Cost-aware Bayesian Optimization via the Pandora's Box Gittins Index

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Joint work with Raul Astudillo, Peter Frazier, Ziv Scully, and Alexander Terenin

INFORMS'24 Data Mining Best General Paper Competition

Coauthors

Raul Astudillo

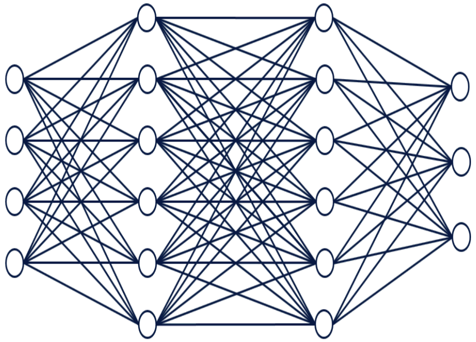
Peter Frazier

Ziv Scully

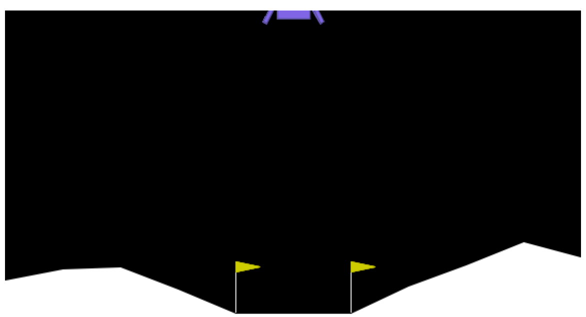
Alexander Terenin

World of Parameter Optimization

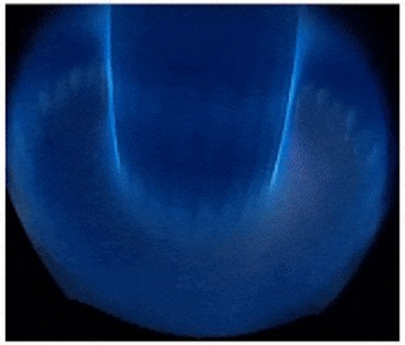
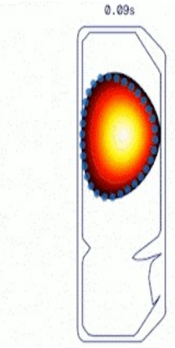
Hyperparameter tuning:

Training parameters →  → Accuracy

Control optimization:

Control parameters →  → Reward

Plasma physics:

Reactor parameters →  

→ Stability

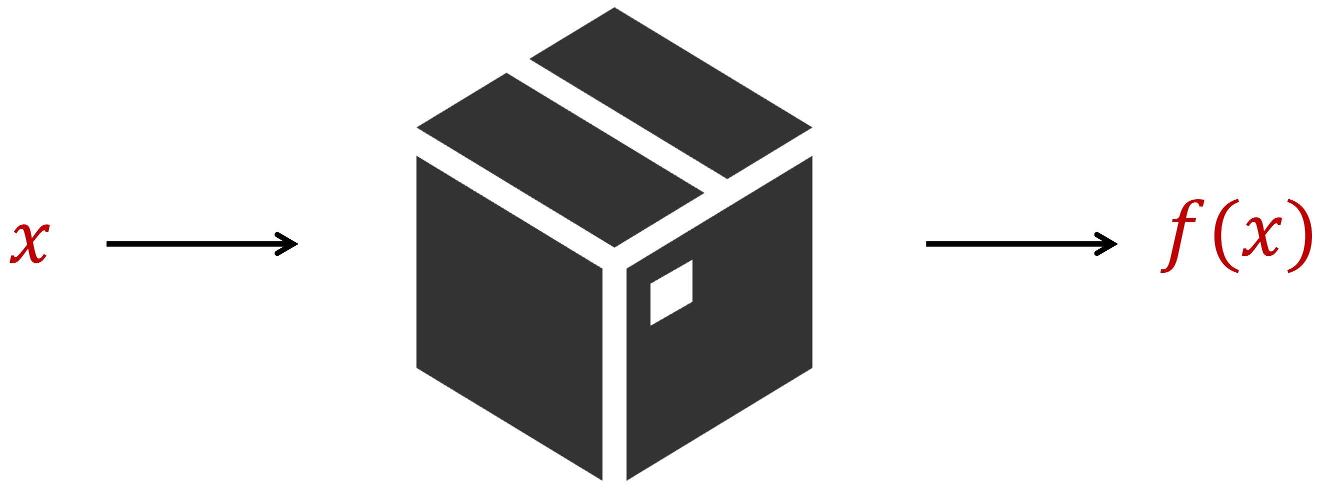
World of Parameter Optimization

Black-box optimization:

Input parameters ⟶  ⟶ Performance metrics

World of Parameter Optimization

Black-box optimization:

