

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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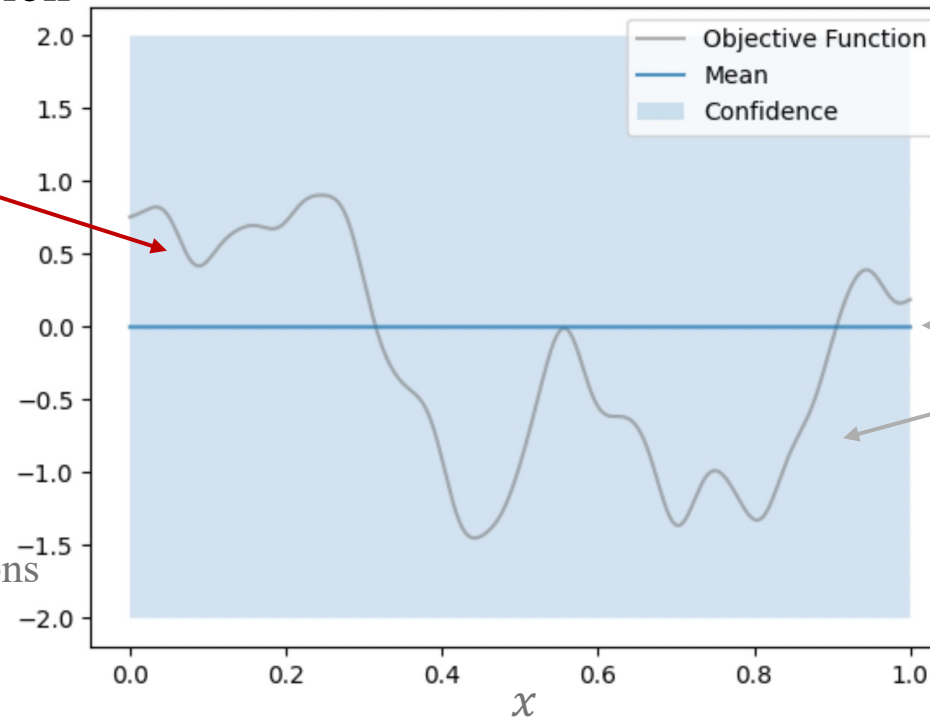
Control design

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:

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x : hyperparameter/configuration

mean: prediction

variance: confidence/uncertainty

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Gaussian process: infinite-dimensional generalization of multivariate normal distributions

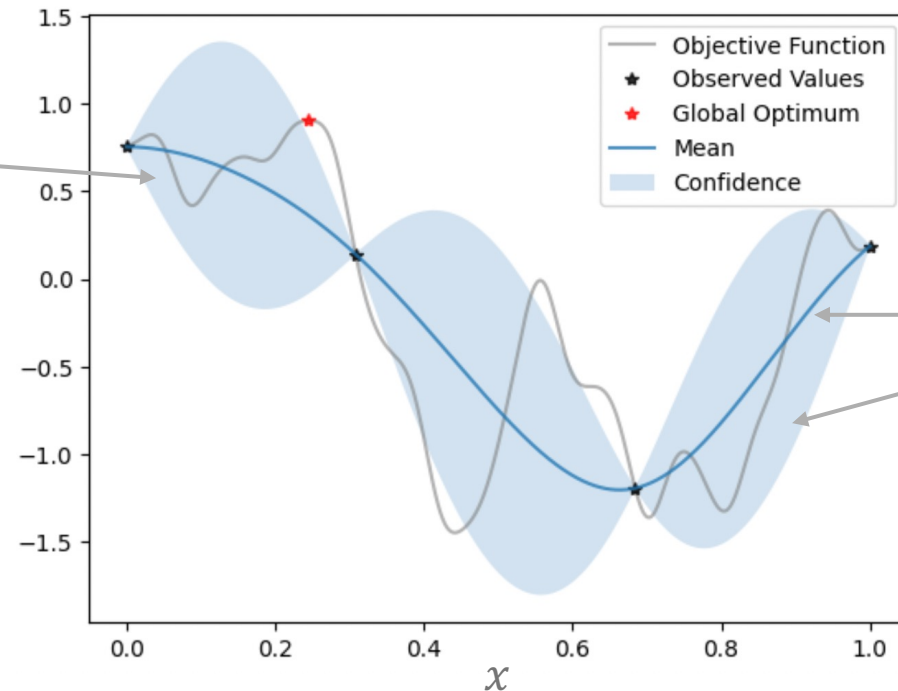
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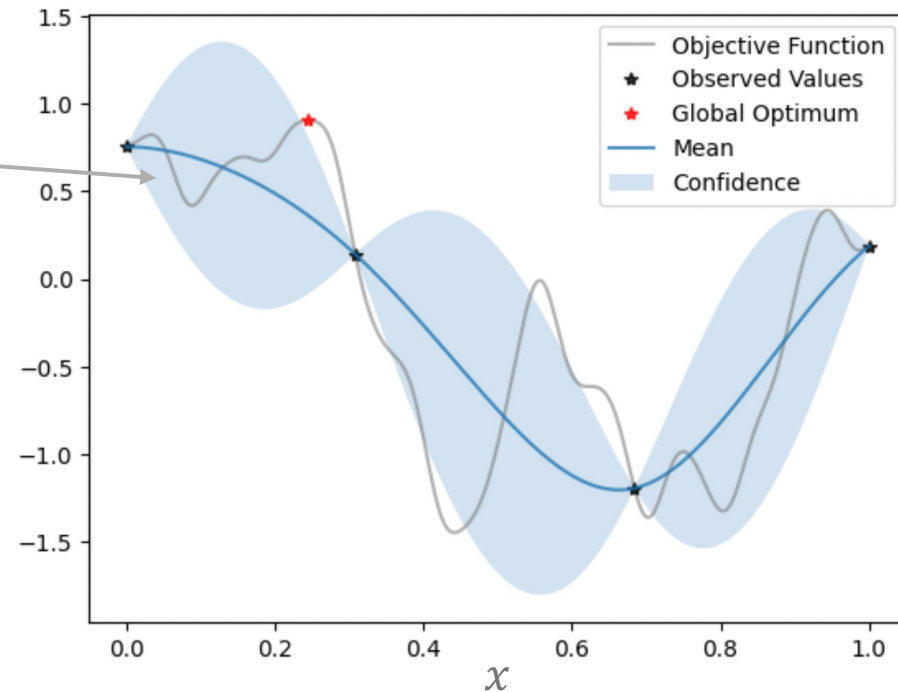
Objective: find global optimum $x^* = \operatorname{argmax}_{x \in \mathcal{X}} f(x)$

Decision: evaluate a set of points

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Applications:

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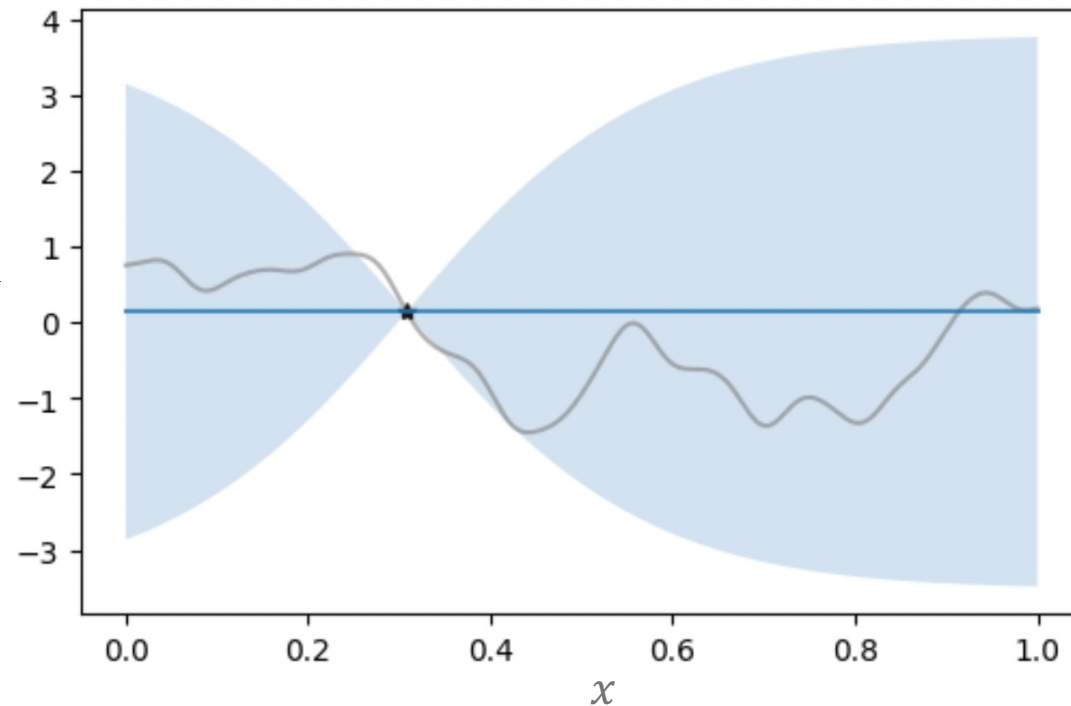
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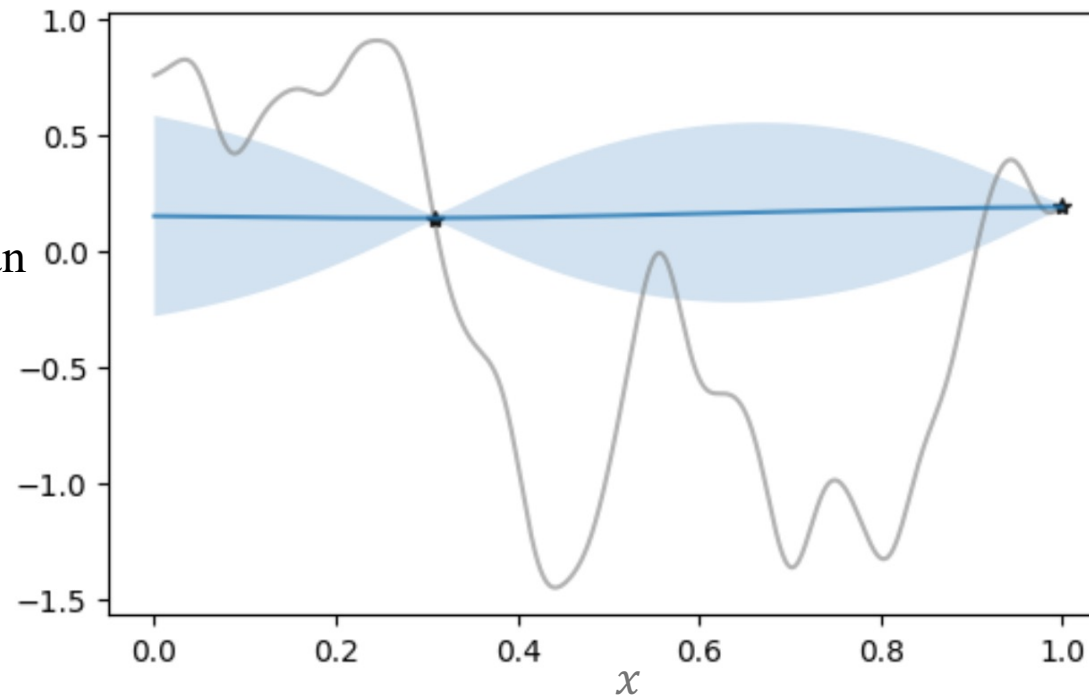
adaptively

