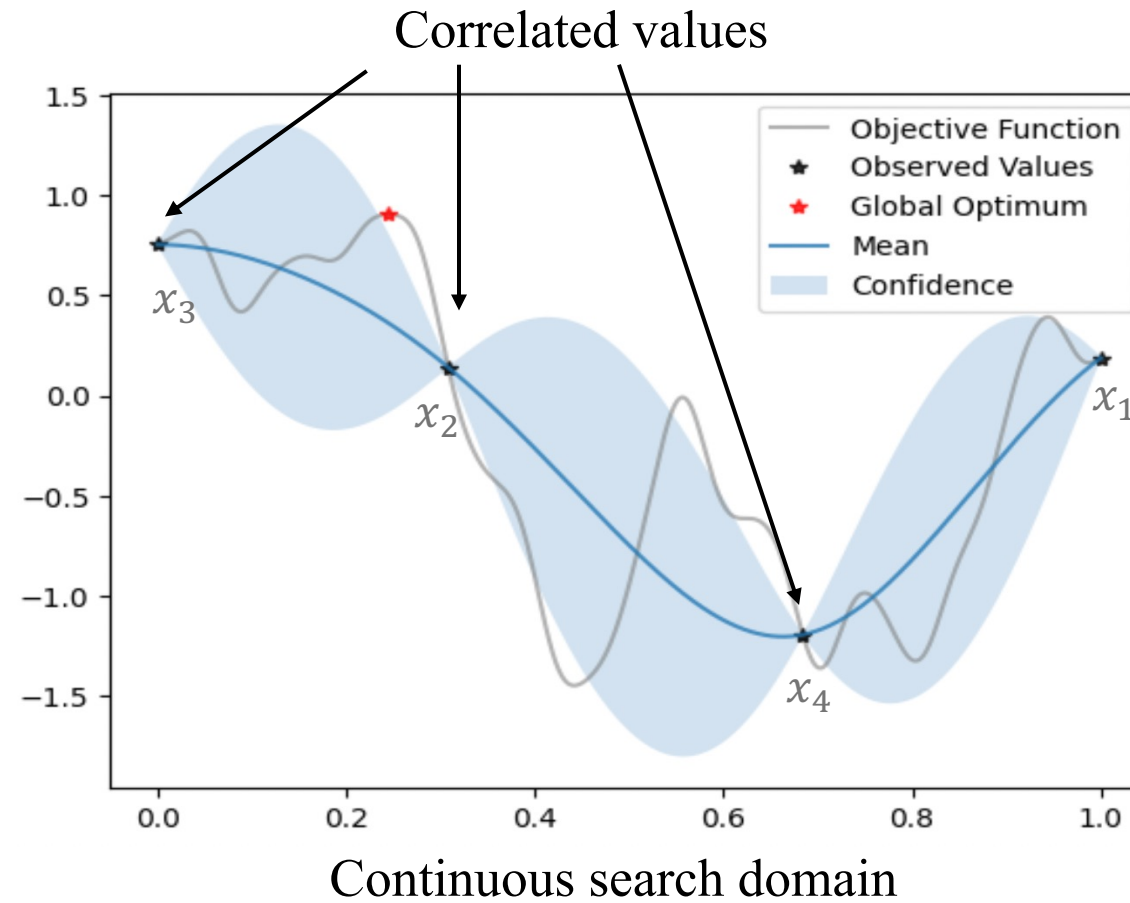
~~$t=4$~~







\vdots

~~$t=T$~~

Why is it hard?

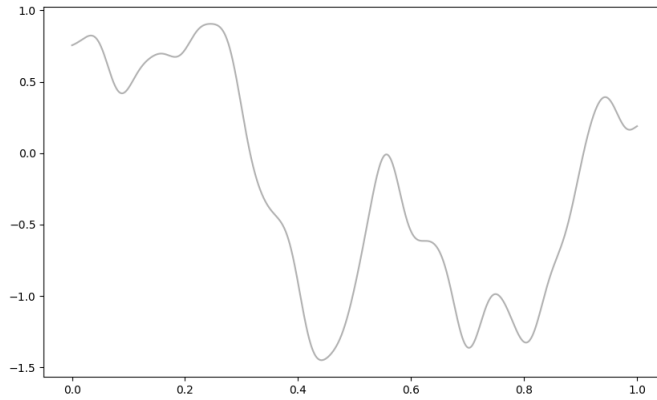


Hard budget constraint

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

\Rightarrow Optimal policy unknown!