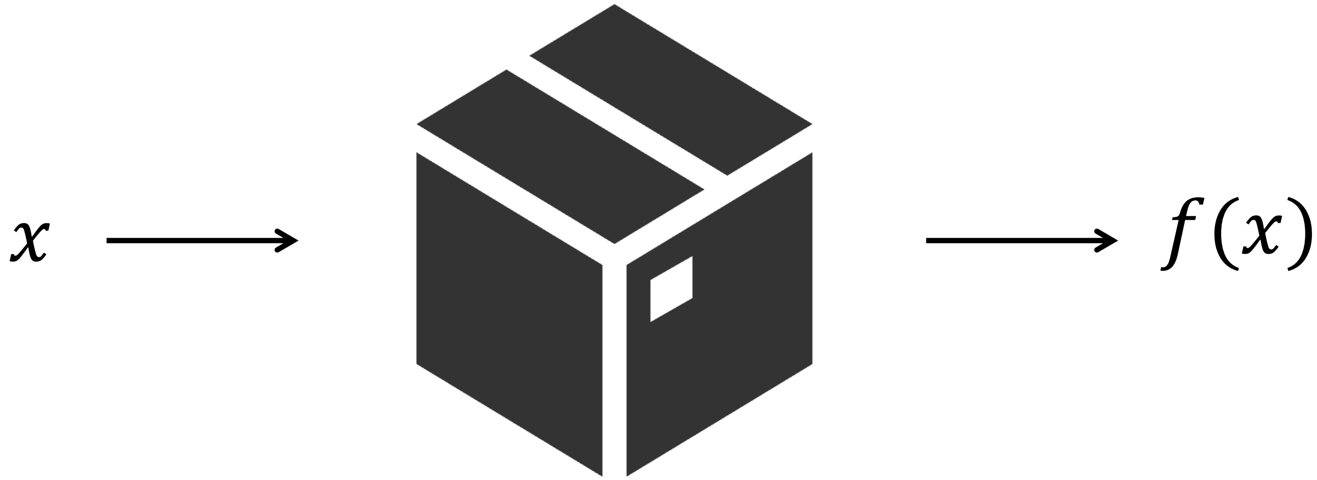


Optimizing Black-box Functions

x ⟶  ⟶ $f(x)$

Goal: $\mathbf{max}_{x \in \mathcal{X}}\, f(x)$

Optimizing Black-box Functions



Goal: $\mathbf{max}_{x \in \mathcal{X}}\, f(x)$

$f \sim$Stochastic Process

Optimizing Black-box Functions

$x \longrightarrow$

$\longrightarrow f(x)$

expensive-to-evaluate

Goal: $\mathbf{max}_{x \in \mathcal{X}} f(x)$

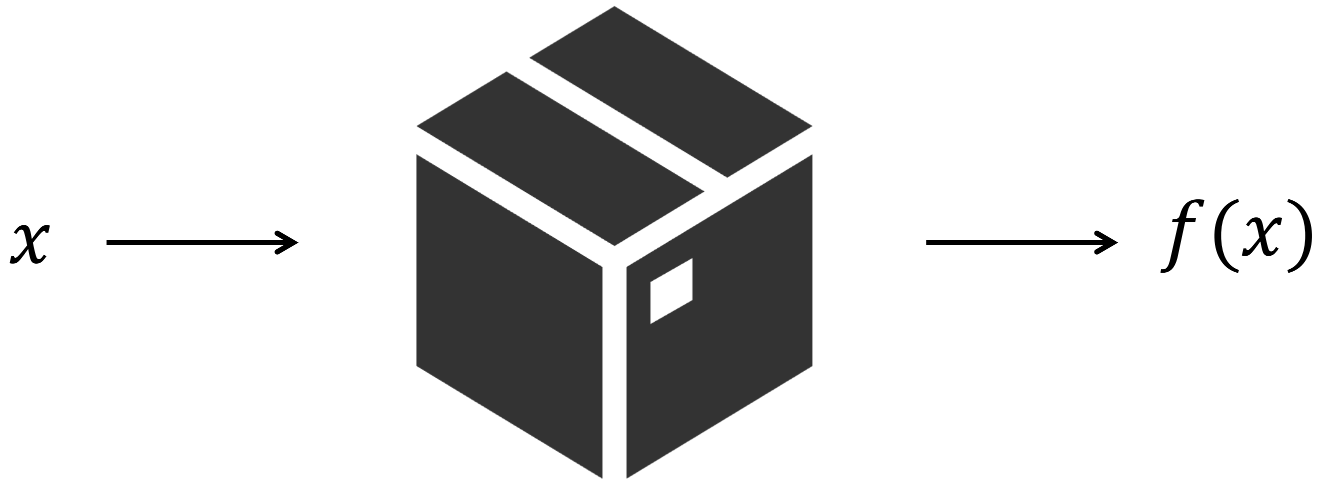
Optimizing Black-box Functions

$x \longrightarrow$

$\longrightarrow f(x)$

Goal: $\mathbf{max}\ \mathbb{E} \max_{t=1,2,\ldots,T} f(x_t)$

Optimizing Black-box Functions



Goal: $\mathbf{max}\ \mathbb{E} \max_{t=1,2,\ldots,T} f(x_t)$

$f \sim$ Gaussian Process

Bayesian Optimization

$x \longrightarrow$  $\longrightarrow f(x)$

Goal: $\mathbf{max}\ \mathbb{E} \max_{t=1,2,\ldots,T} f(x_t)$

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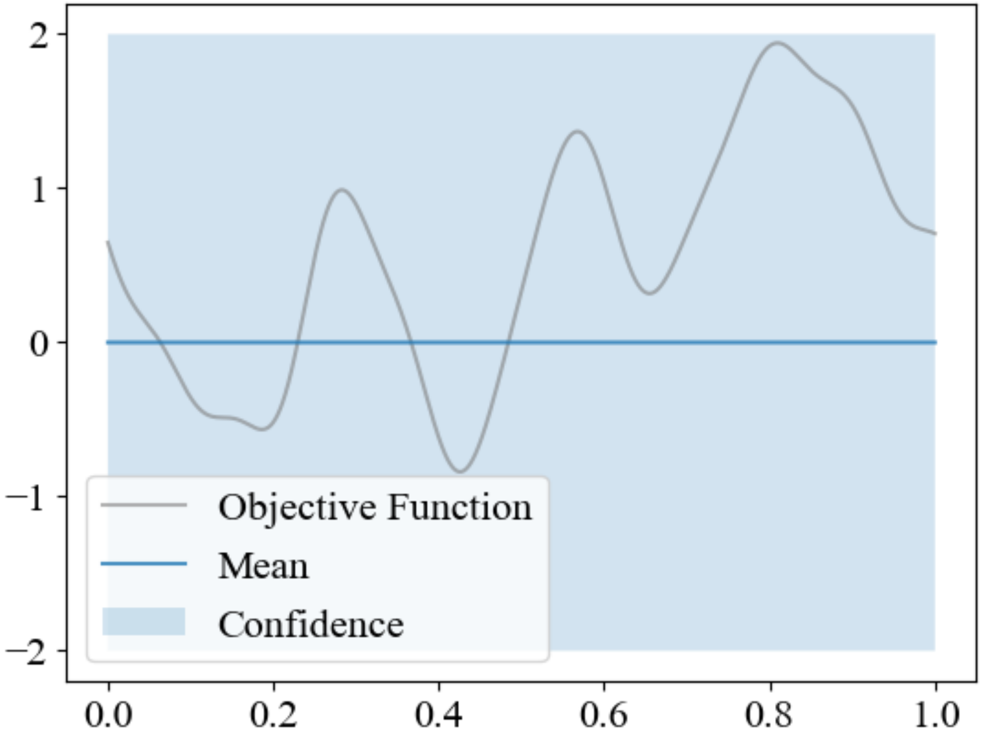
Bayesian Optimization



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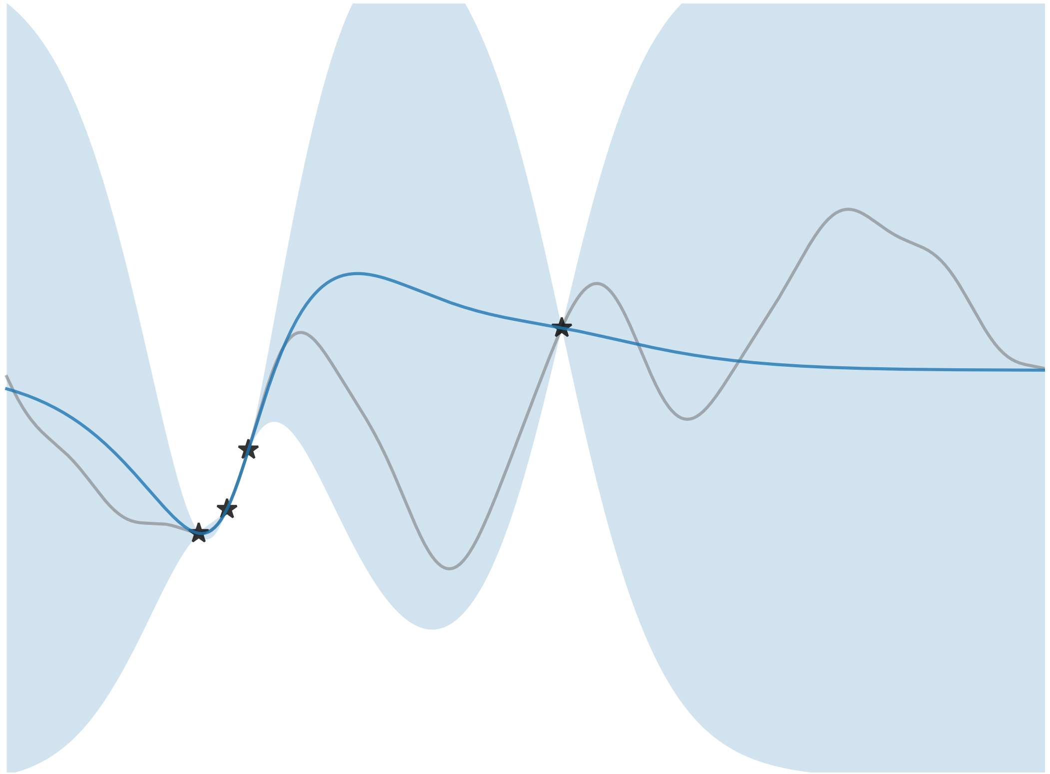
Bayesian Optimization



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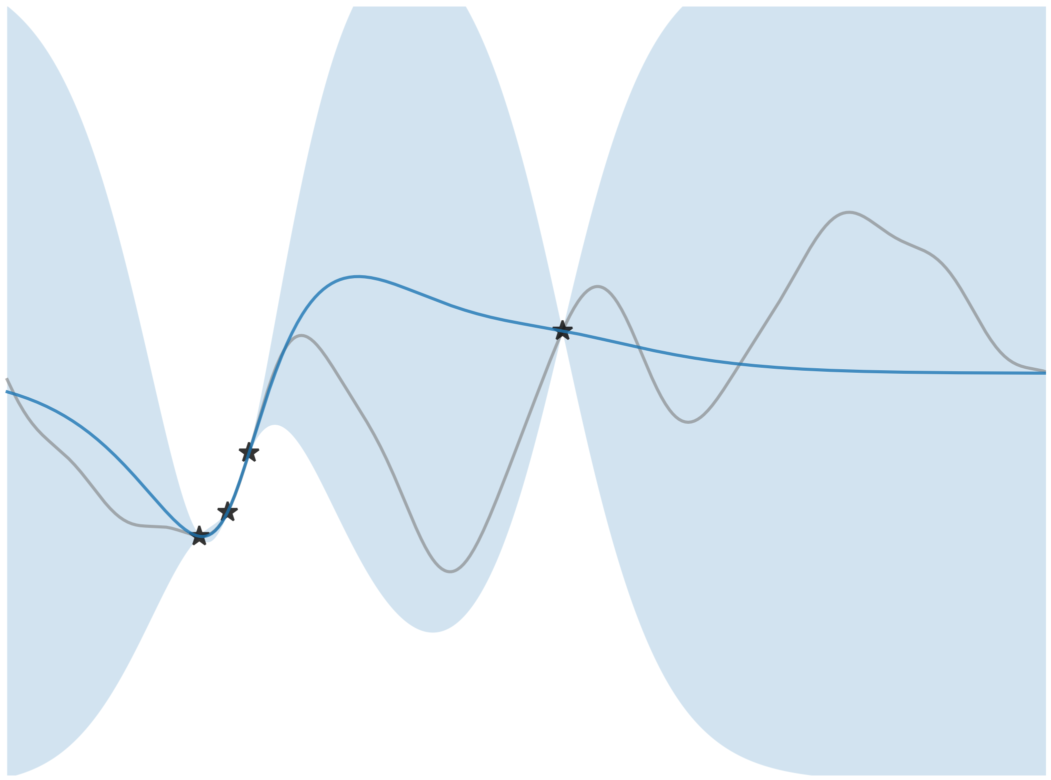
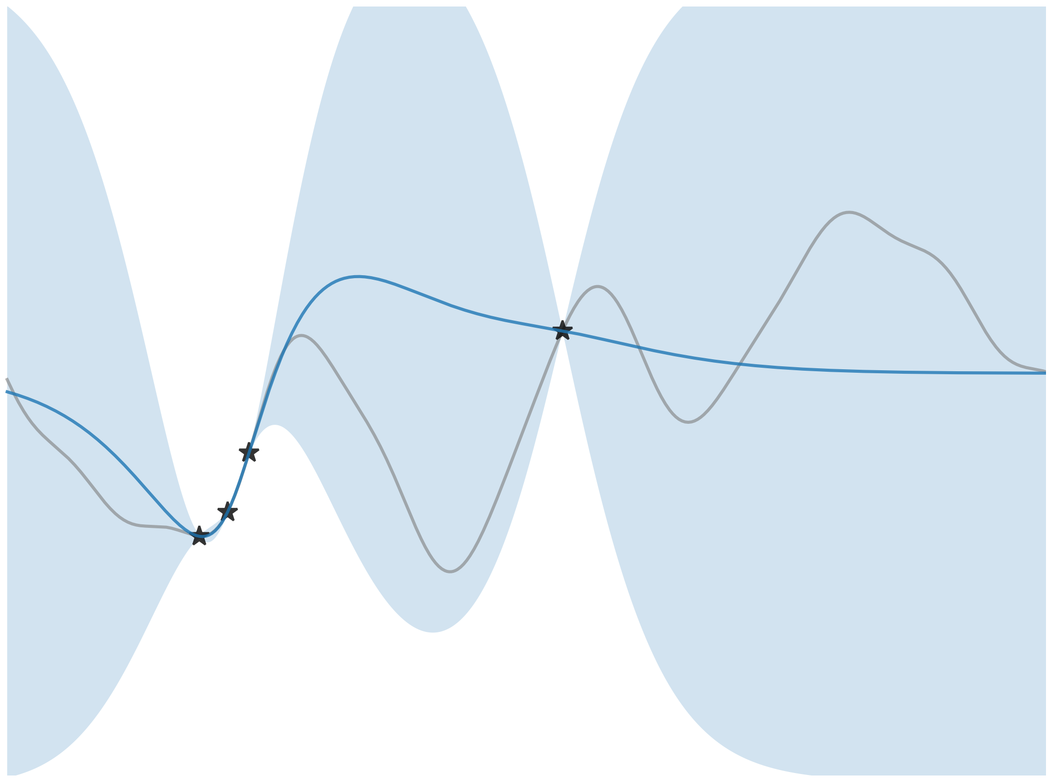
Bayesian Optimization