Decision: evaluate a set of points

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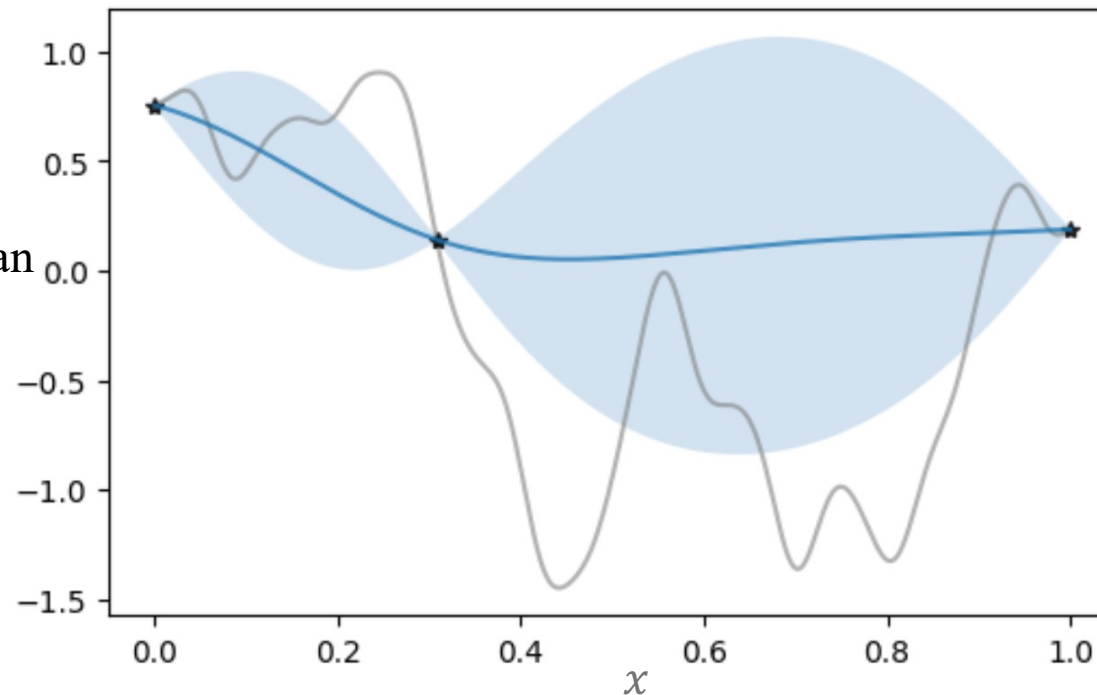
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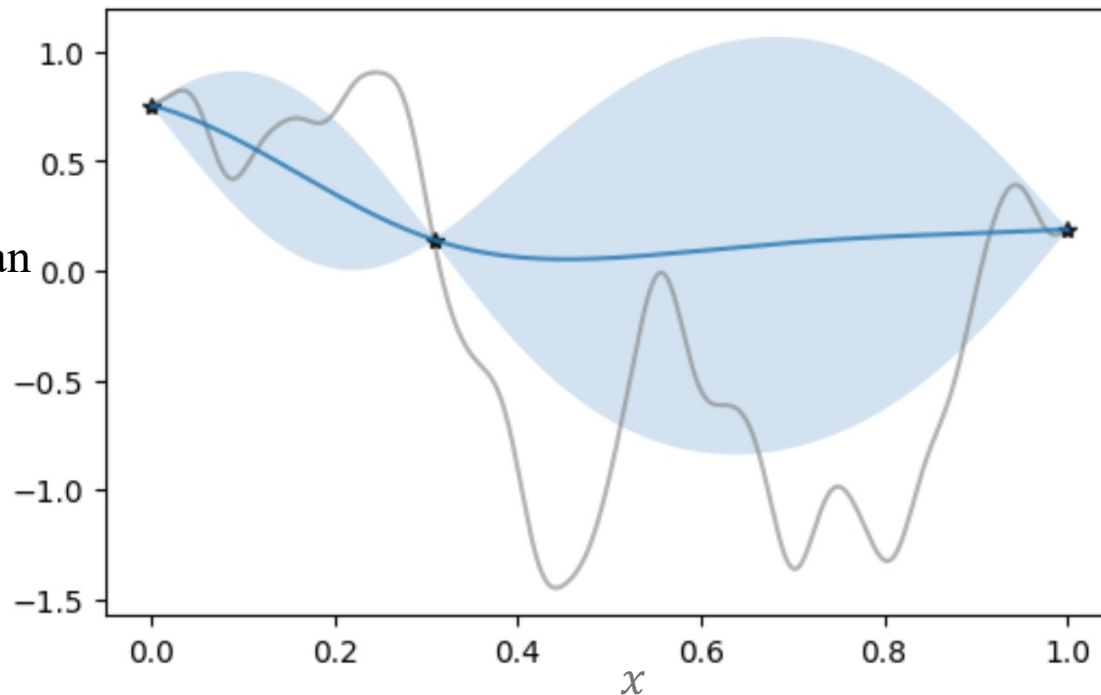
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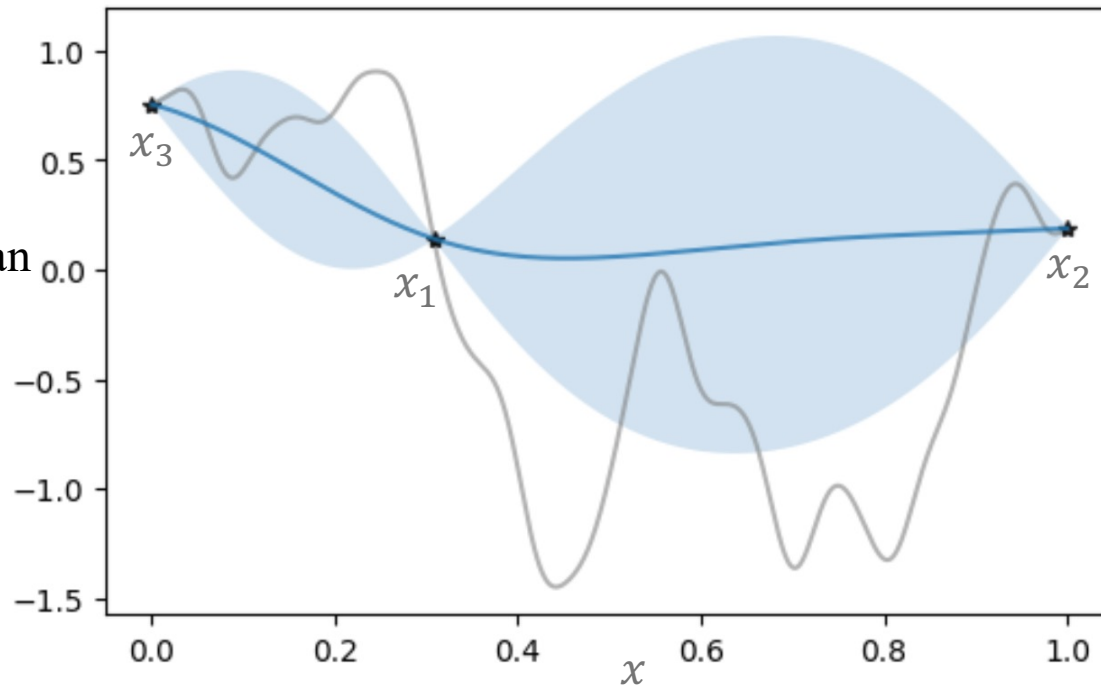
$x_1, x_2, \dots, x_T \in \mathcal{X}$

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

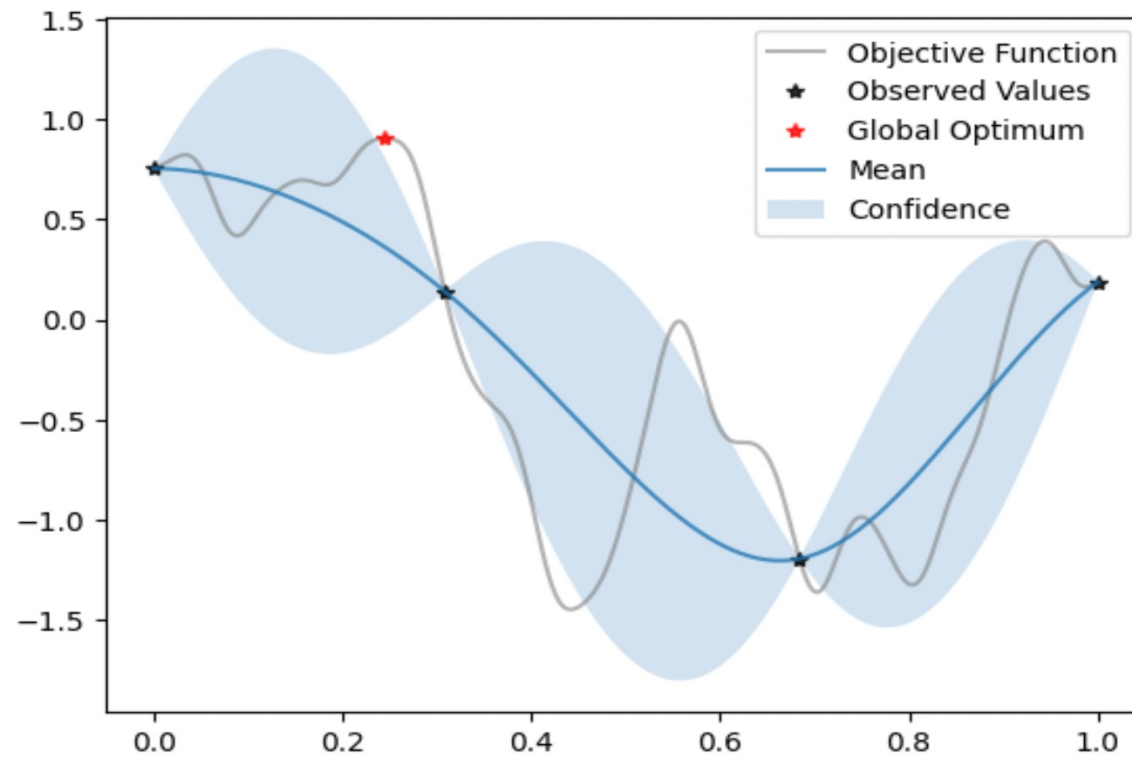
Decision: **adaptively** evaluate a set of points