Bayesian Optimization

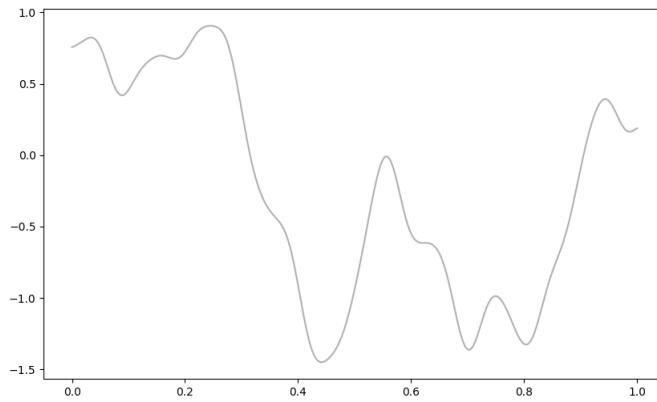


Continuous

Correlated

Hard budget constraint

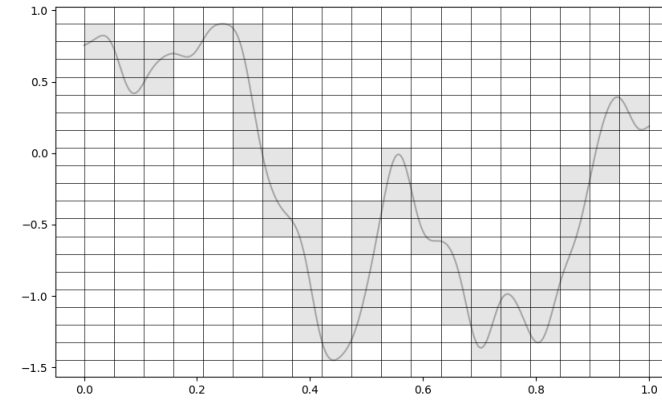
Bayesian Optimization



Continuous

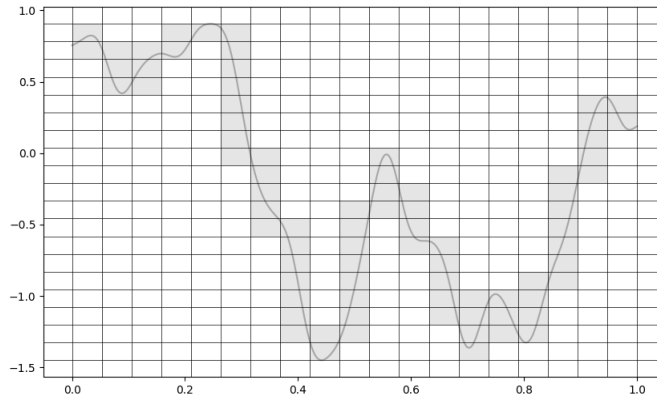
Correlated

Hard budget constraint



Discrete

Bayesian Optimization



Continuous

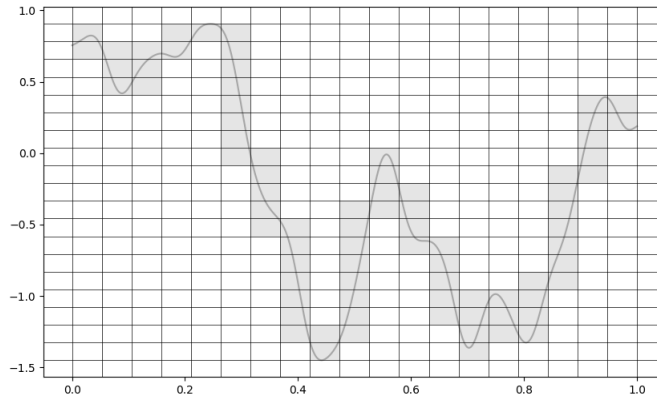


Discrete

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Hard budget constraint

Bayesian Optimization



Continuous



Discrete

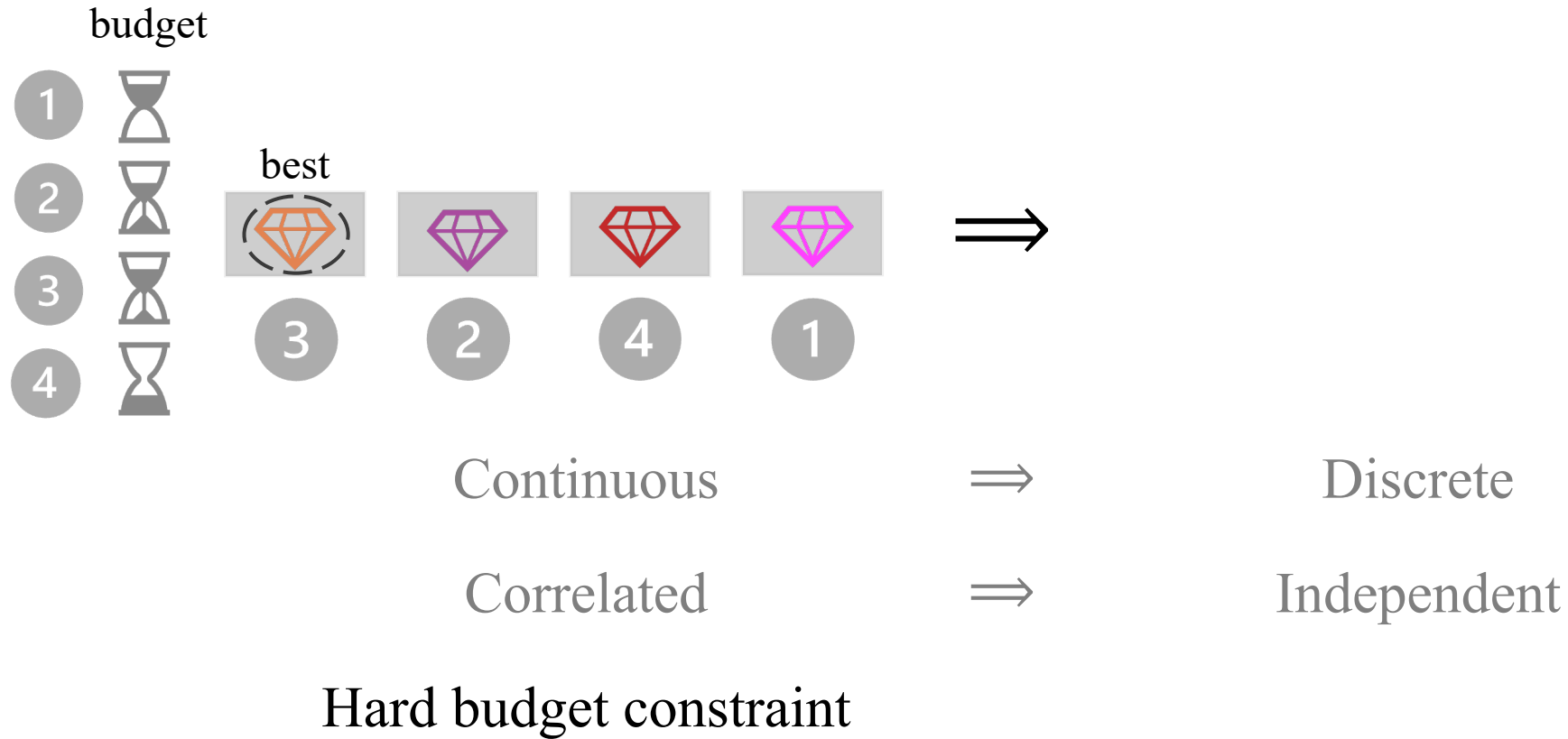
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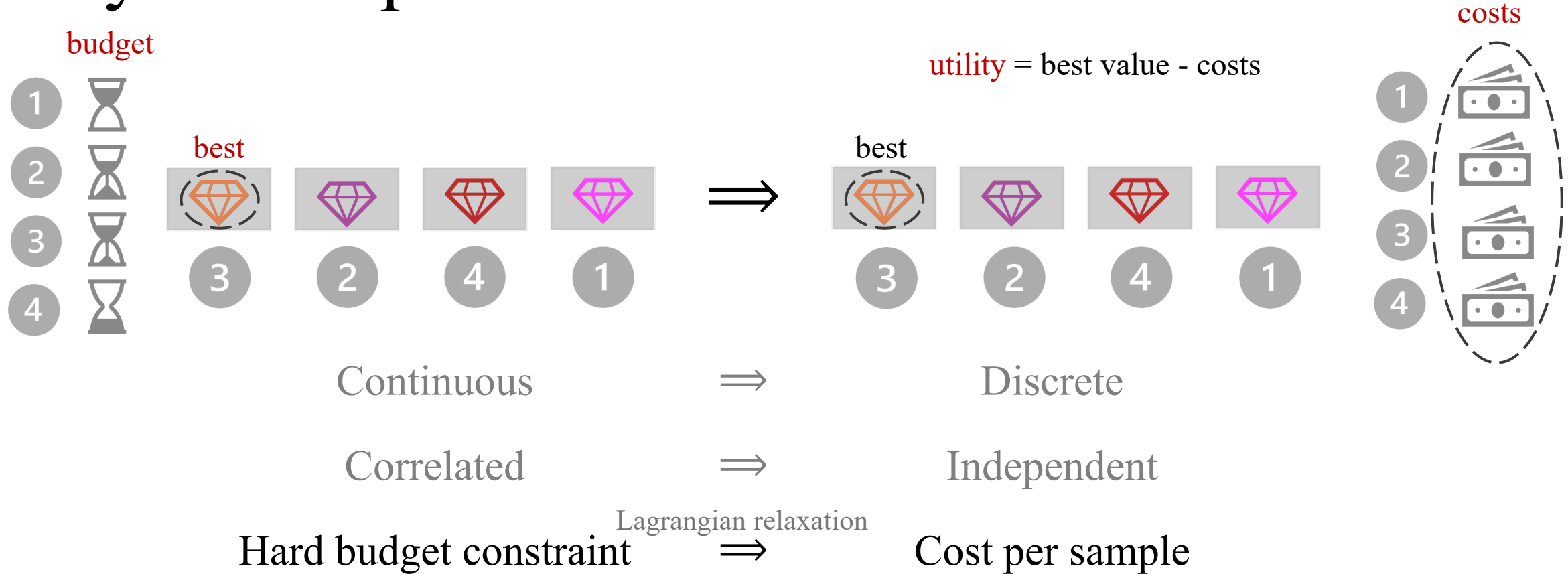
Independent