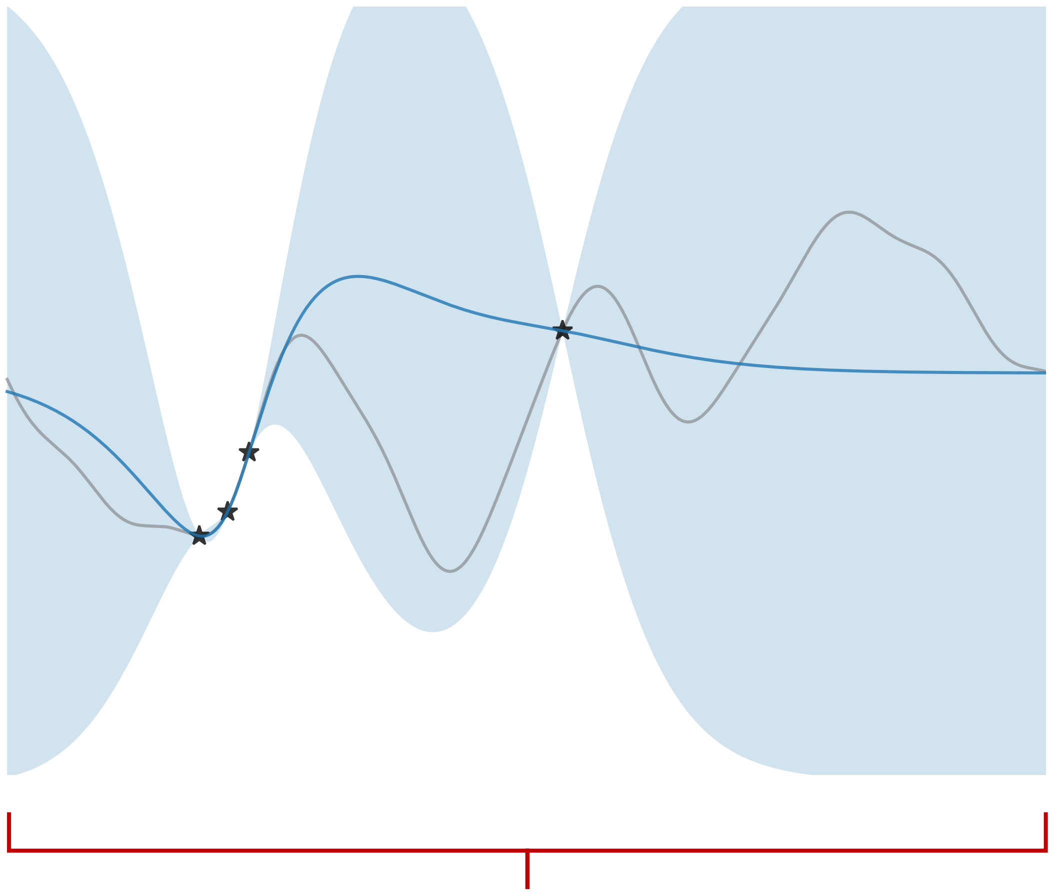
What to evaluate next?

Bayesian Optimization



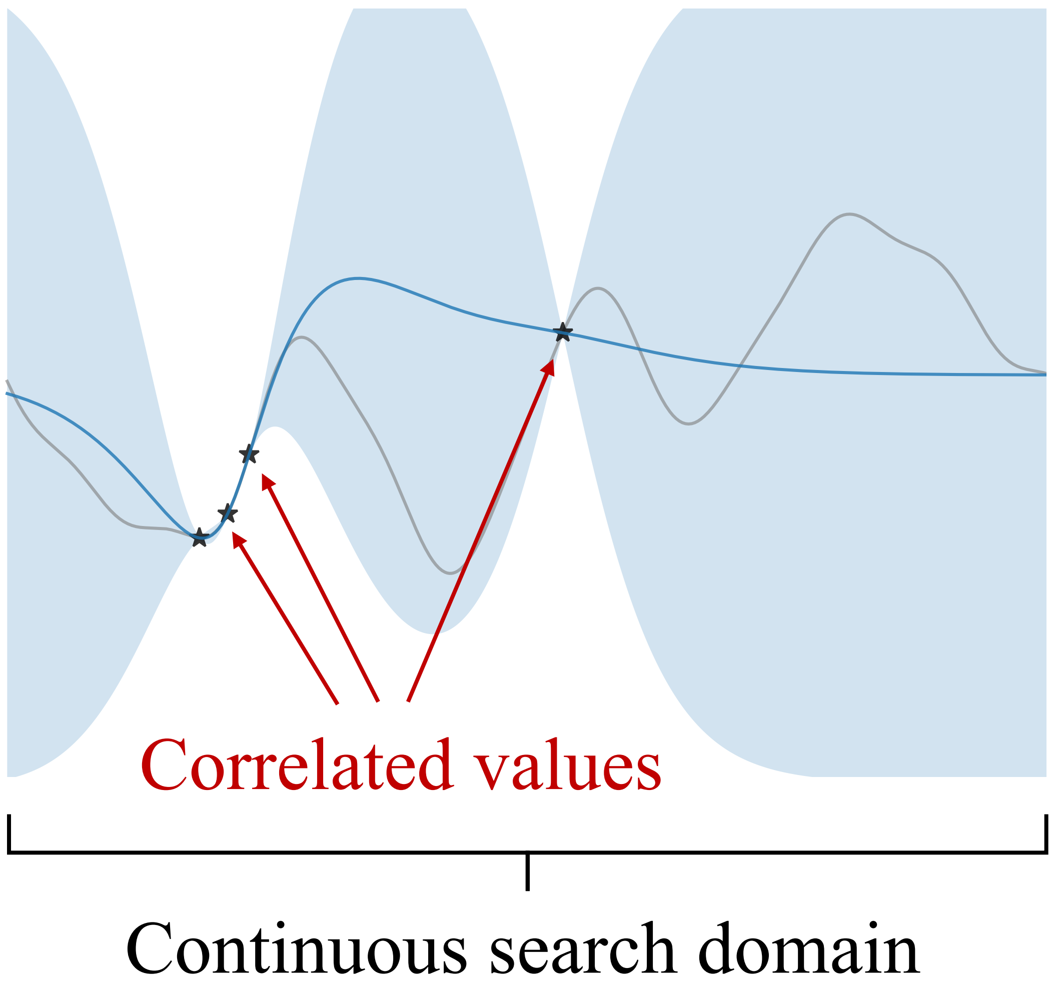
Optimal policy?