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

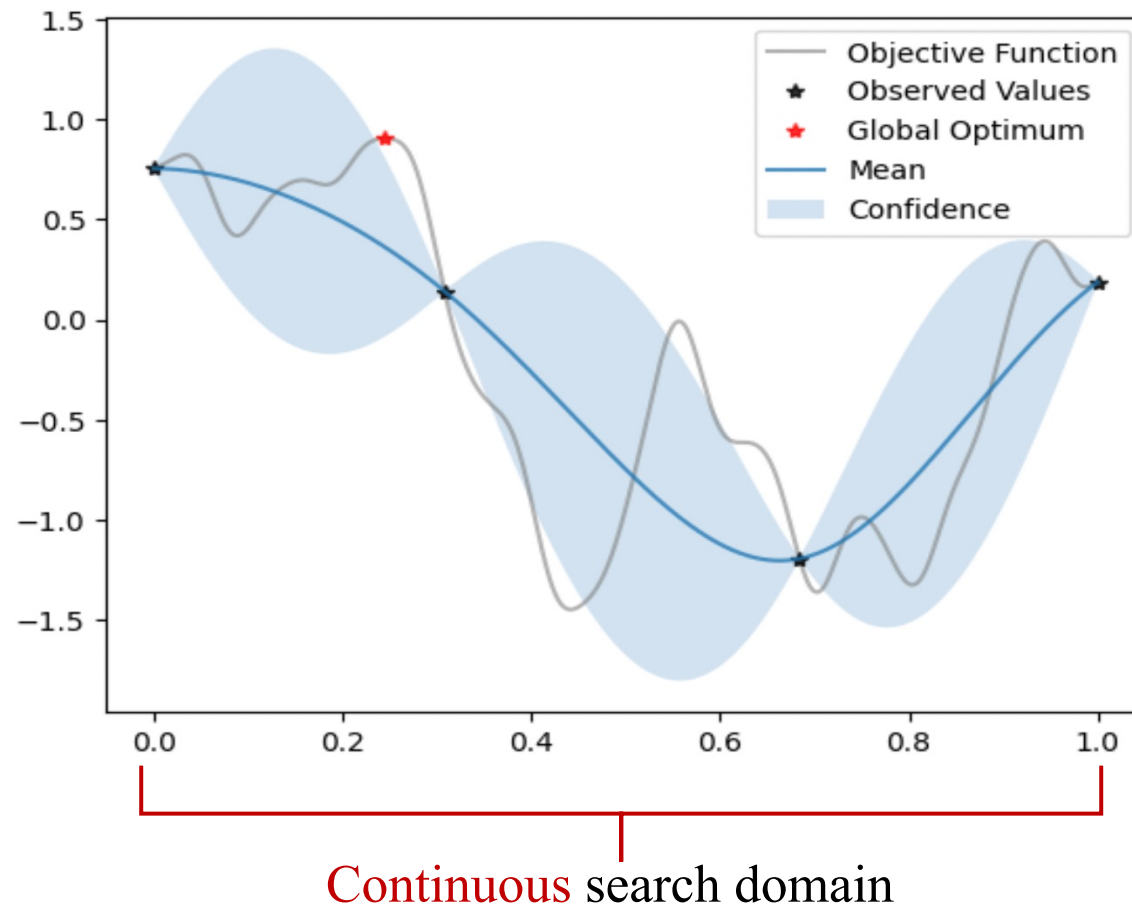
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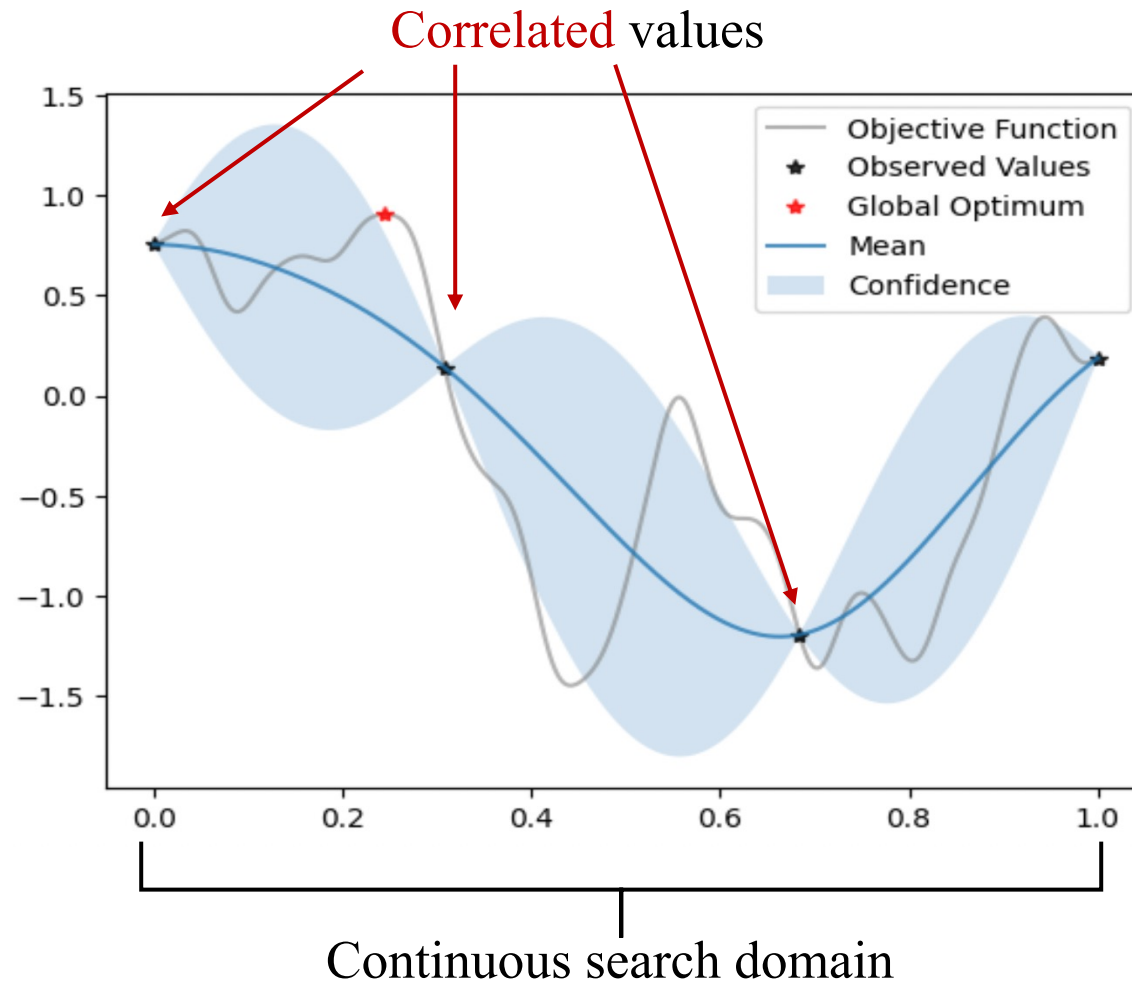
Why is it hard?



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Hard budget **constraint**

~~$t=1$~~



~~$t=2$~~



~~$t=3$~~

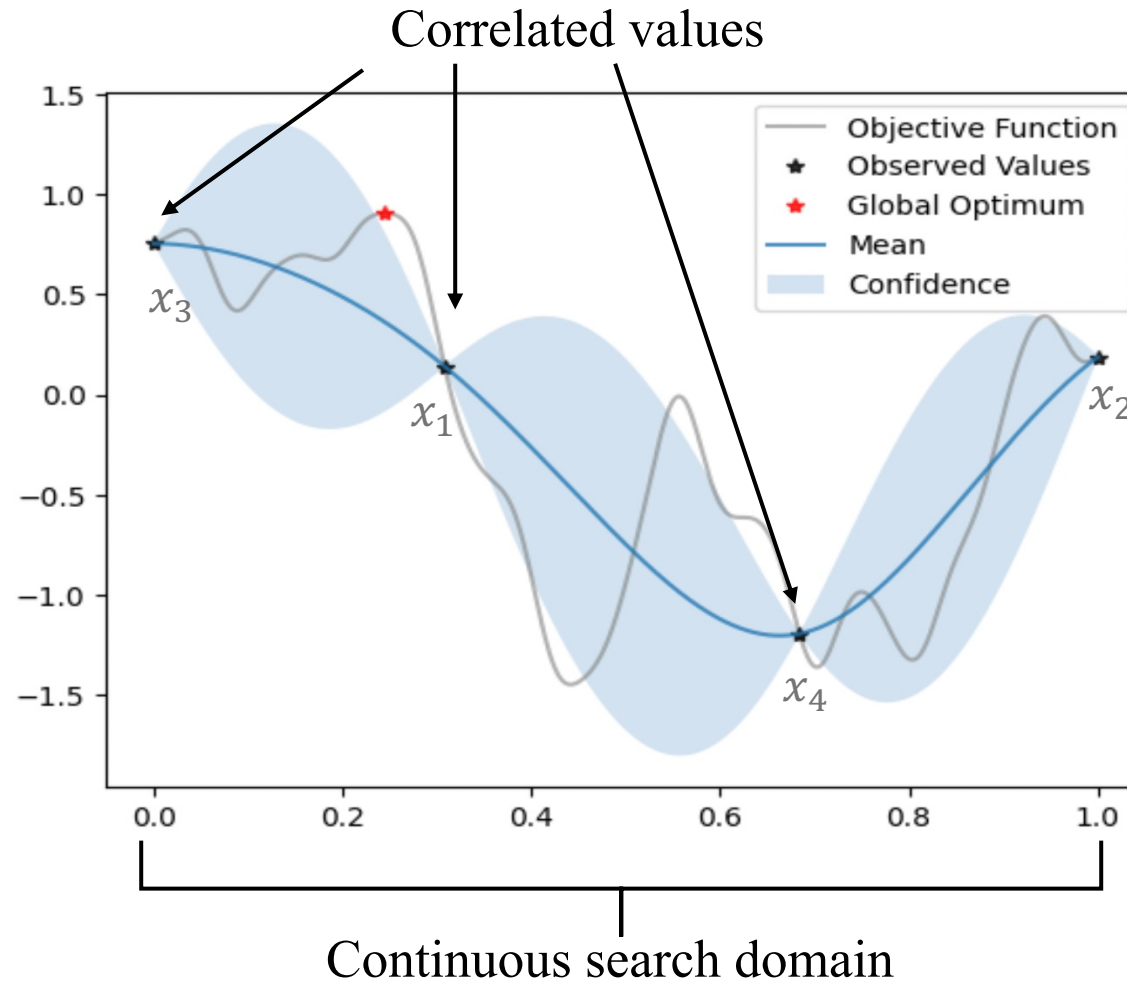


~~$t=4$~~







\vdots

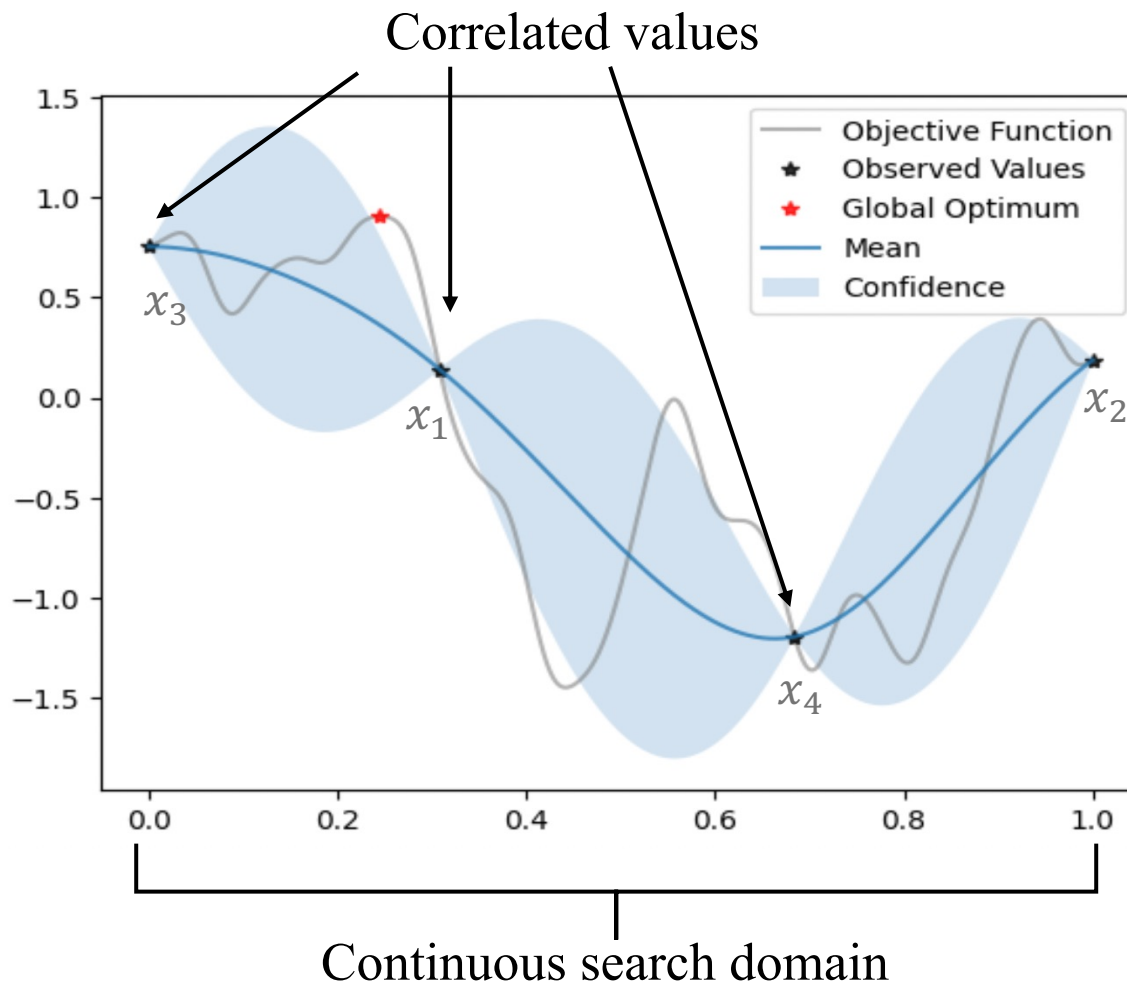
$t = T$



Why is it hard?