Hard budget constraint

Bayesian Optimization

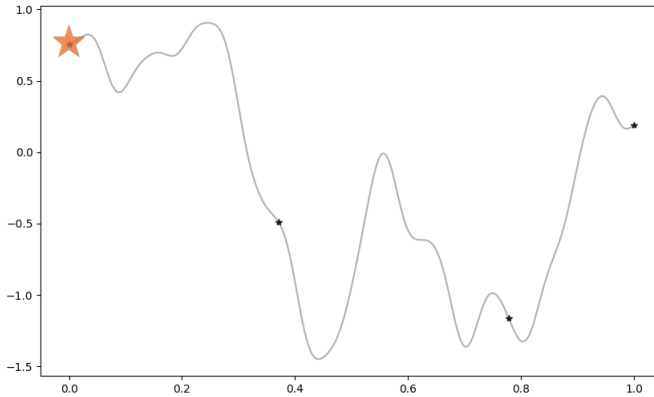


Bayesian Optimization



Bayesian Optimization \Rightarrow Pandora's Box

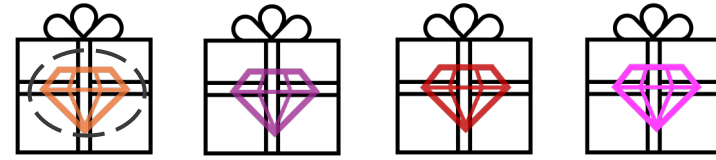
Special case of Markovian/
Bayesian multi-armed bandits



Continuous

Correlated

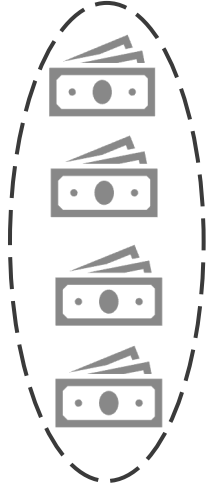
Hard budget constraint



Discrete

Independent

Cost per sample

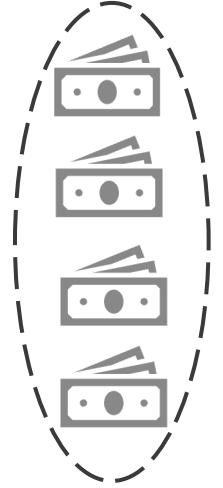
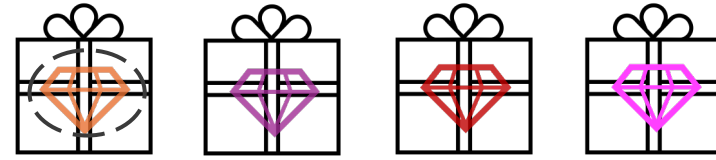


Bayesian Optimization \Rightarrow Pandora's Box

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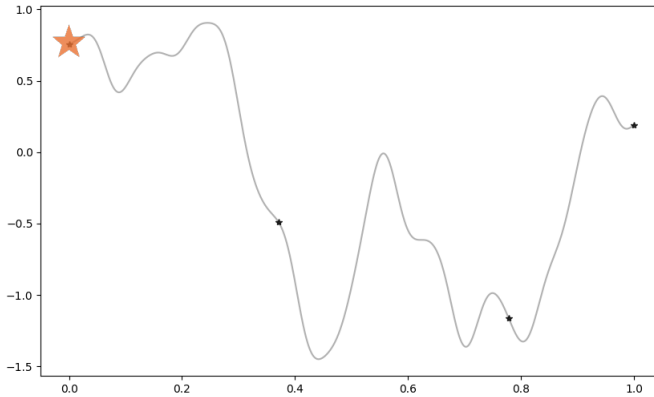
Hard budget constraint



Cost per sample

Optimal policy: Gittins index

Bayesian Optimization \Rightarrow Pandora's Box

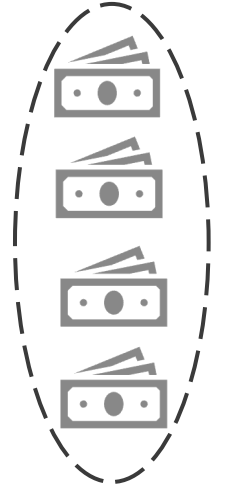
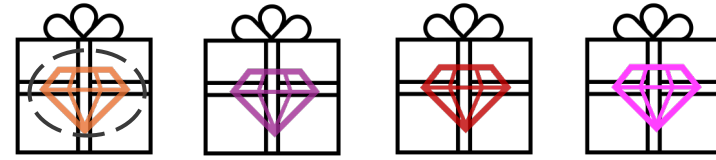


Continuous

Correlated

Hard budget constraint

Is Gittins index good?