Challenges of Bayesian Optimization

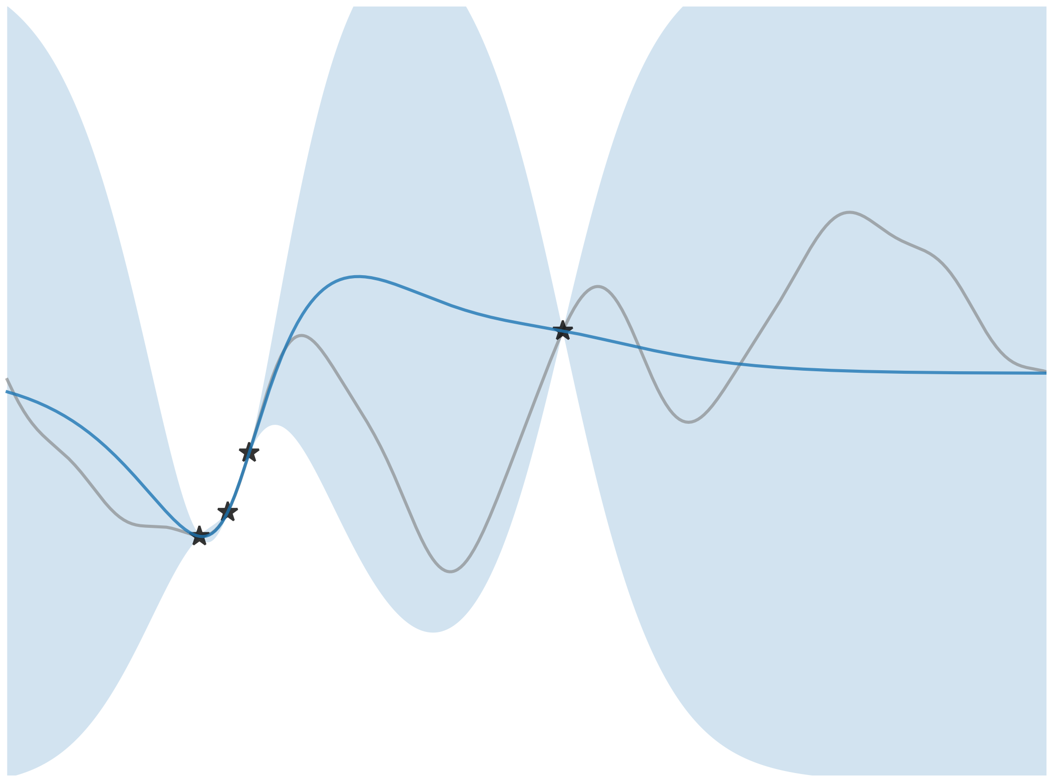


Continuous search domain

Challenges of Bayesian Optimization

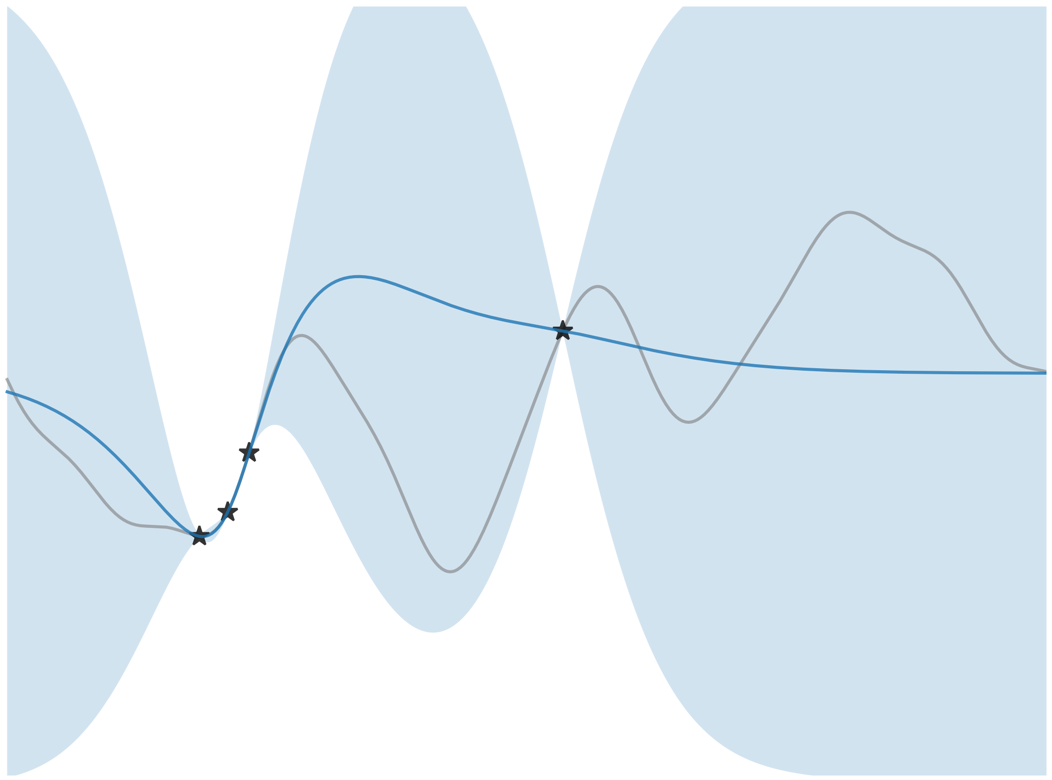


Challenges of Bayesian Optimization



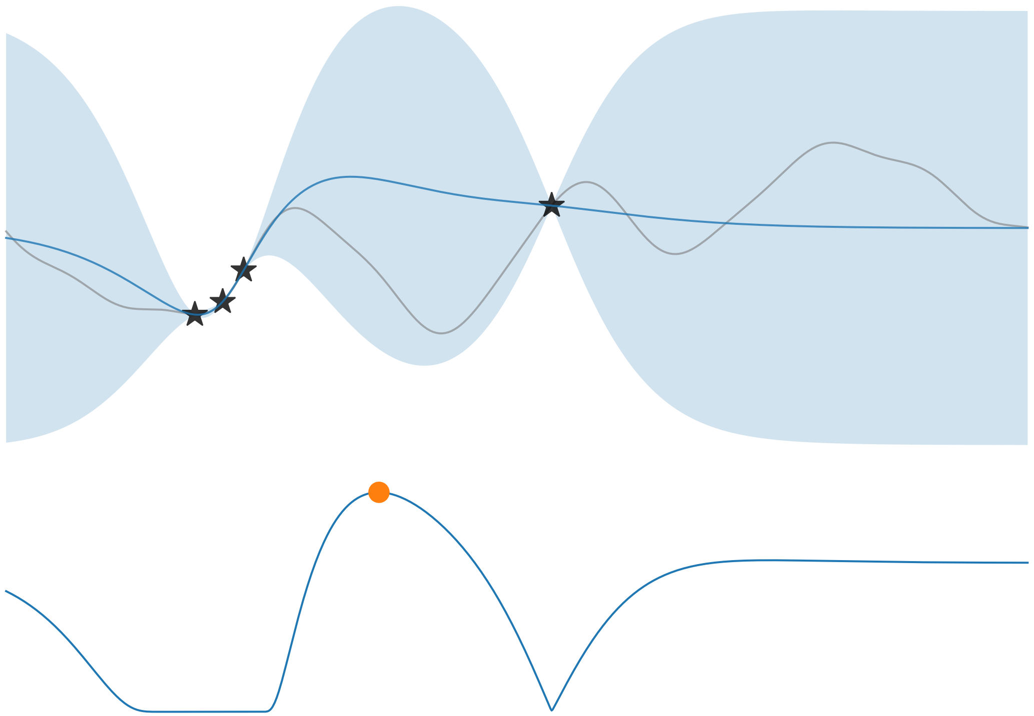
Correlation & continuity $\Longrightarrow$ Intractable MDP

Challenges of Bayesian Optimization



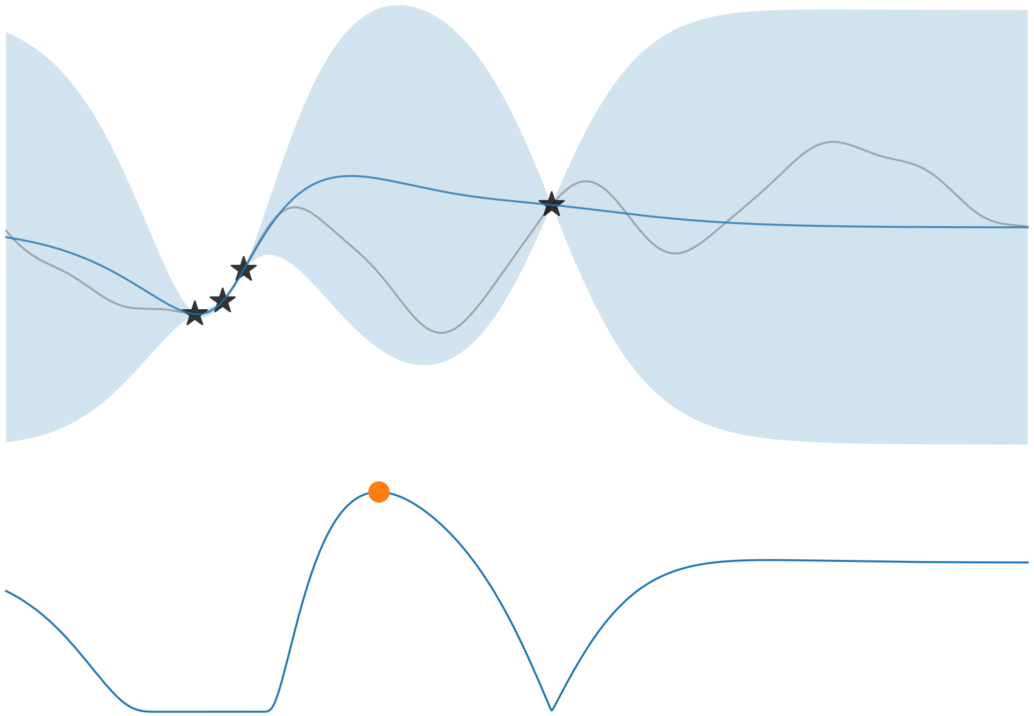
Intractable MDP $\Longrightarrow$ Optimal policy unknown

Popular Policy: Expected Improvement



$$\text{EI}(x) = \mathbb{E}[\underbrace{\max(f(x) - \overset{\text{current best observed}}{y_{\text{best}}}, 0)}_{\text{"improvement"}} \mid \overset{\text{data}}{D}]$$

Popular Policy: Expected Improvement

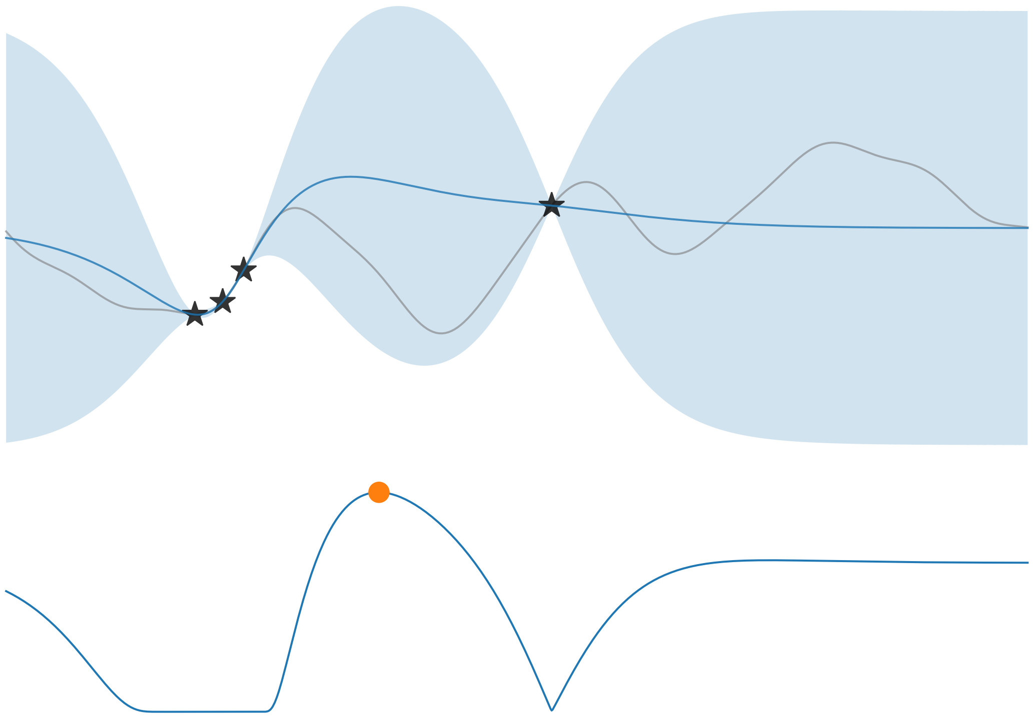


current best observed data

$$\mathrm{EI}(x) = \mathbb{E}[\underbrace{\max(f(x) - y_{\text{best}}, 0)}_{\text{“improvement”}} \mid D]$$