Hard budget **constraint**

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



Evaluation **costs** handling



cheap

risk-seeking

exploration



uniform



expensive

risk-averse





exploitation

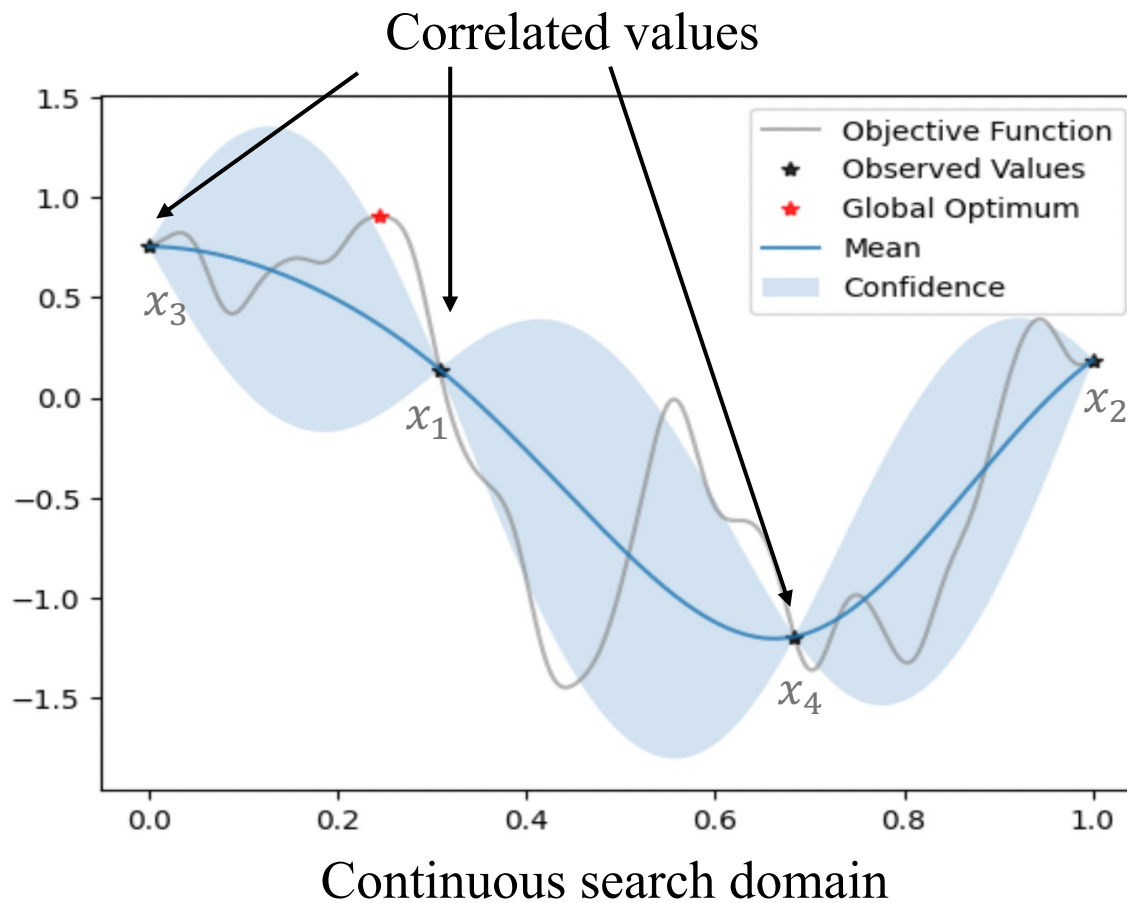


heterogeneous

Why is it hard?

Hard budget constraint

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 \vdots
 $t=T$



Evaluation costs handling



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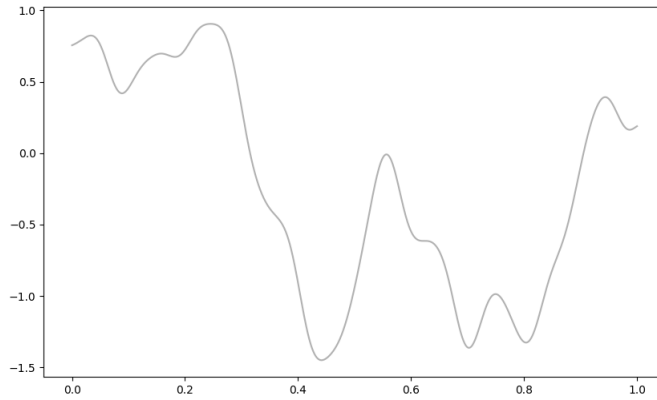
exploitation



heterogeneous

⇒ Optimal policy unknown!