Discrete



Independent

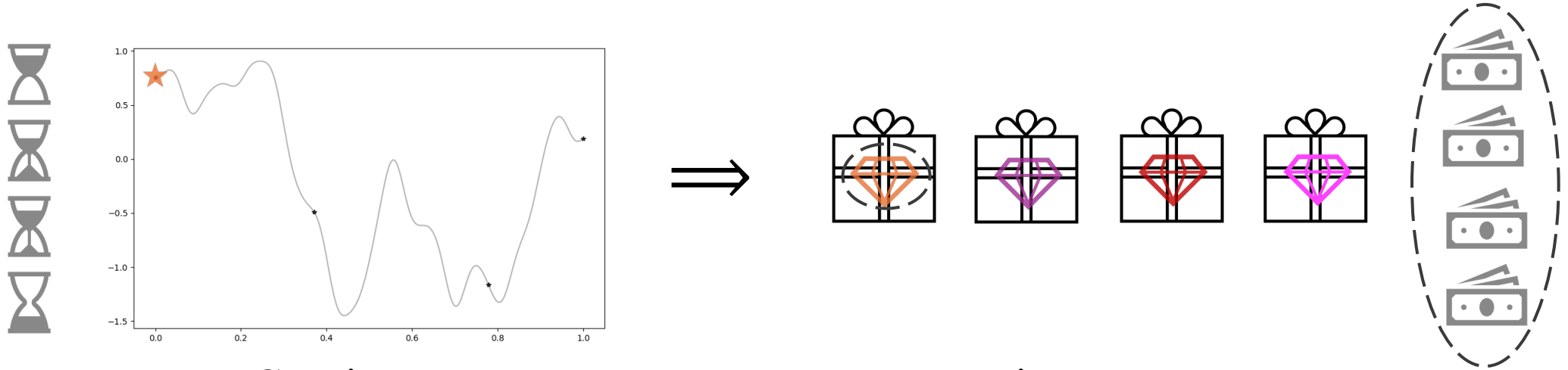


Cost per sample



Optimal policy: Gittins index

Bayesian Optimization \Rightarrow Pandora's Box



Continuous

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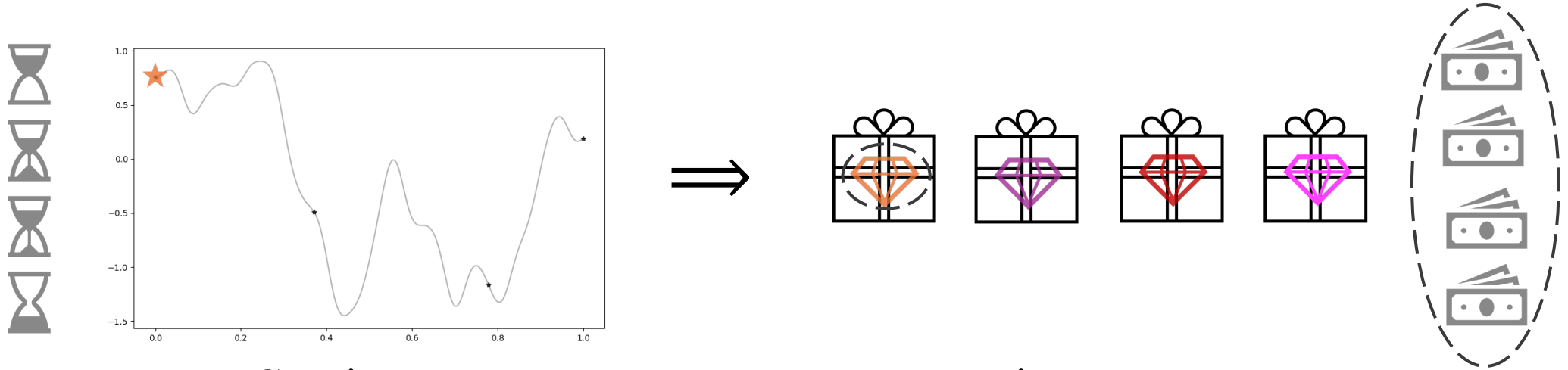
Independent

Hard budget constraint

Cost per sample

Is Gittins index good? $\xRightarrow{\text{How to translate?}}$ Optimal policy: Gittins index

Bayesian Optimization \Rightarrow Pandora's Box



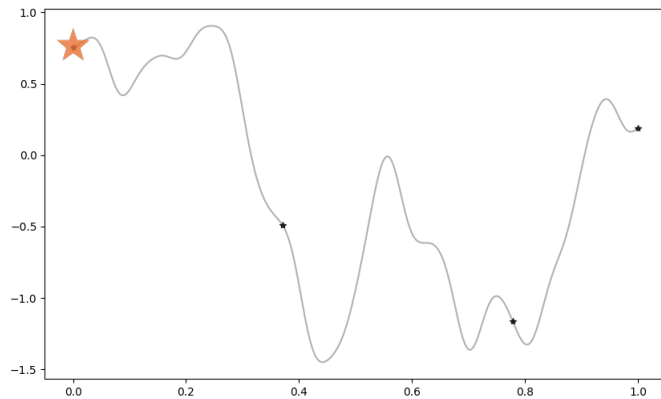
Is Gittins index good? How to translate?

\Leftarrow Optimal policy: Gittins index

Our contributions!

Our Contributions

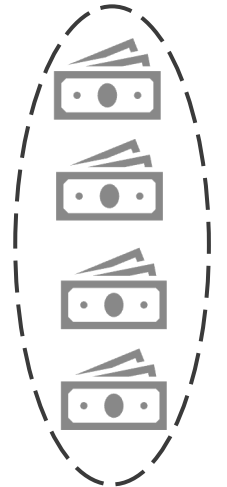
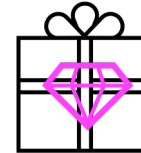
- How to translate?
- Is Pandora's Box Gittins index (PBGI) good?



?

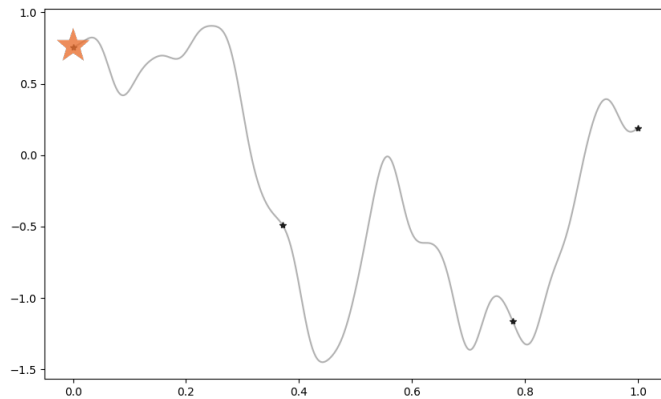


Pandora's Box Gittins index

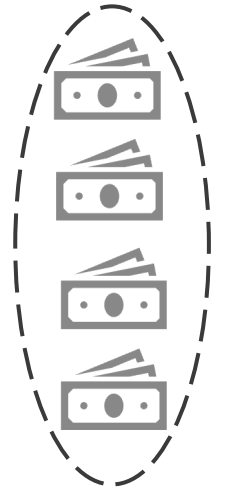
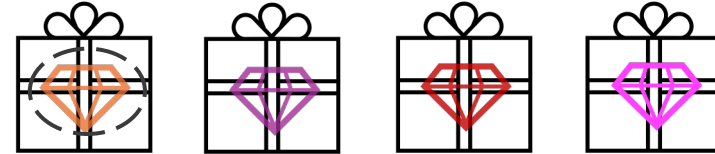