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

Popular Policy: Expected Improvement



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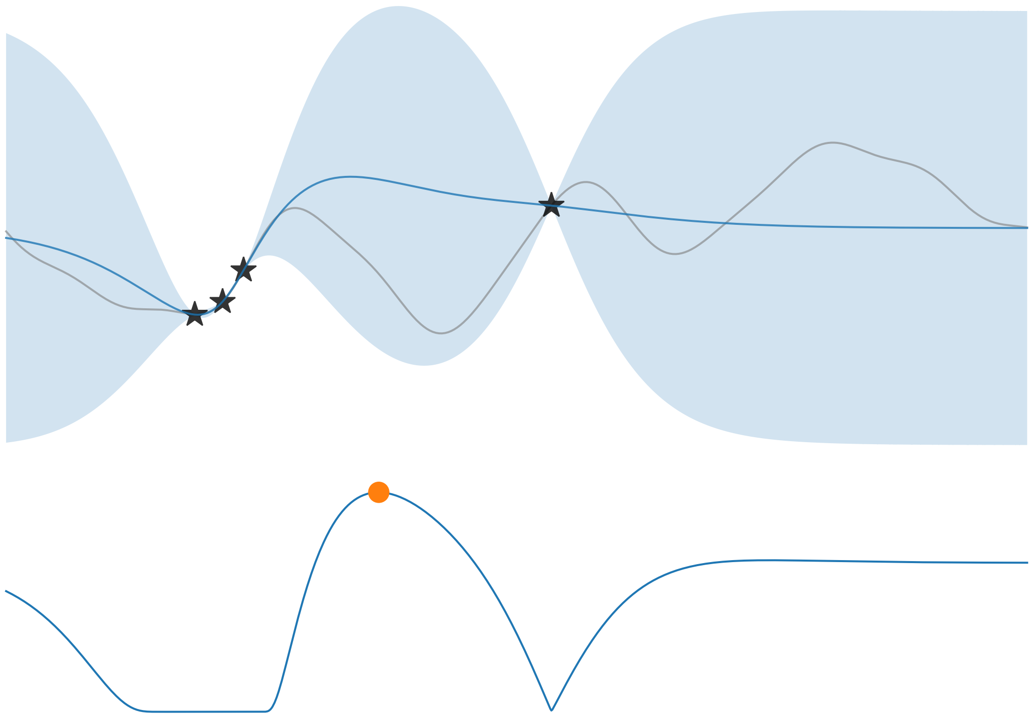
One-step approximation to MDP

Popular Policy: Expected Improvement



Other improvement-based policy:

- Probability of Improvement
- Knowledge Gradient
- Multi-step Lookahead EI
- …

Approaches to Bayesian Optimization

- Improvement-based:
  - Expected Improvement
  - Probability of Improvement
  - Knowledge Gradient
  - Multi-step Lookahead EI

Approaches to Bayesian Optimization

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Approaches to Bayesian Optimization

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- Our work: Gittins Index

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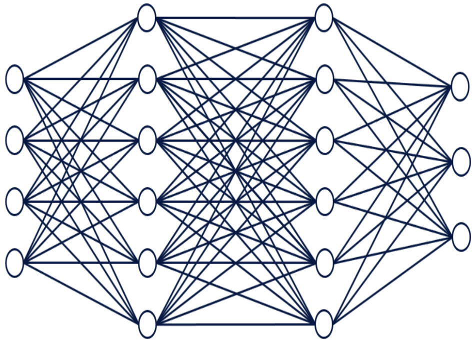
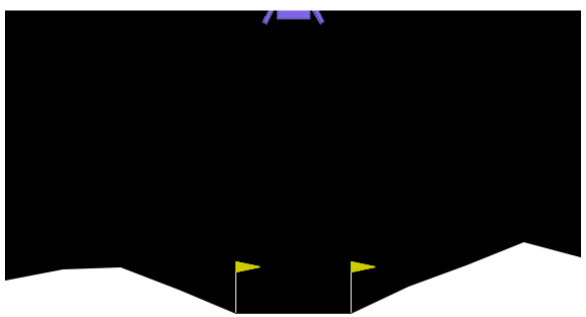
Why another approach?

Another Challenge: Varying Evaluation Costs

Hyperparameter tuning:

Training parameters →  → Accuracy

Control optimization:

Control parameters →  → Reward

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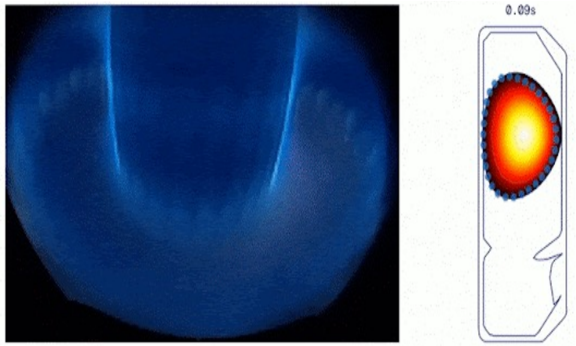
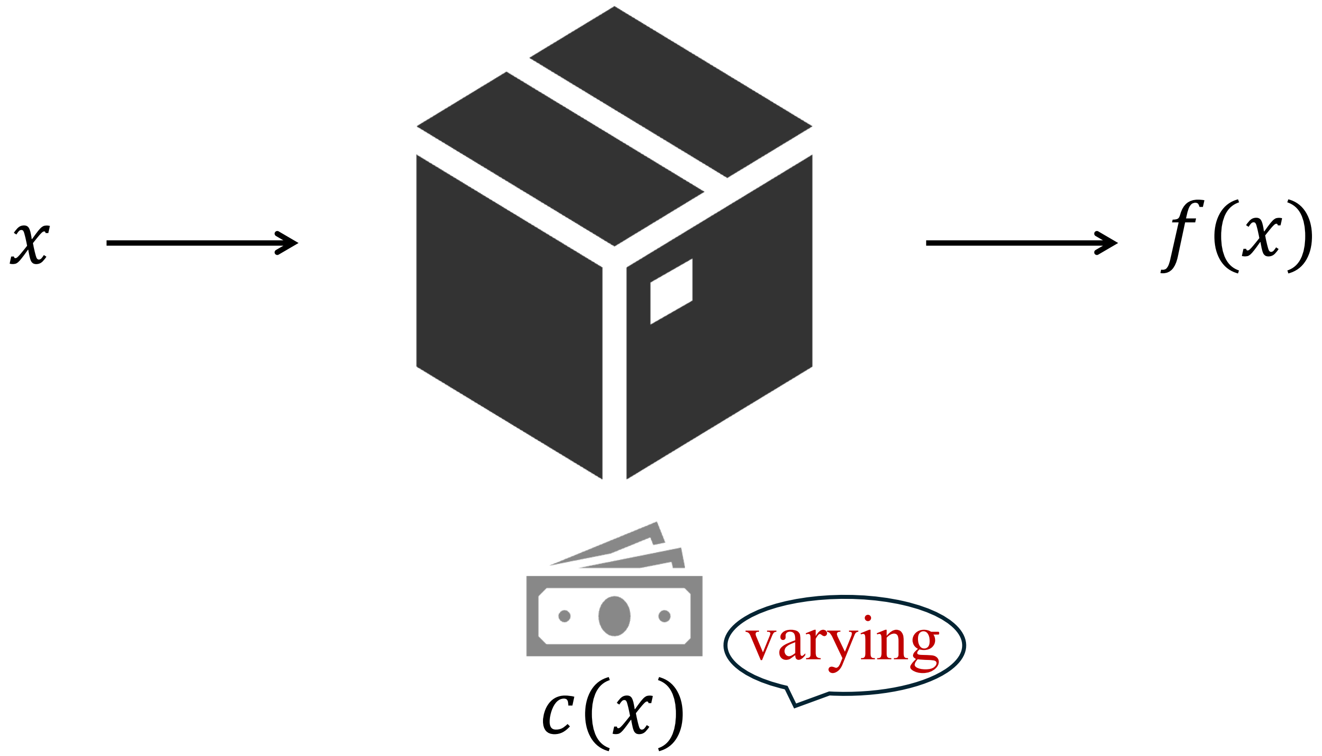
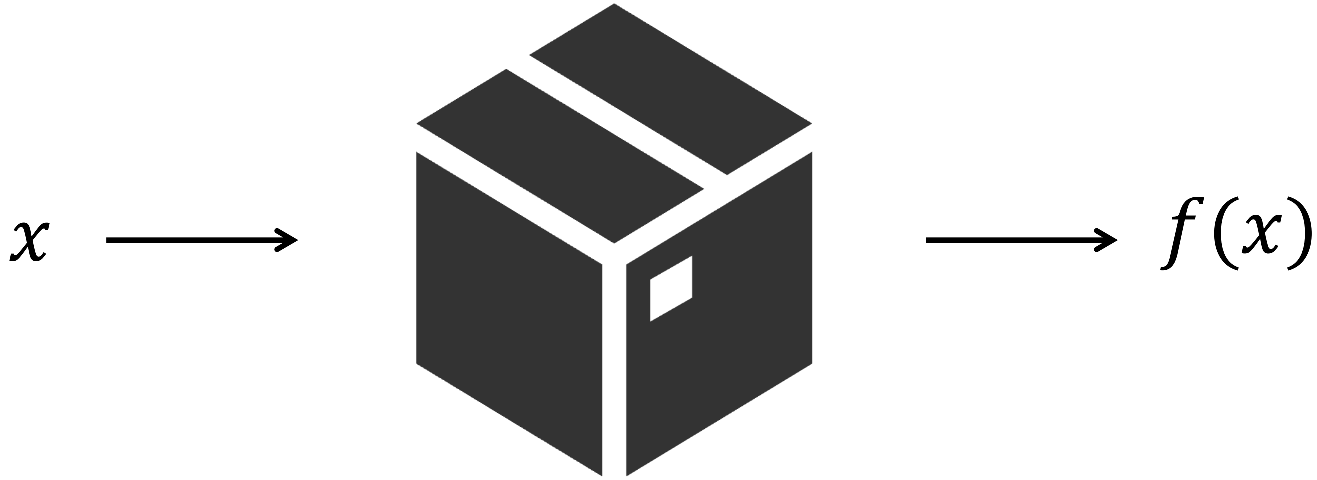
Reactor parameters → 