Bayesian Optimization

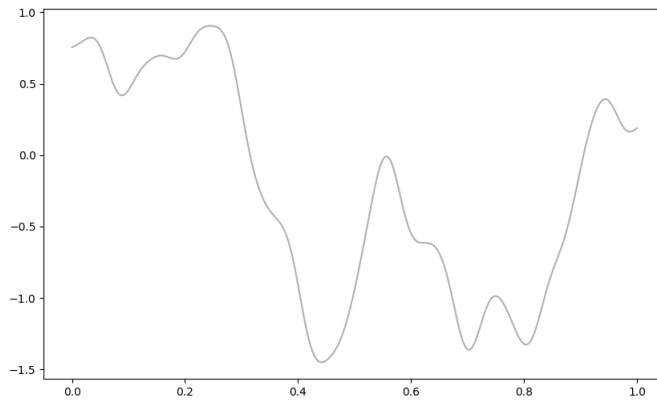


Continuous

Correlated

Hard budget constraint

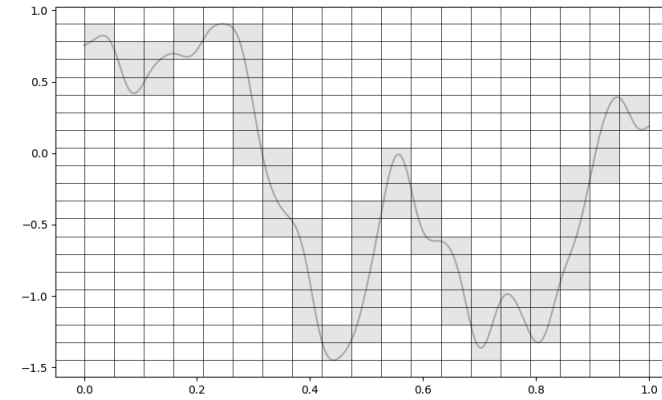
Bayesian Optimization



Continuous

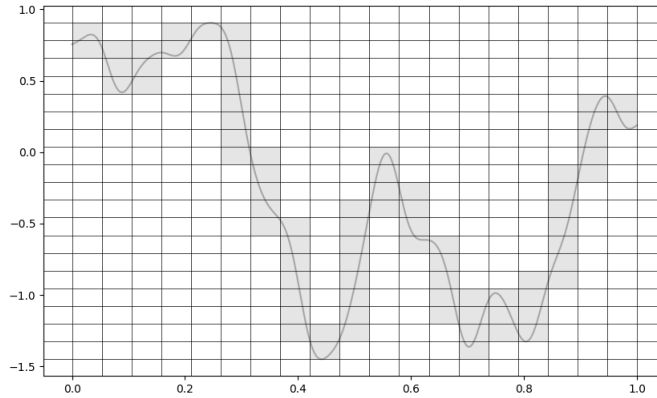
Correlated

Hard budget constraint



Discrete

Bayesian Optimization



Continuous

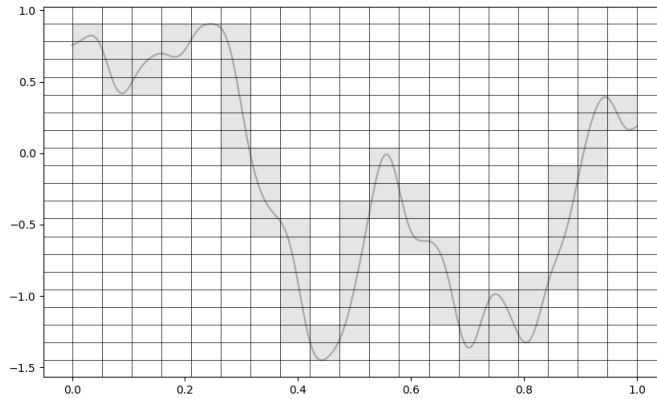


Discrete

Correlated

Hard budget constraint

Bayesian Optimization



Continuous



Discrete

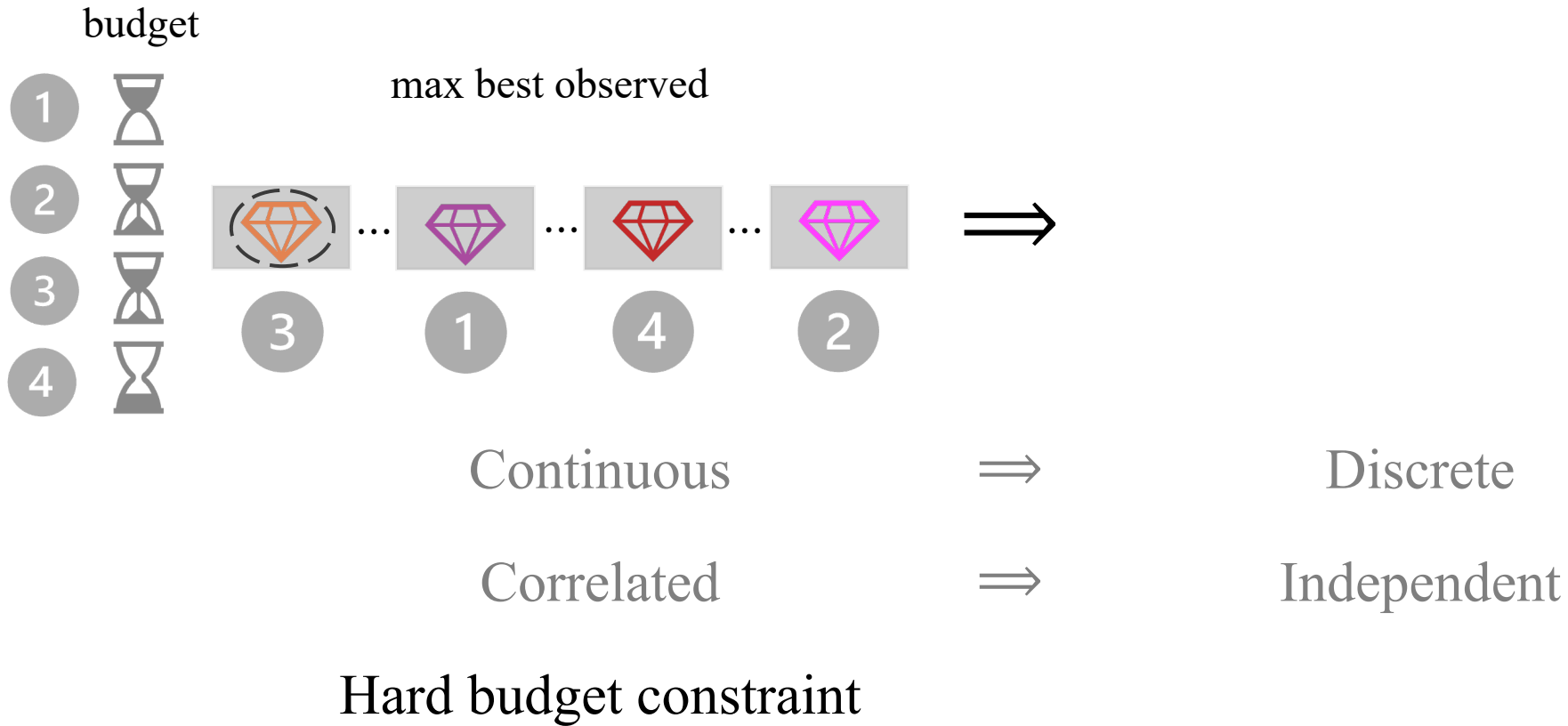
Correlated



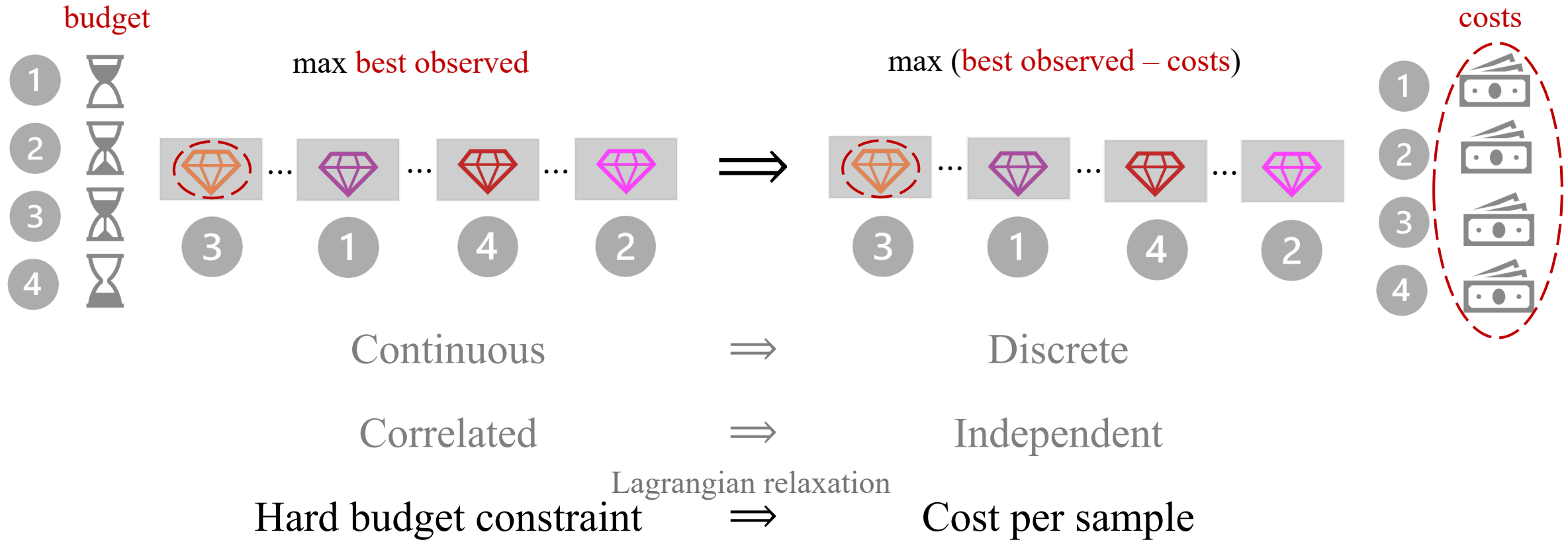
Independent

Hard budget constraint

Bayesian Optimization



Bayesian Optimization

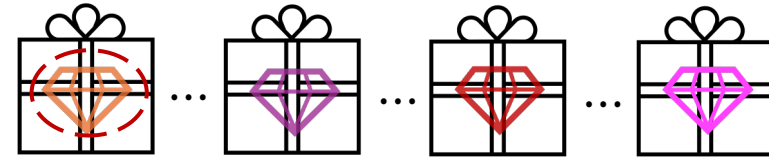


Bayesian Optimization \Rightarrow Pandora's Box

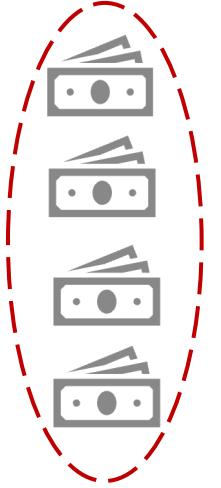
[Weitzman'79]



Continuous



Discrete



Correlated



Independent

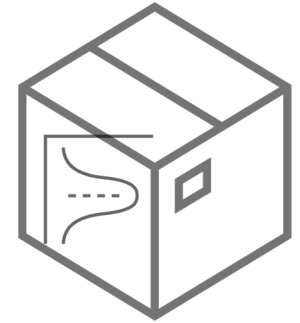
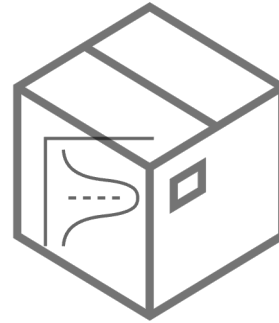
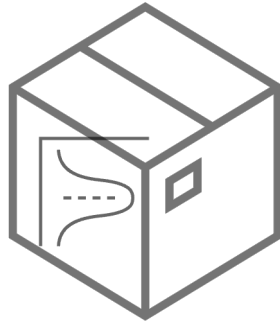
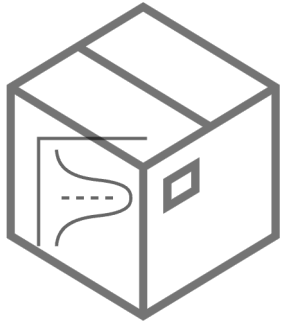
Hard budget constraint



Cost per sample

Pandora's Box

$t = 0$

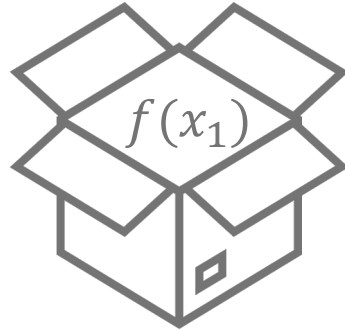
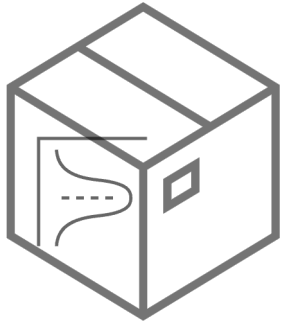


Objective: maximize net utility

Decision: adaptively evaluate a set of points

Pandora's Box

$t = 1$



$c(x_1)$

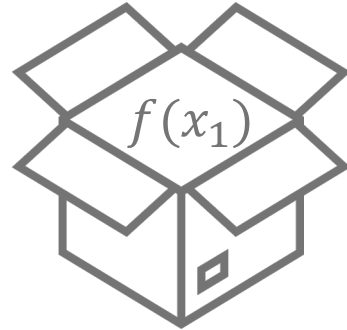
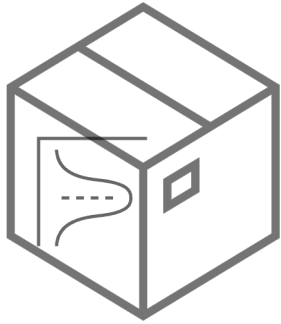


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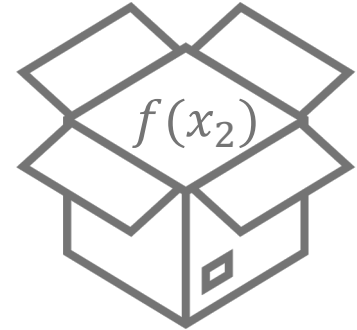
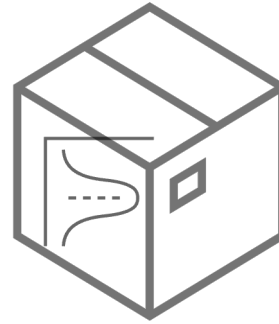
Decision: adaptively evaluate a set of points

Pandora's Box

$t = 2$



$c(x_1)$



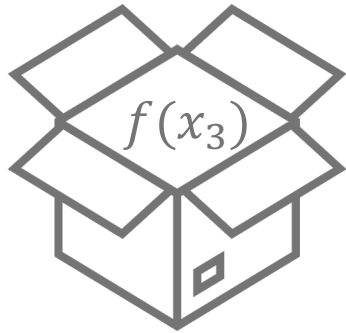
$c(x_2)$

Objective: maximize net utility

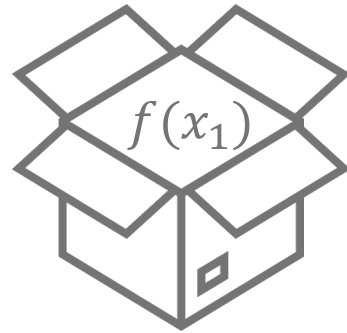
Decision: adaptively evaluate a set of points

Pandora's Box

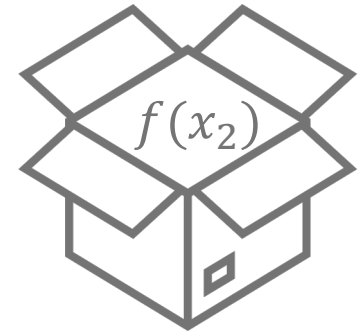
$t = 3$



$c(x_3)$



$c(x_1)$



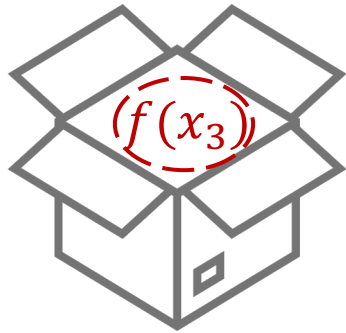
$c(x_2)$

Objective: maximize net utility

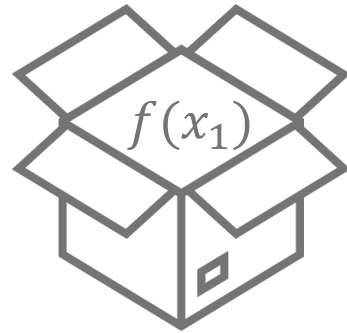
Decision: adaptively evaluate a set of points

Pandora's Box

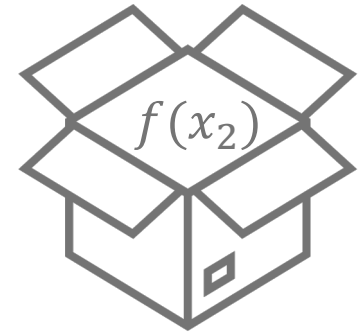
$t = 3$



$c(x_3)$



$c(x_1)$



$c(x_2)$

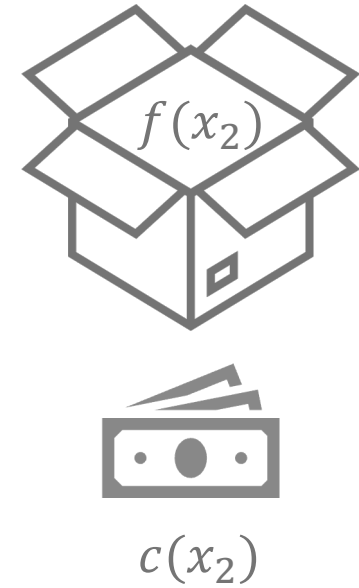
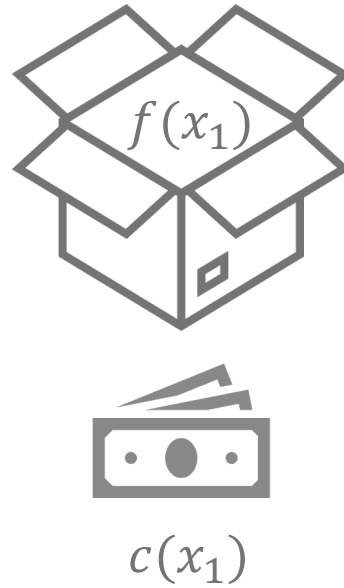
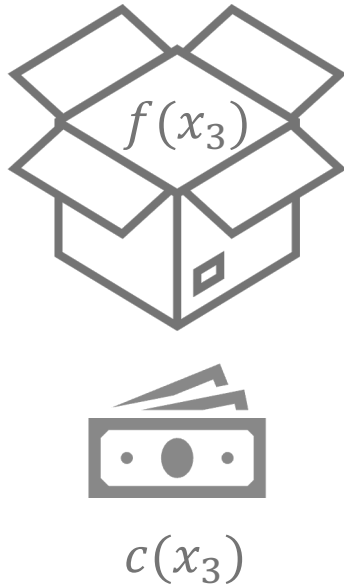
Objective: maximize net utility

Decision: adaptively evaluate a set of points

$\max \mathbb{E}(\text{best observed value} - \text{total evaluation costs})$

Pandora's Box

$t = 3$



Objective: maximize **net utility**

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

Decision: adaptively evaluate a set of points

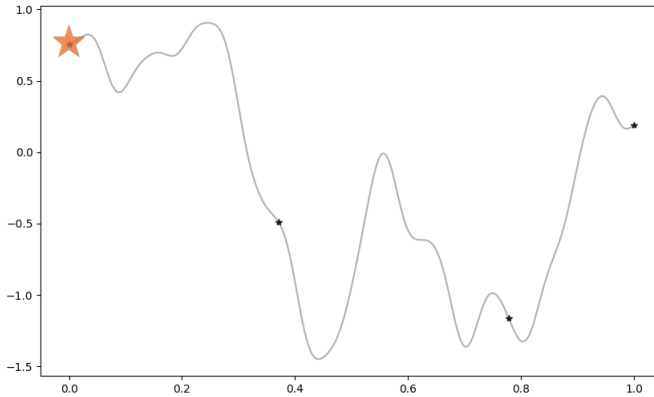
$$x_1, x_2, \dots, x_T \in \mathcal{X}$$