Our Contributions

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



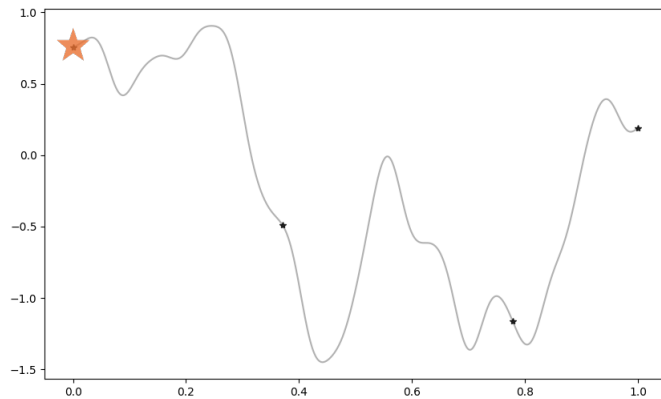
Our work



Pandora's Box Gittins index

Our Contributions

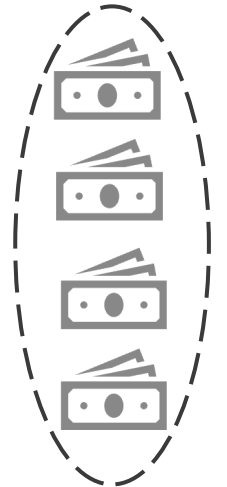
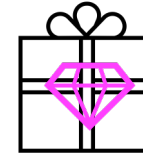
- Develop PBGI policy for Bayesian optimization
- Show **performance** against baselines on synthetic & empirical experiments



Our work

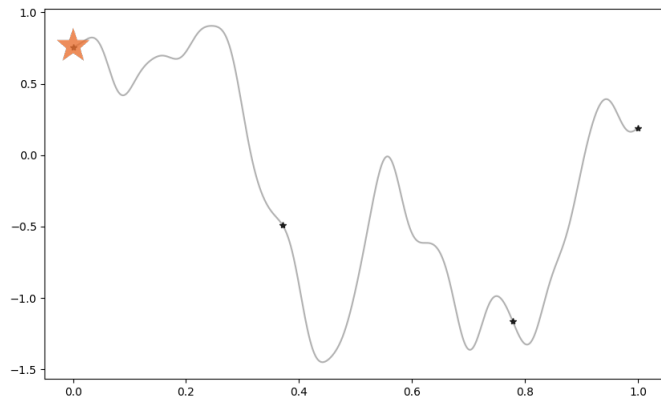


Pandora's Box Gittins index



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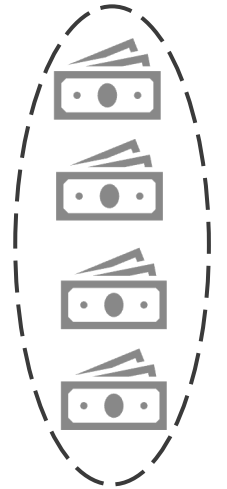
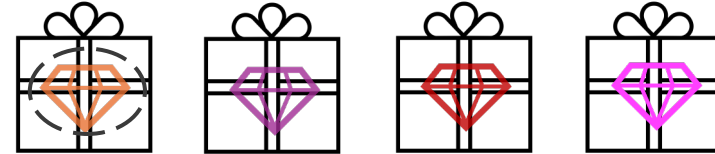
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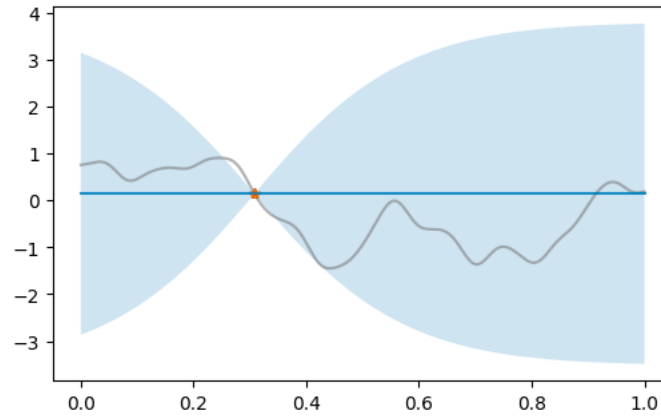


Pandora's Box Gittins index



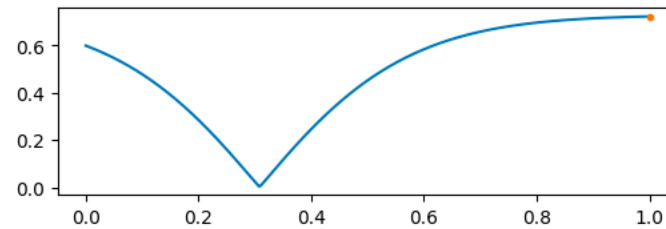
How is our PBGI policy different from baselines?

Popular One-step Heuristic: EI



mean: prediction

variance: confidence/uncertainty



Trade-off between

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

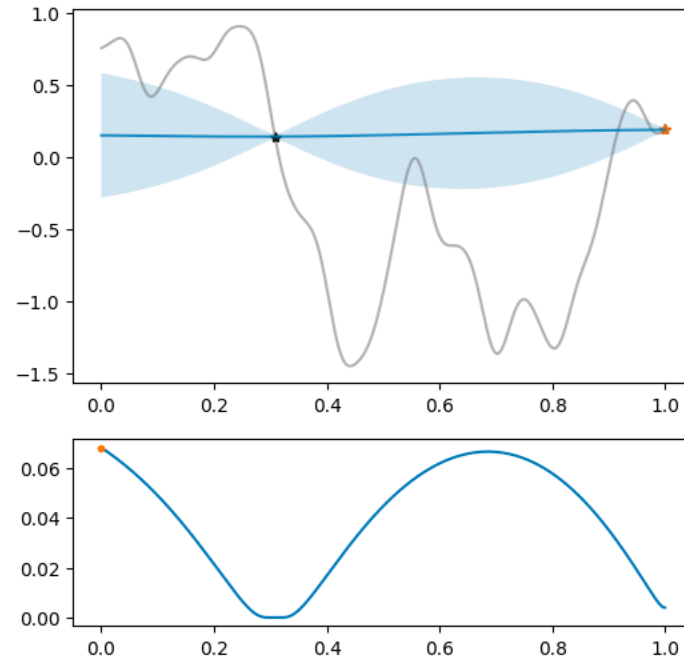
Expected improvement

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

y_{best} : current best observed value

EI policy: evaluate $\text{argmax}_x \text{EI}_f(x; y_{\text{best}})$

Popular One-step Heuristic: EI



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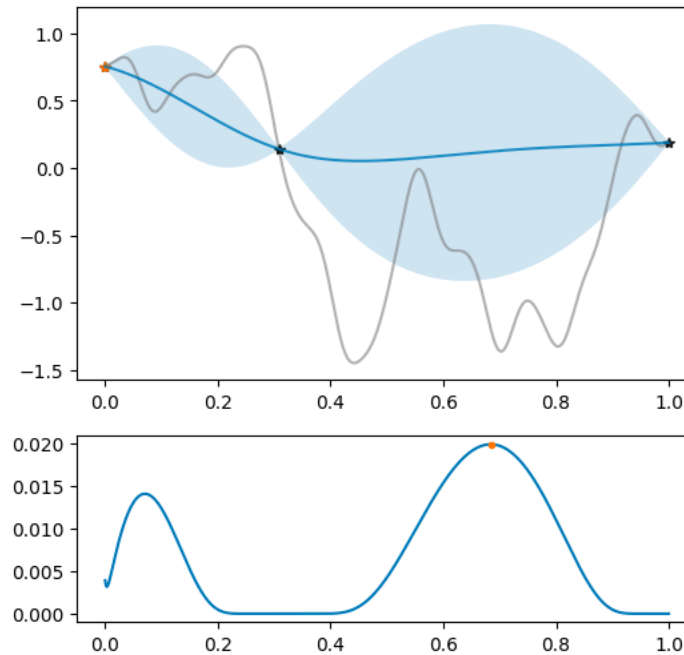
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Popular One-step Heuristic: EI