→ Stability

Another Challenge: Varying Evaluation Costs



Cost-aware Bayesian Optimization



$$\text{Goal: } \mathbf{max}\ \mathbb{E} \max_{t=1,2,\ldots,T} f(x_t)$$

$$\text{s.t. } \mathbb{E} \textstyle\sum_{t=1}^{T} c(x_t) \le B$$

"Cost-aware Bayesian Optimization." [Lee, Perrone, Archambeau, Seeger'21]

"Multi-step Budgeted .. Unknown Evaluation Costs" [Astudillo, Jiang, Balandat, Bakshy, Frazier'21]

Cost-aware Bayesian Optimization

	Uniform costs	Varying costs
One-step	Expected improvement $\max_x \mathrm{EI}_{f\mid D}(x; y_{\text{best}})$	

Cost-aware Bayesian Optimization

	Uniform costs	Varying costs
One-step	Expected improvement	Expected improvement per cost
	$\max_x \mathrm{EI}_{f\|D}(x; y_{\text{best}})$	[Snoek, Larochelle, Adams'21]

Cost-aware Bayesian Optimization

	Uniform costs	Varying costs
One-step	Expected improvement	Expected improvement per cost
	$\max_x \mathrm{EI}_{f\|D}(x; y_{\text{best}})$	$\max_x \mathrm{EI}_{f\|D}(x; y_{\text{best}})/c(x)$

Cost-aware Bayesian Optimization

	Uniform costs	Varying costs
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Why divide?

Cost-aware Bayesian Optimization

	Uniform costs	Varying costs
One-step	Expected improvement	Expected improvement per cost
	$\max_x \mathrm{EI}_{f\|D}(x; y_{\mathrm{best}})$	$\max_x \mathrm{EI}_{f\|D}(x; y_{\mathrm{best}})/c(x)$

EI and EIPC policy can be arbitrarily bad under varying costs!

[Astudillo, Jiang, Balandat, Bakshy, Frazier'21]

Cost-aware Bayesian Optimization

	Uniform costs	Varying costs
One-step	Expected improvement	Expected improvement per cost
Multi-step	Multi-step Lookahead EI	Budgeted Multi-step Lookahead EI

slow

[Astudillo, Jiang, Balandat, Bakshy, Frazier'21]

Cost-aware Bayesian Optimization

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	Upper Confidence Bound	?
	Thompson Sampling	?

Cost-aware Bayesian Optimization

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Multi-step	Multi-step Lookahead EI	Budgeted Multi-step Lookahead EI
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	⋮	⋮

Our view: lack of a guidance to incorporate costs

Cost-aware Bayesian Optimization

	Uniform costs	Varying costs
One-step	Expected improvement	Expected improvement per cost
Multi-step	Multi-step Lookahead EI	Budgeted Multi-step Lookahead EI
	Upper Confidence Bound	?
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	⋮	⋮

New design principle: Gittins Index

Cost-aware Bayesian Optimization

	Uniform costs	Varying costs
One-step	Expected improvement	Expected improvement per cost
Multi-step	Multi-step Lookahead EI	Budgeted Multi-step Lookahead EI
	Upper Confidence Bound	?
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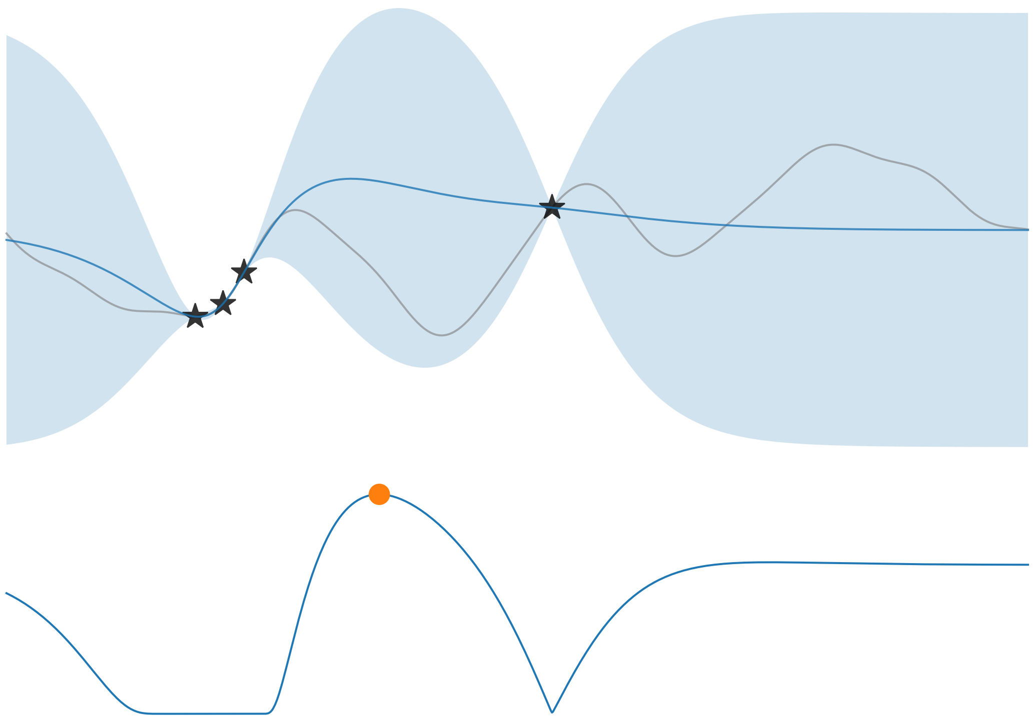
	⋮	⋮