\mathcal{X} : discrete

T : random stopping time

Bayesian Optimization \Rightarrow Pandora's Box

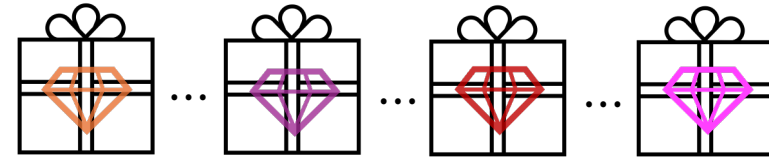
Special case of Markovian/
Bayesian multi-armed bandits



Continuous

Correlated

Hard budget constraint



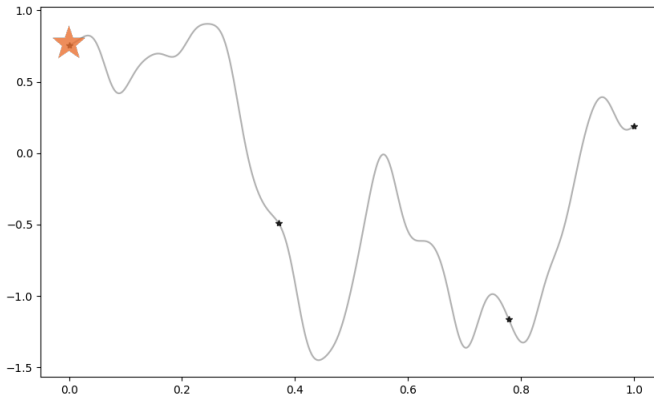
Discrete

Independent

Cost per sample

Optimal policy: Gittins index [Weitzman'79]

Bayesian Optimization \Rightarrow Pandora's Box

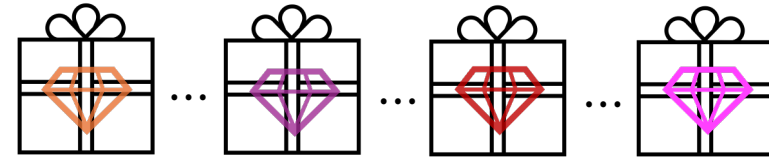


Continuous

Correlated

Hard budget constraint

Is Gittins index good?



Discrete

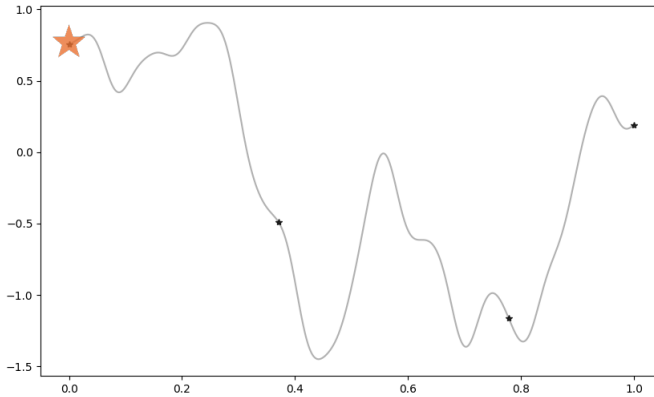
Independent

Cost per sample

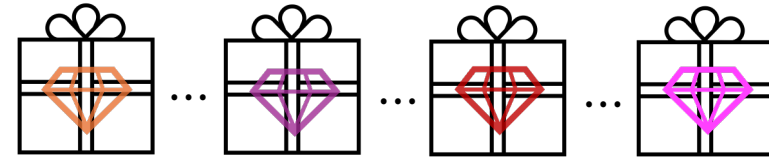
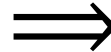
Optimal policy: Gittins index



Bayesian Optimization \Rightarrow Pandora's Box



Continuous



Discrete

Correlated



Independent

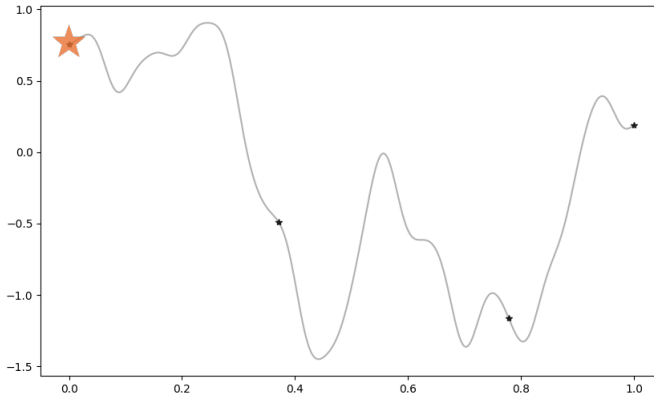
Hard budget constraint



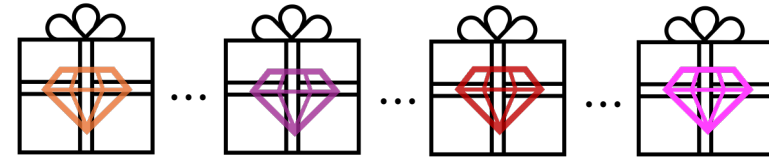
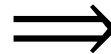
Cost per sample

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

Bayesian Optimization \Rightarrow Pandora's Box



Continuous



Discrete

Correlated



Independent

Hard budget constraint



Cost per sample

Is Gittins index good?

How to translate?

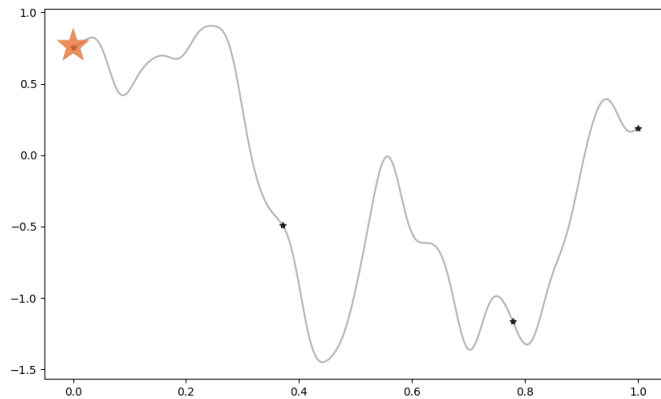


Optimal policy: Gittins index

Our contributions!

Our Contributions

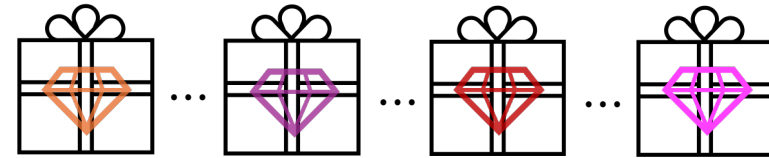
- How to translate?
- Is Pandora's Box Gittins index (PBGI) good?



?

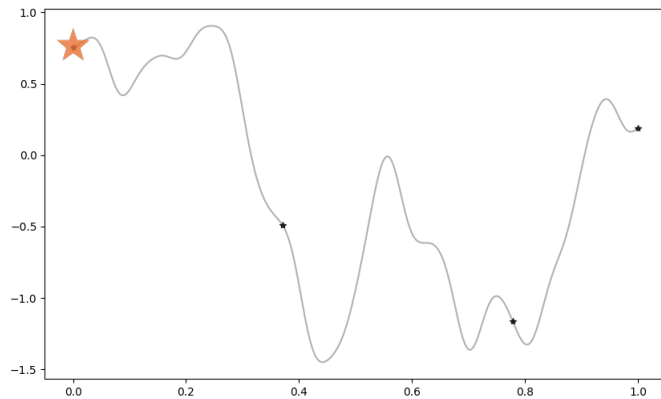


Pandora's Box Gittins index

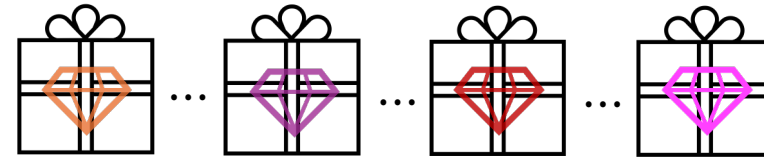


Our Contributions

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



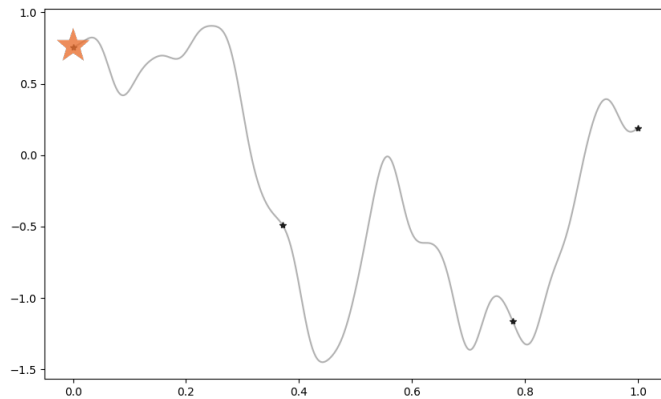
Our work



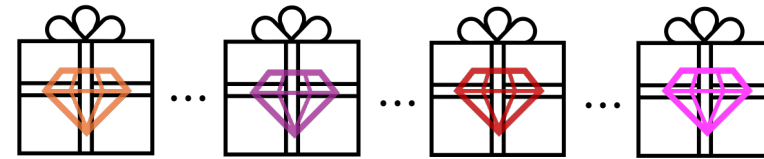
Pandora's Box Gittins index

Our Contributions

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



Our work

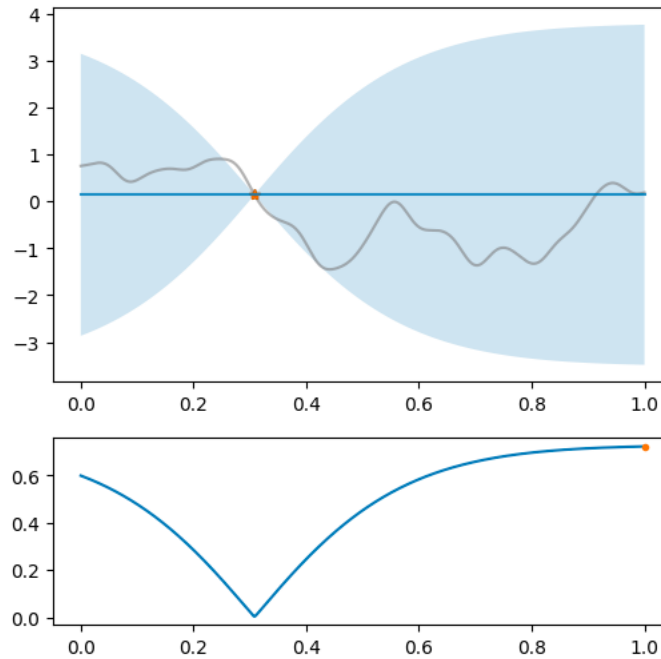


Pandora's Box Gittins index



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

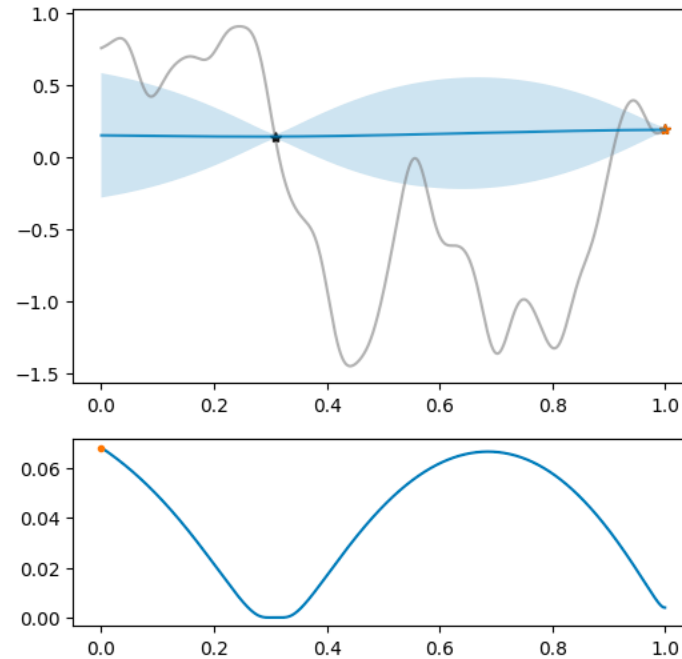
$$\text{EI}_{f|D}(x; y) = \mathbb{E}[(f|D)(x) - y]^+$$