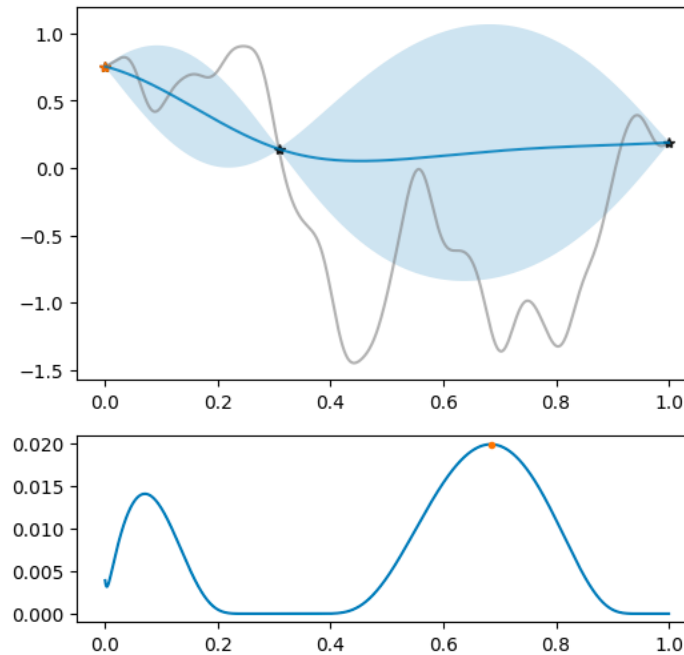
Other heuristics:

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
- exploration (high uncertainty)

Expected improvement

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

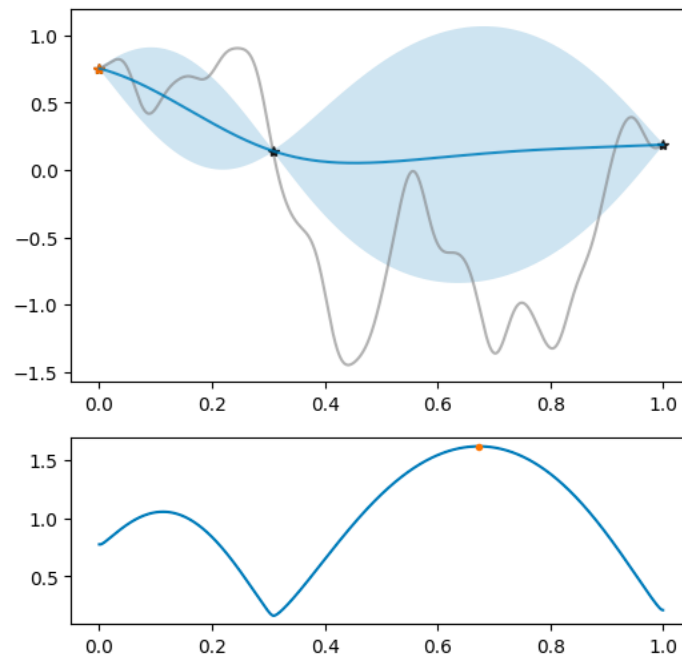
y_{best} : current best observed value

EI policy: evaluate $\arg\max_x \text{EI}_f(x; y_{\text{best}})$

New One-step Heuristic: PBGI

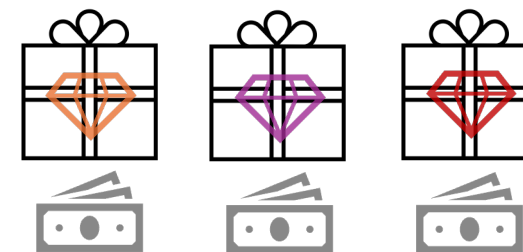
Other heuristics:

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



Pandora's box Gittins index

Pandora's box



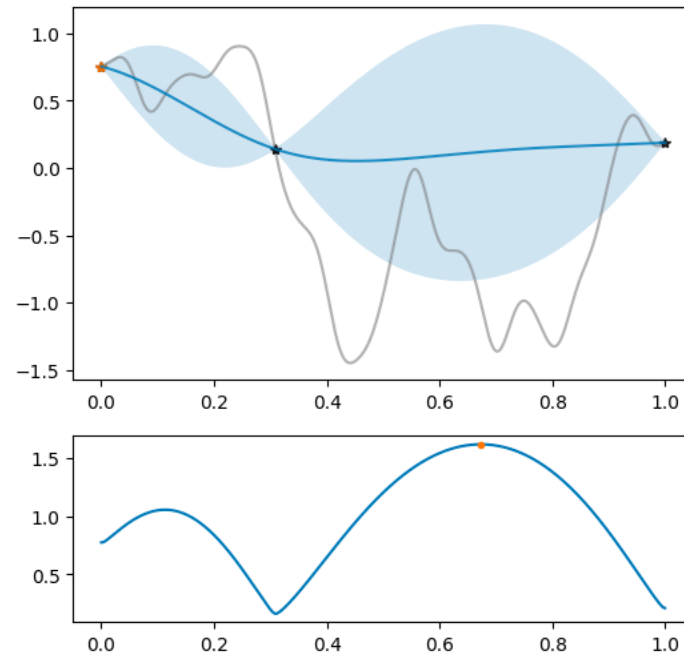
PBGI policy: evaluate $\operatorname{argmax}_x \alpha^*(x)$

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

New One-step Heuristic: PBGI

Other heuristics:

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



Pandora's box Gittins index

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

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

$\alpha^*(x)$: solution to $EI_f(x; \alpha^*(x)) = \lambda$

Pandora's box



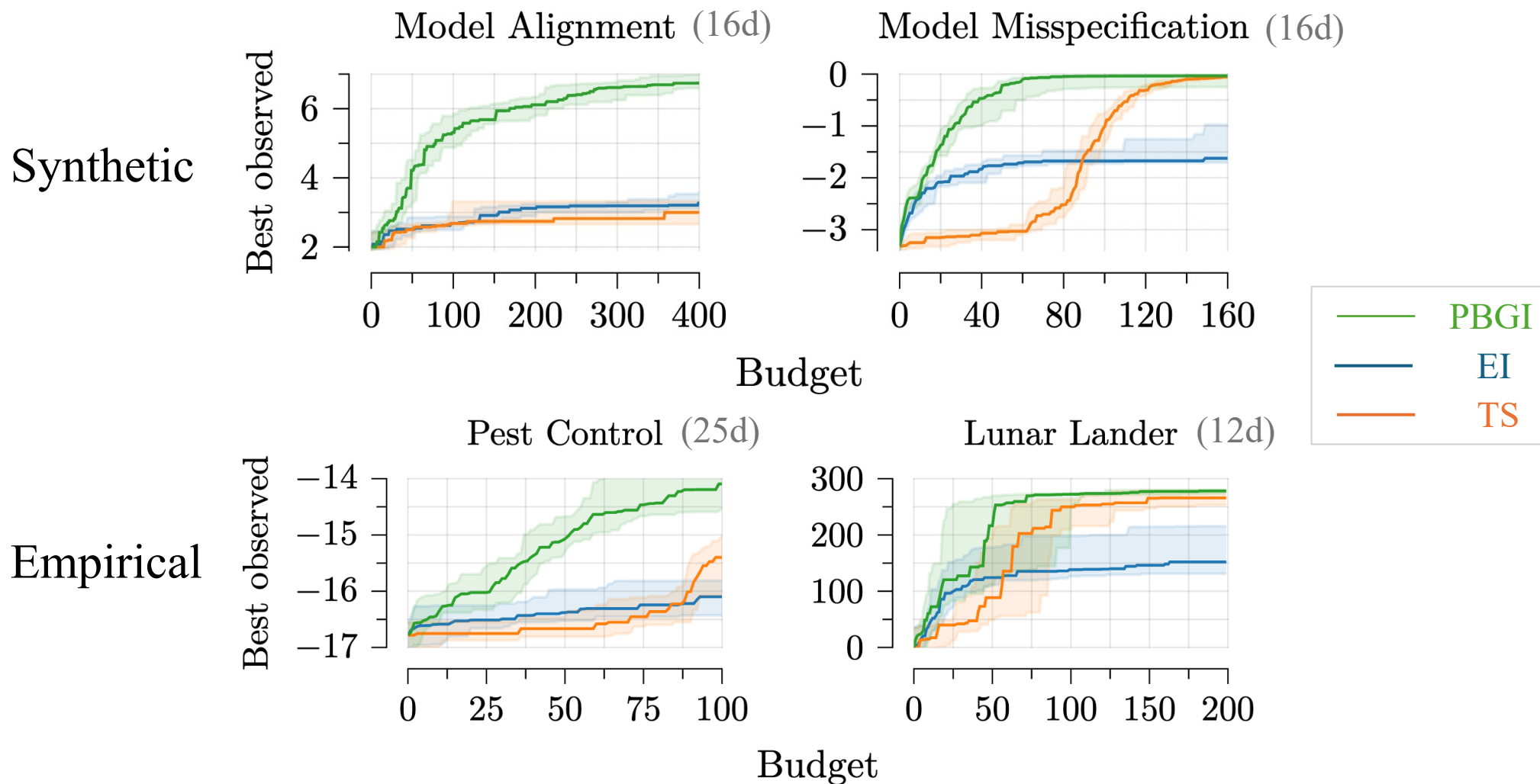
λ

λ

λ

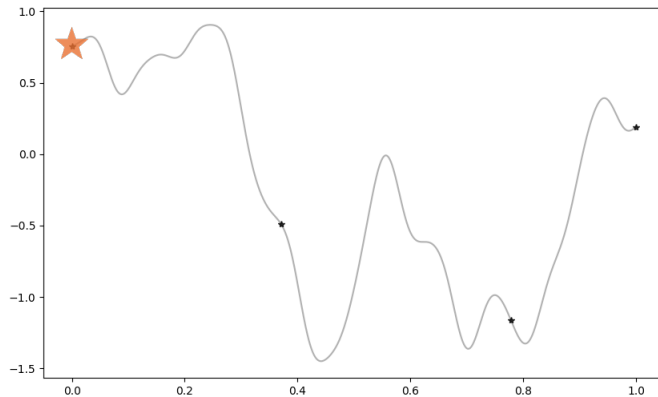
λ : cost-per-sample
(Lagrange multiplier)

Experiment Results: PBGI vs EI vs TS

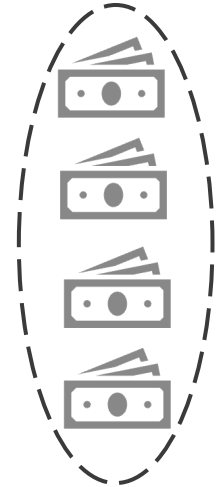
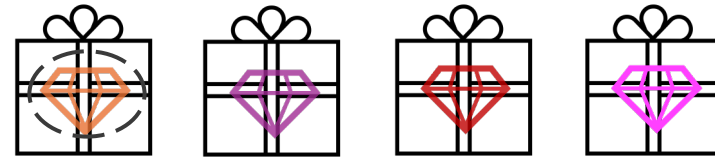


Conclusions

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



Our work

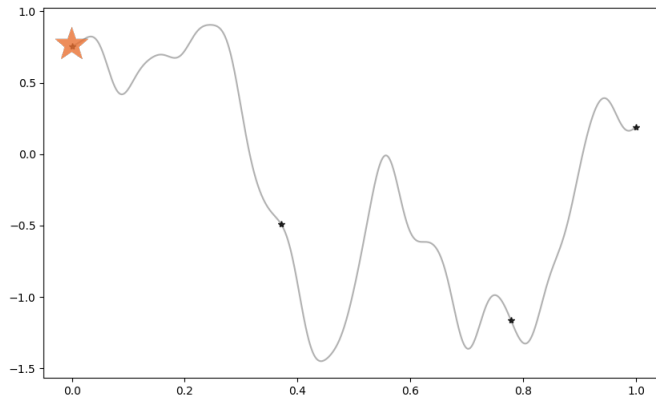


Pandora's box Gittins index

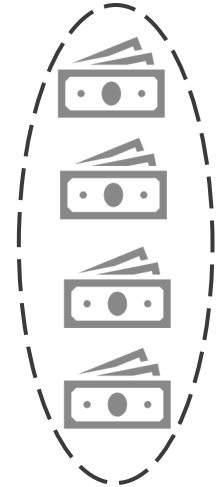
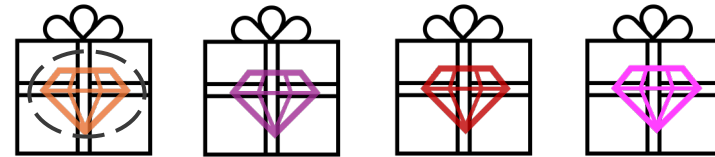
Check our preprint on arXiv!