New design principle: Gittins Index

naturally cost-aware

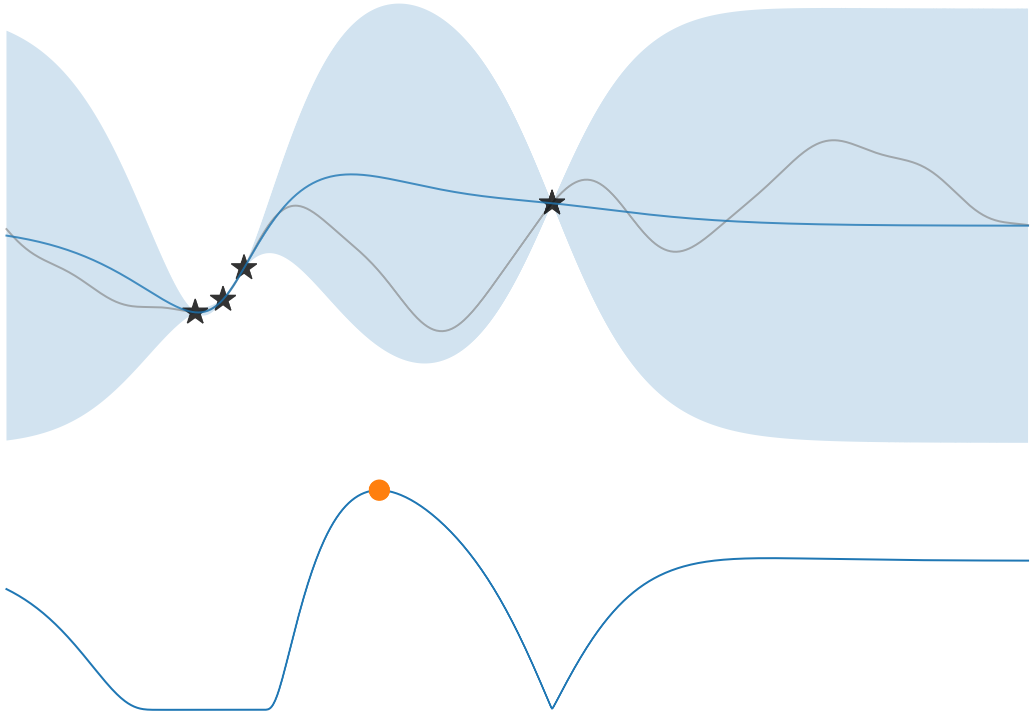
Expected Improvement



$$\mathrm{EI}_{f|D}(x) = \mathbb{E}[\max(f(x) - y_{\mathrm{best}}, 0) \mid D]$$

$$\max_x \mathrm{EI}_{f|D}(x; y_{\mathrm{best}})$$

Expected Improvement



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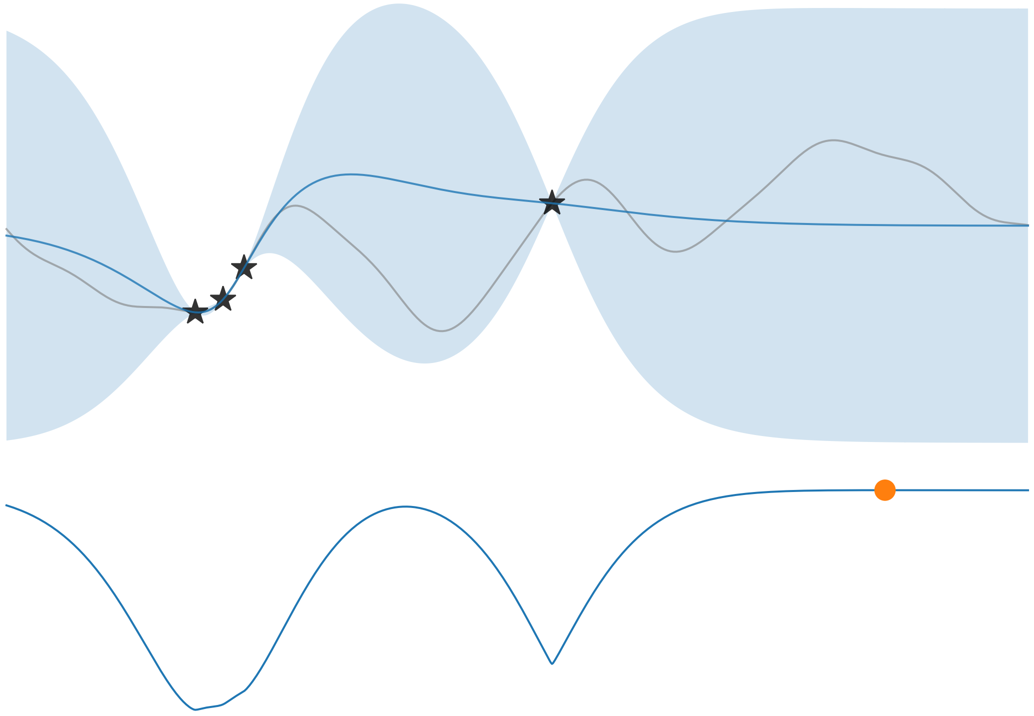
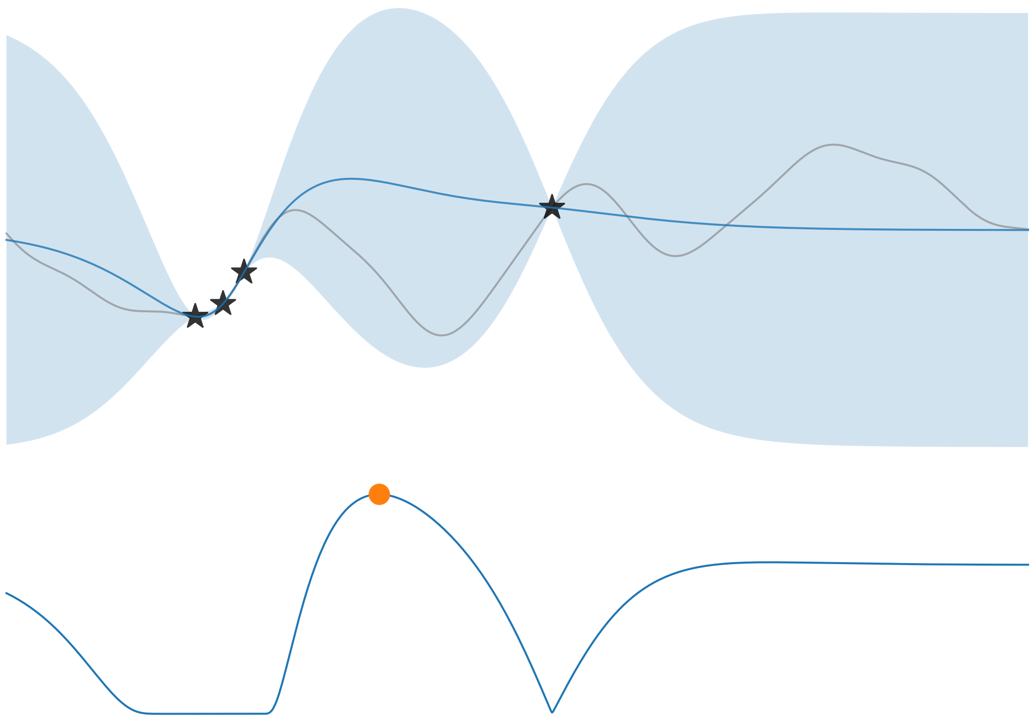
Gittins Index



$$\color{red}{\mathrm{GI}_{f|D}(x)} = g \text{ s.t. } \mathrm{EI}_{f|D}(x; \color{red}{g}) = c(x)$$

$$\max_x \mathrm{GI}_{f|D}(x)$$

Expected Improvement



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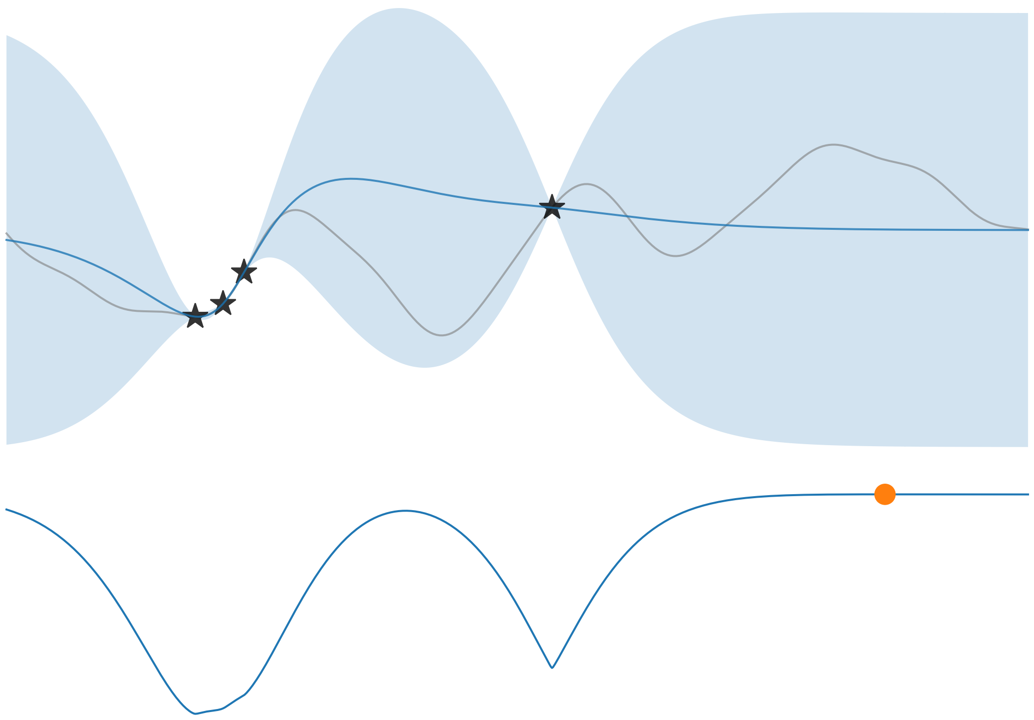
One-step approximation to MDP