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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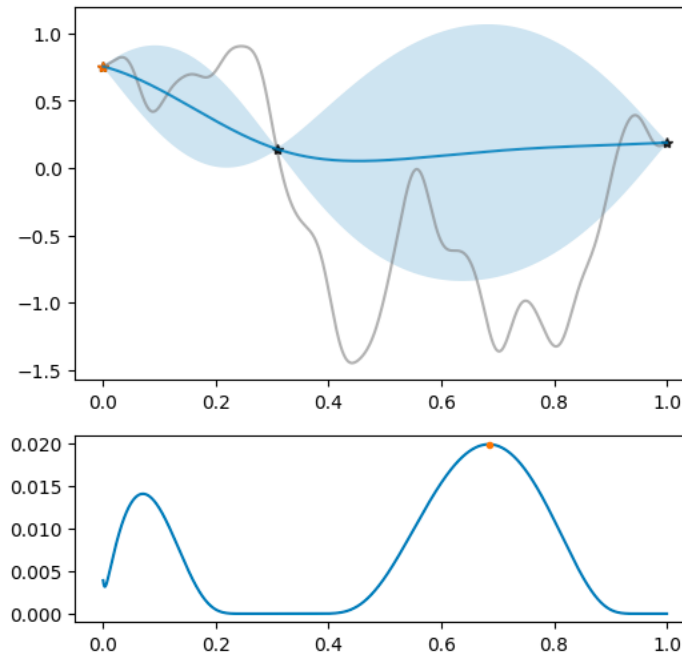
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Popular One-step Heuristic: EI



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Popular One-step Heuristic: EI

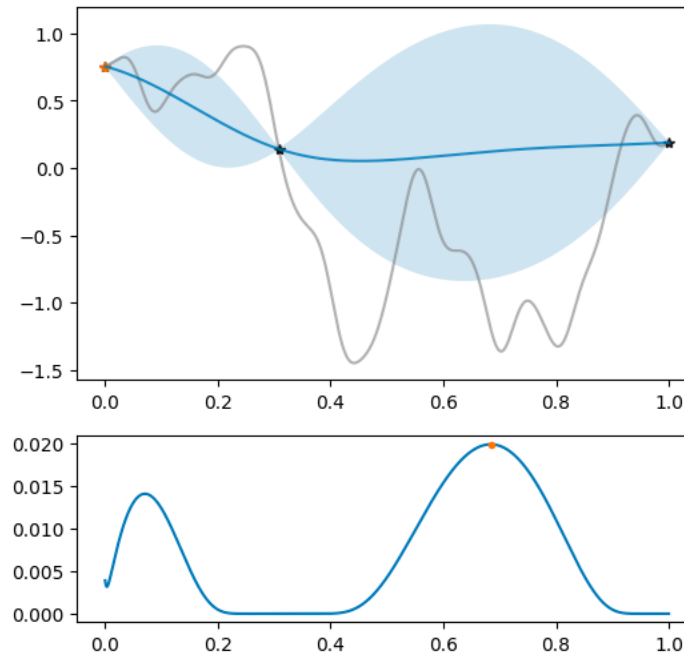
Other heuristics:

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

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

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

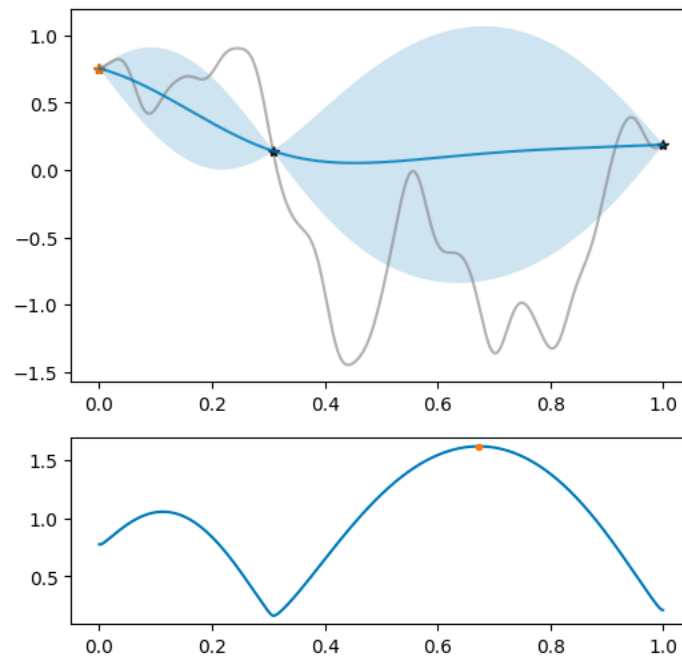
D : observed data

y_{best} : current best observed value

New One-step Heuristic: PBGI

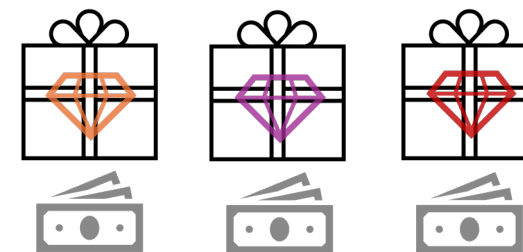
Other heuristics:

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



Pandora's box Gittins index

Pandora's box



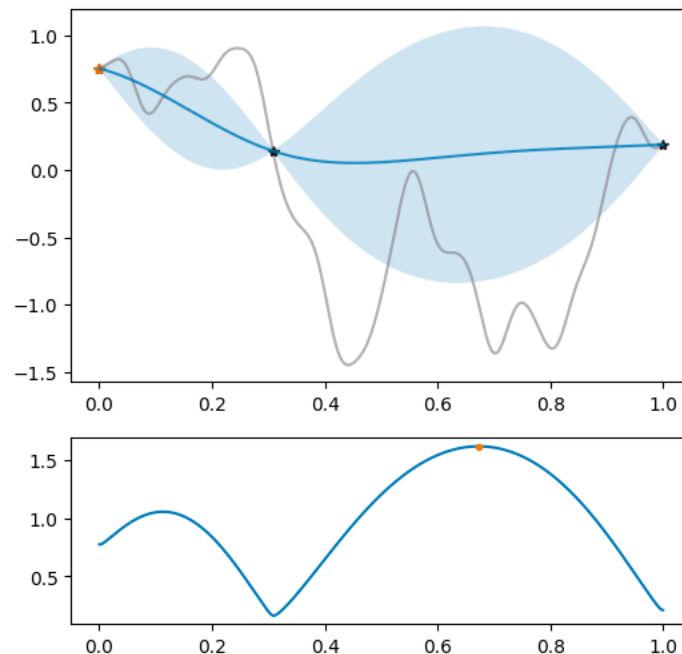
PBGI policy: evaluate $\arg\max_x \alpha^*(x)$

$\alpha^*(x)$: 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

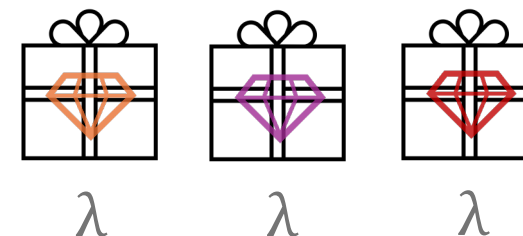


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$$\text{EI}_{f|D}(x; y) = \mathbb{E}[(f|D)(x) - y]^+$$

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

Pandora's box



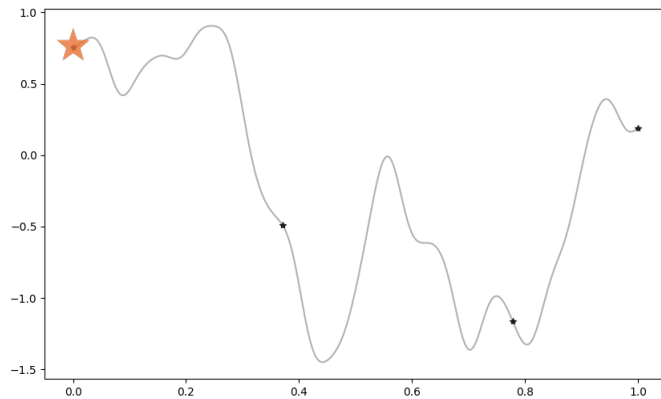
λ : cost-per-sample
(Lagrange multiplier)

D : observed data

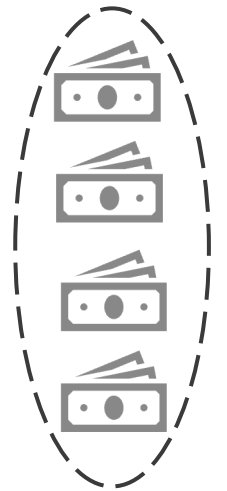
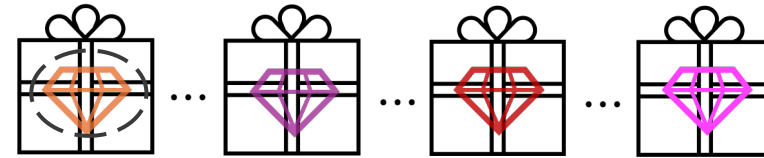
$\alpha^*(x)$: solution to $\text{EI}_{f|D}(x; \alpha^*(x)) = \lambda$