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

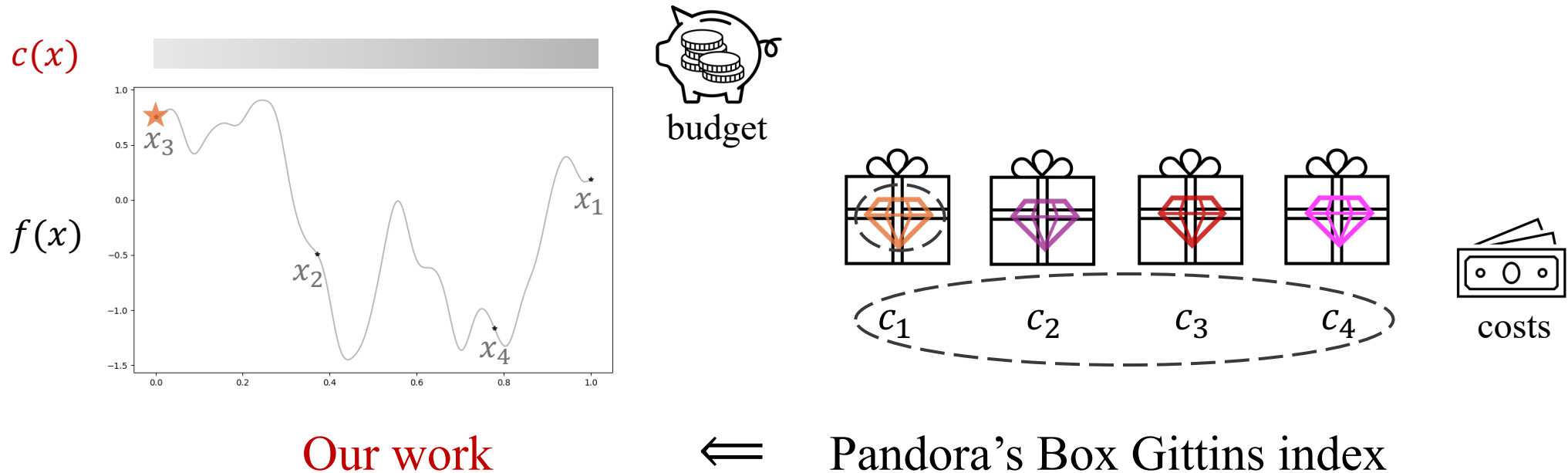


Pandora's box Gittins index

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Conclusions

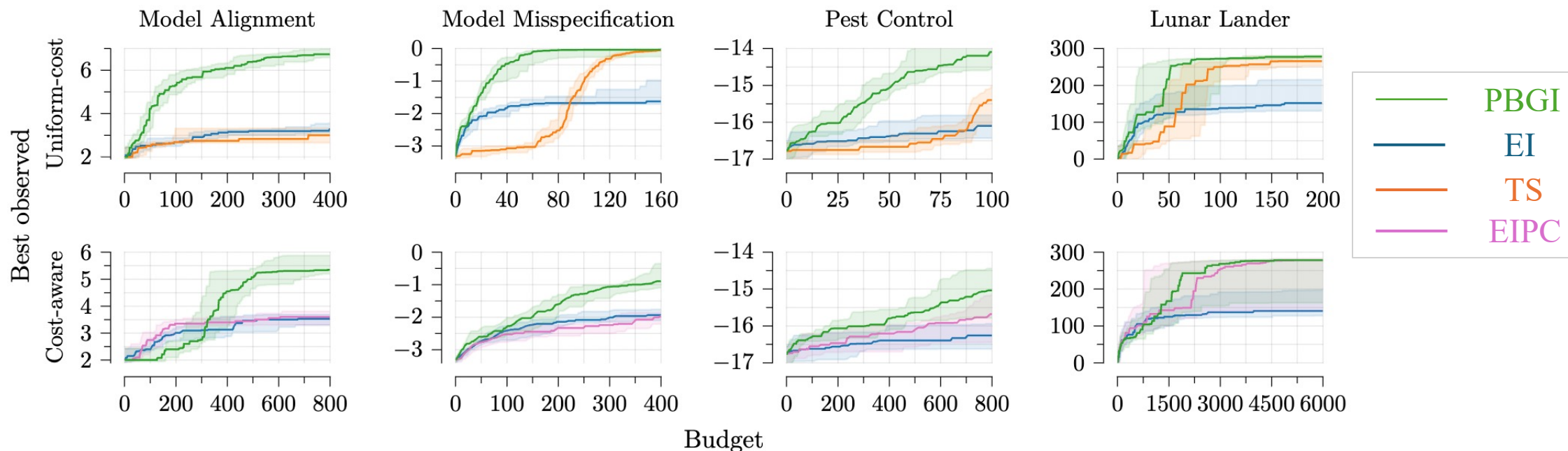
- Propose easy-to-compute Gittins index function for Bayesian optimization
- Show the effectiveness of PBGI on synthetic & empirical experiments
- Extend to Bayesian optimization with **heterogeneous evaluation costs**



Check our preprint on arXiv!

Heterogeneous-cost Experiment Results

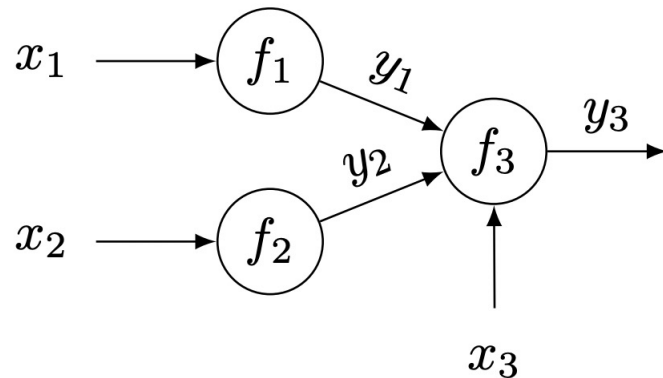
- Show the effectiveness of PBGI on synthetic & empirical experiments
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Conclusions

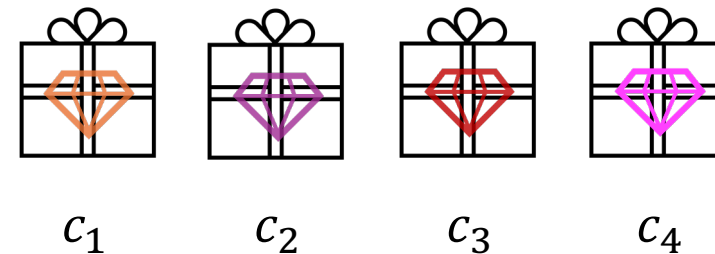
- Propose easy-to-compute PBGI policy for Bayesian optimization
- Show the effectiveness of PBGI on synthetic & empirical experiments
- Extend to Bayesian optimization with heterogeneous evaluation costs
- Open door for **exotic BO** (freeze-thaw, multi-fidelity, function network, etc.)



?



Pandora's Box Gittins index



Check our preprint on arXiv!