Our Contributions

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



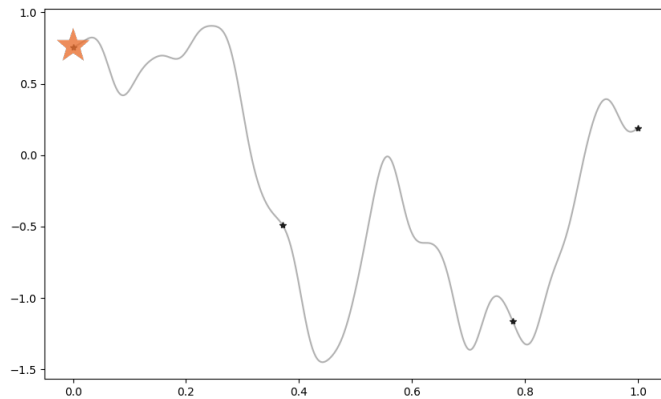
Our work



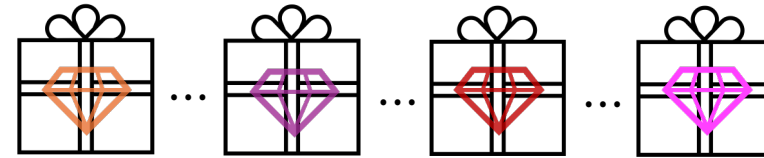
Pandora's Box Gittins index

Our Contributions

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

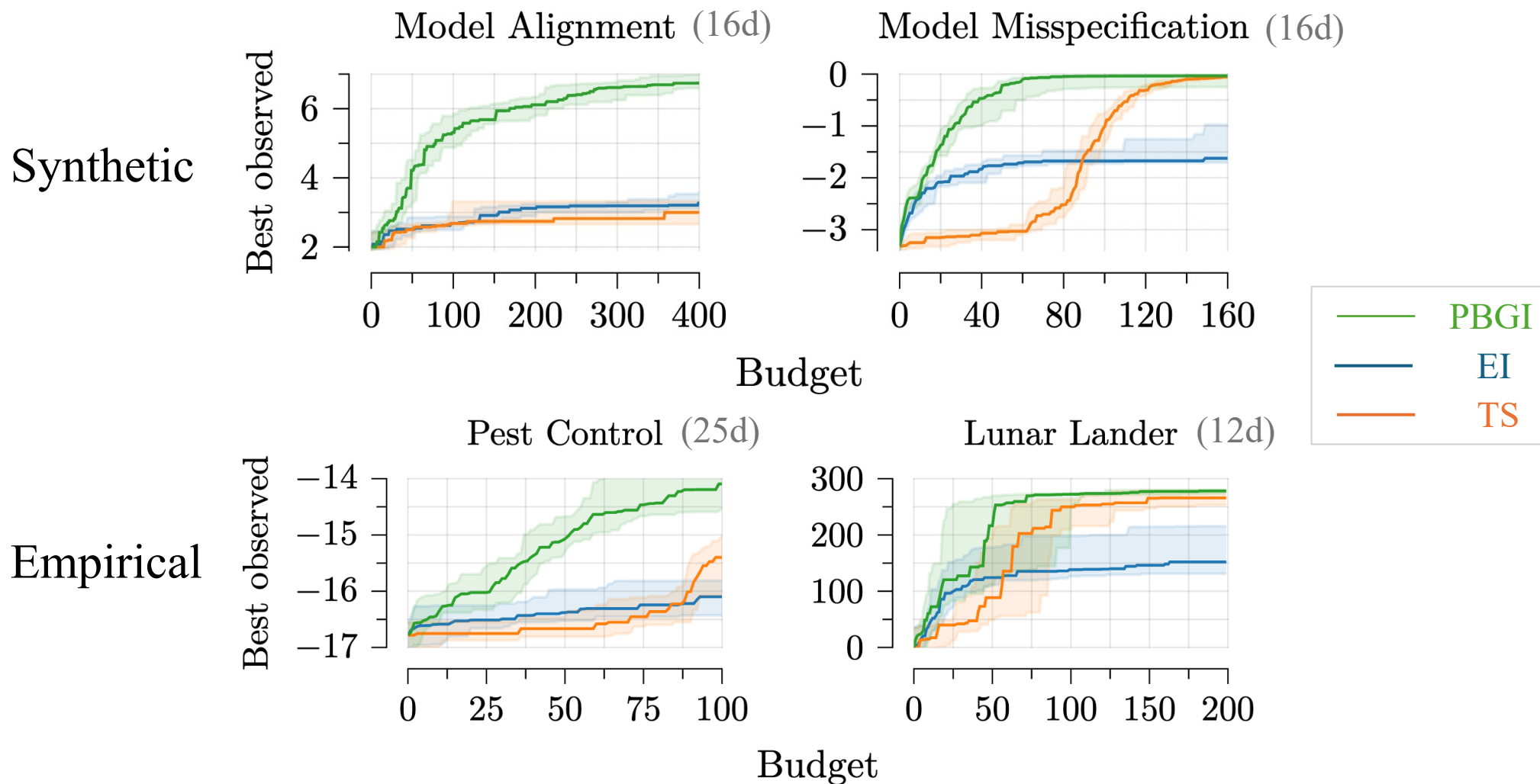


Our work



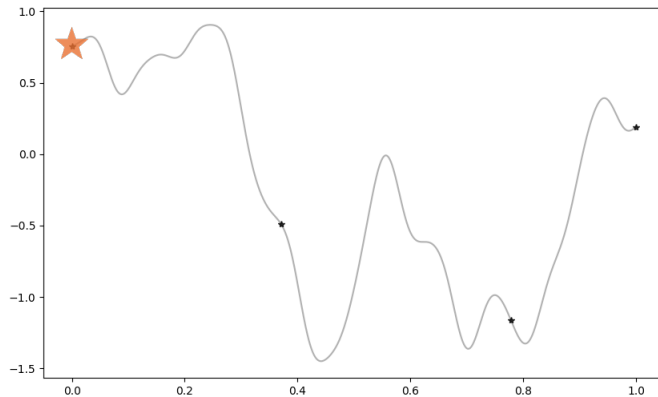
Pandora's Box Gittins index

Experiment Results: PBGI vs EI vs TS

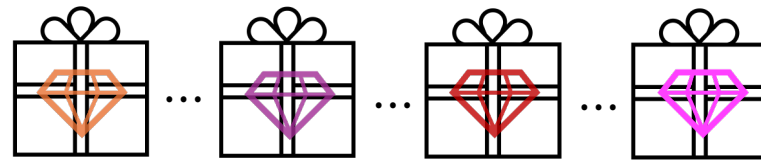


Conclusions

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



Our work

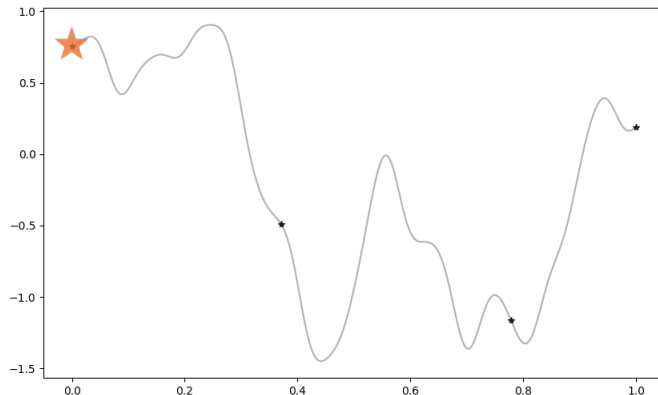


Pandora's box Gittins index

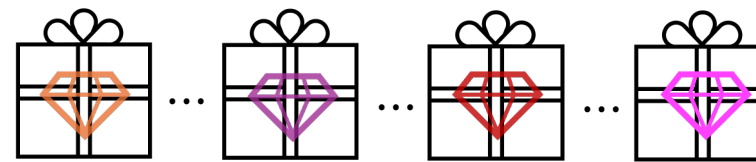
Check our preprint on arXiv!

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

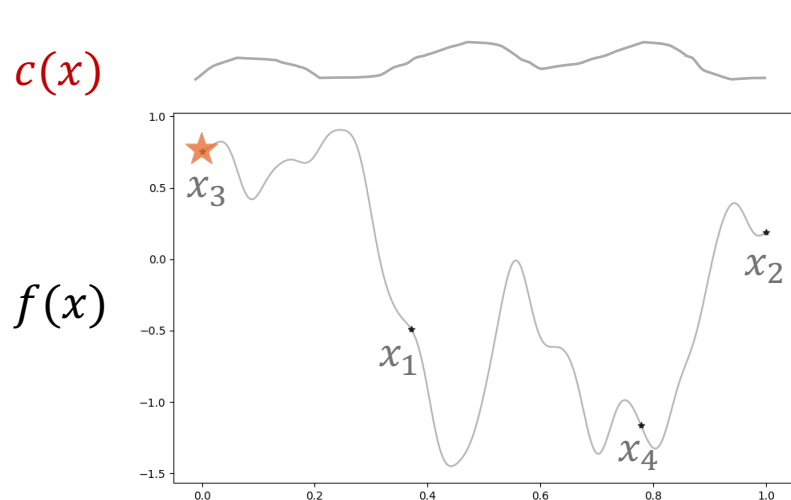


Pandora's box Gittins index

Check our preprint on arXiv!

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**

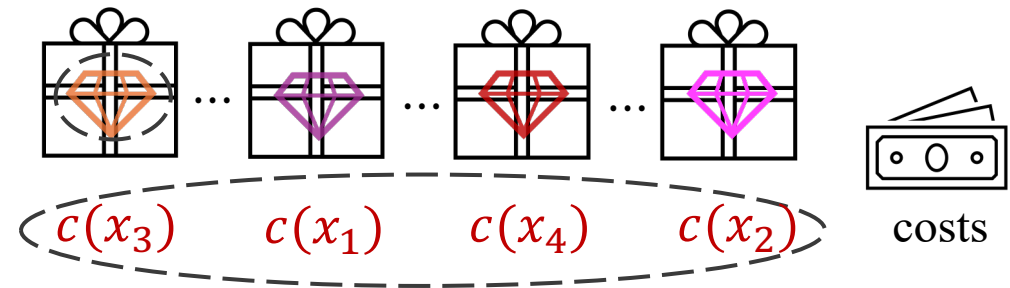


Our work



budget

max (best observed – costs)

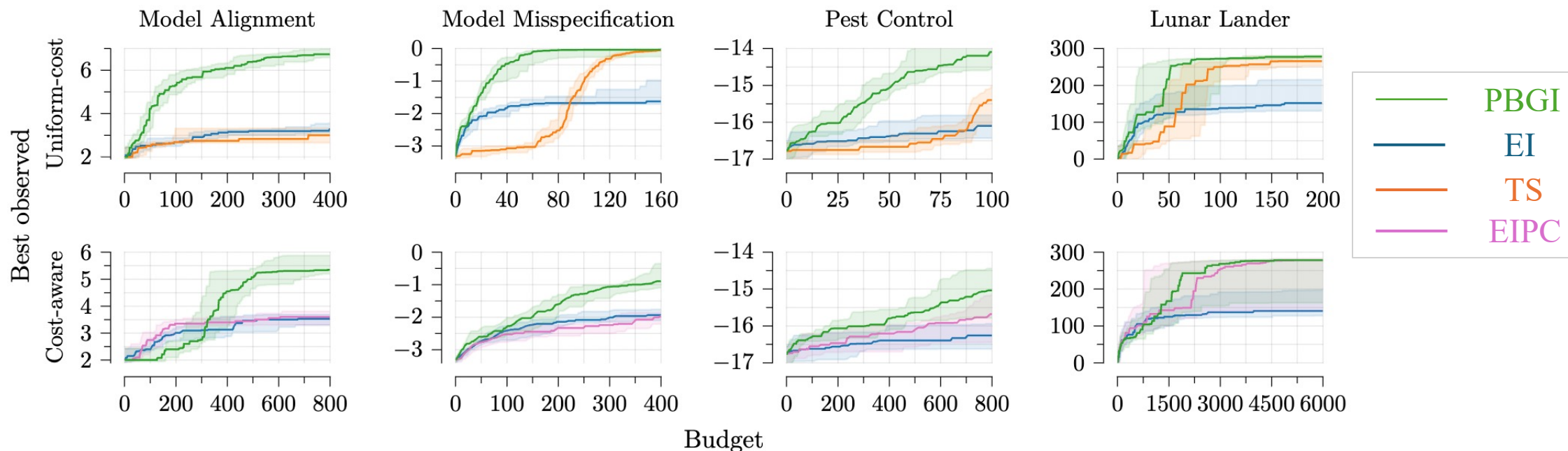


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Heterogeneous-cost Experiment Results

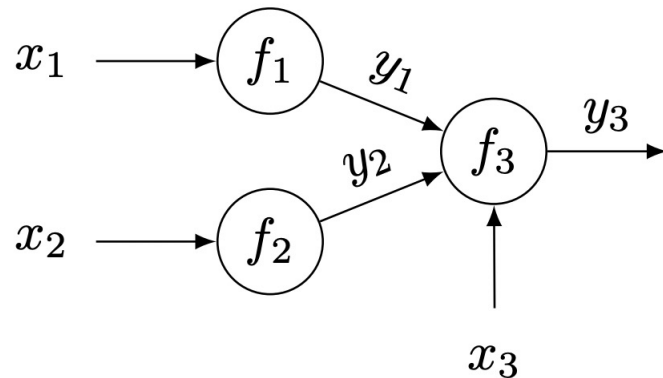
- Show the effectiveness of PBGI on synthetic & empirical experiments
- Extend to Bayesian optimization with **heterogeneous evaluation costs**



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Conclusions

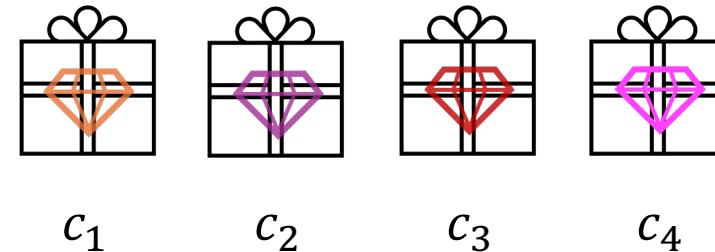
- Propose easy-to-compute PBGI policy for Bayesian optimization
- Show the effectiveness of PBGI on synthetic & empirical experiments
- Extend to Bayesian optimization with heterogeneous evaluation costs
- Open door for **complex BO** (freeze-thaw, multi-fidelity, function network, etc.)



?



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