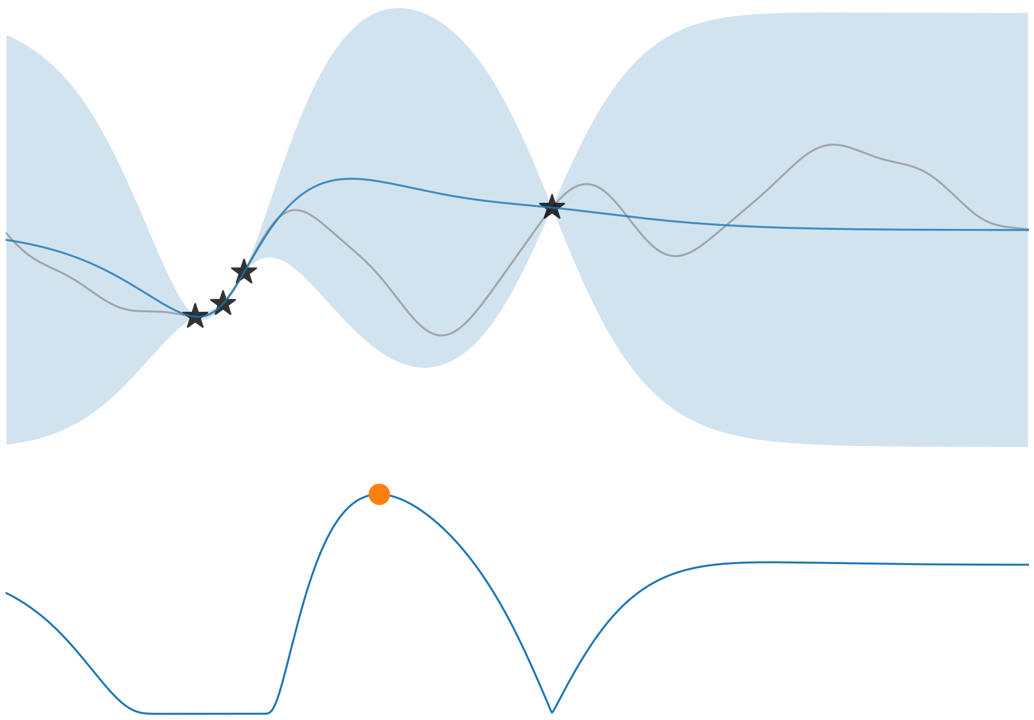
Gittins Index



$$\mathrm{GI}_{f|D}(x) = g \text{ s.t. } \mathrm{EI}_{f|D}(x; g) = c(x)$$

$$\max_x \mathrm{GI}_{f|D}(x)$$

Expected Improvement



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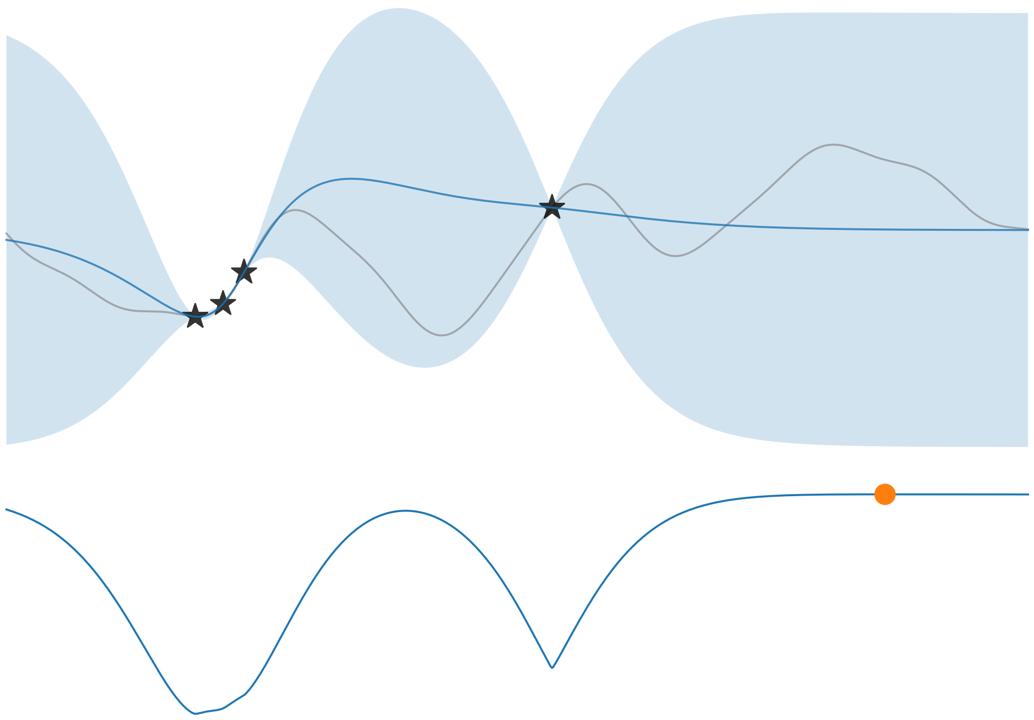
Temporal simplification to MDP

Gittins Index



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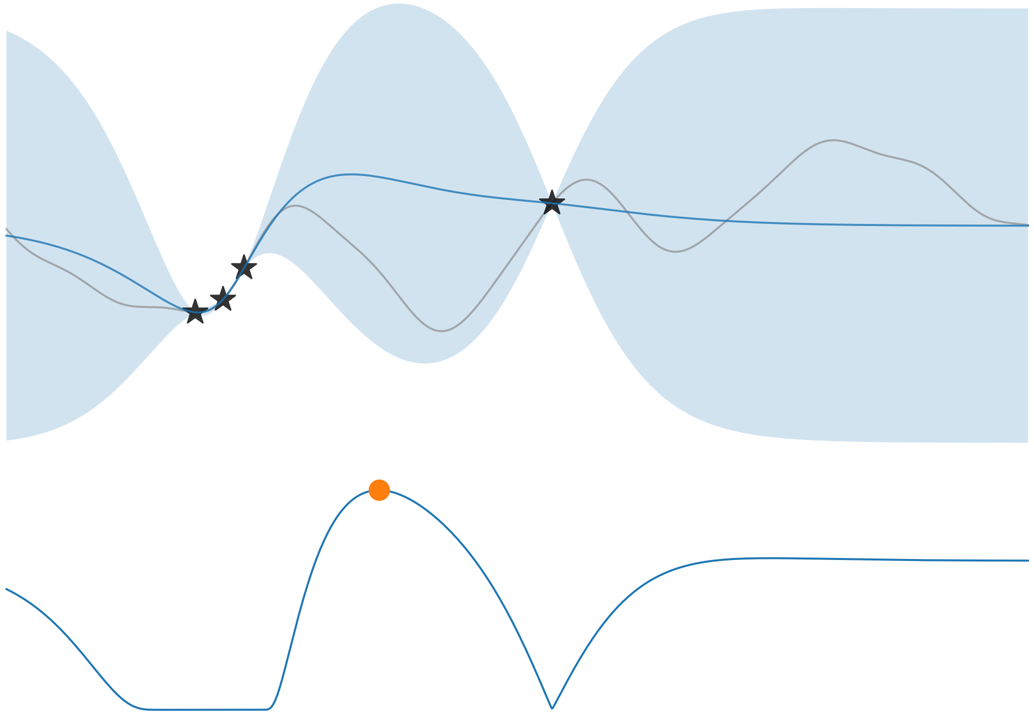
Expected Improvement



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Temporal simplification to MDP

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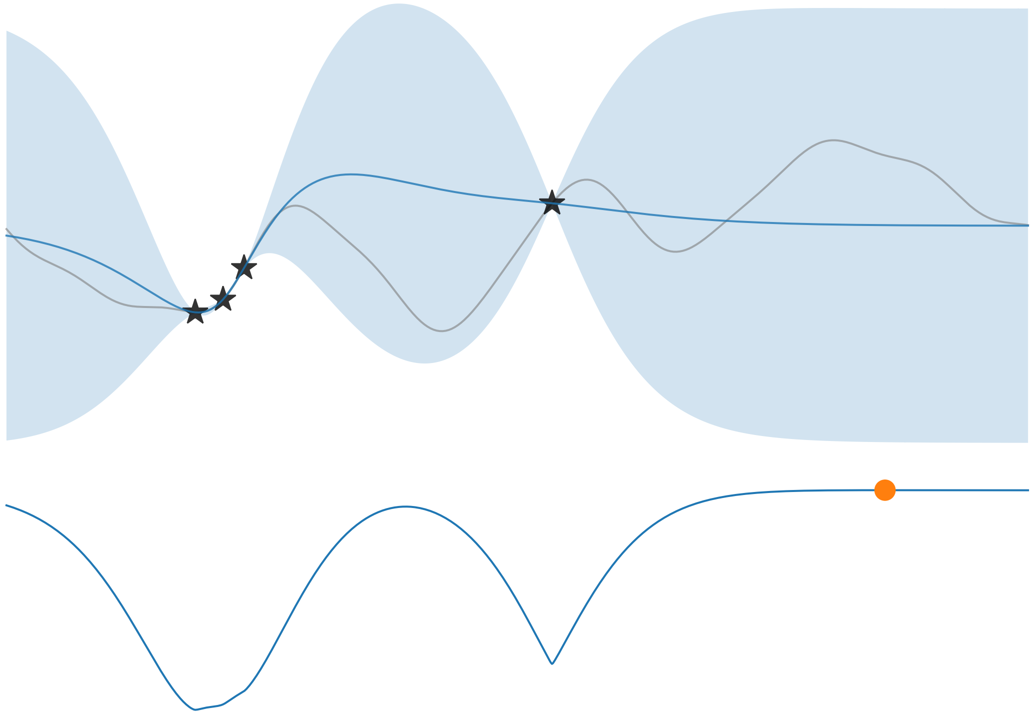
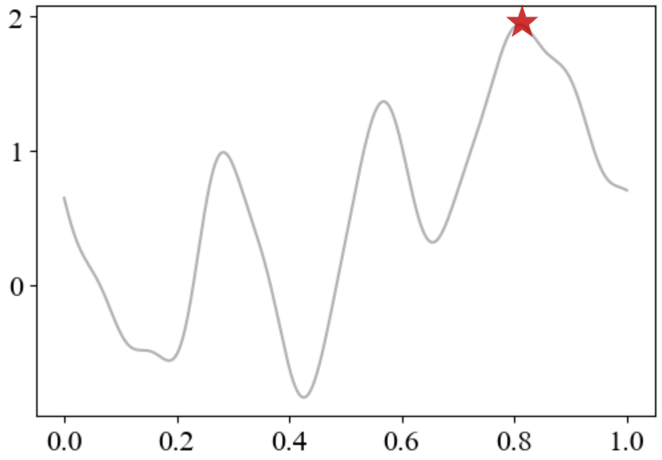


$$\mathrm{GI}_{f|D}(x) = g \text{ s.t. } \mathrm{EI}_{f|D}(x; g) = c(x)$$

$$\max_x \mathrm{GI}_{f|D}(x)$$

Spatial simplification to MDP

Our Approach: Spatial Simplification

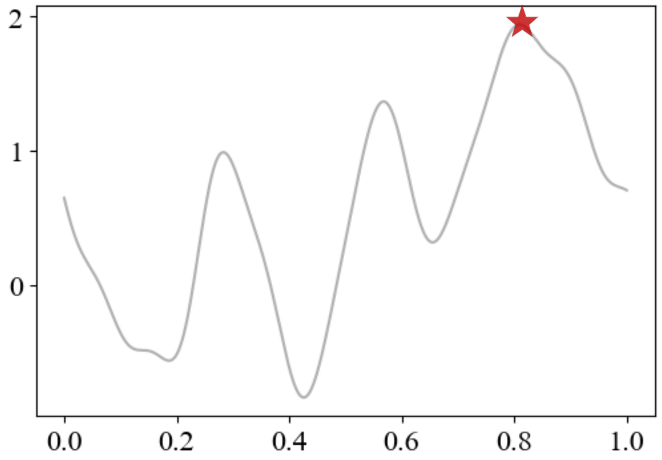


Bayesian Optimization

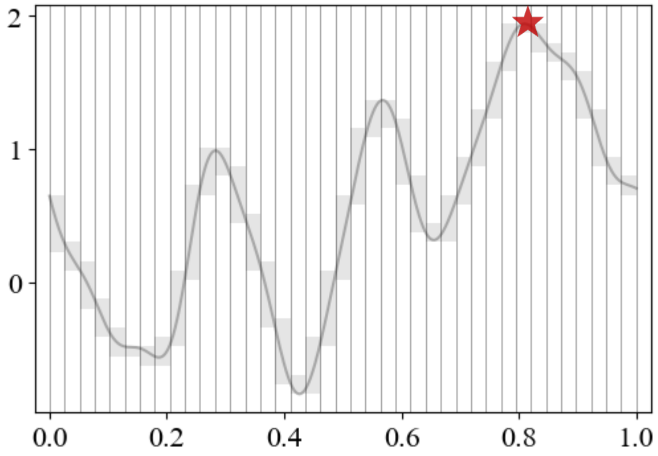
Continuous

Correlated

Our Approach: Spatial Simplification



⟹

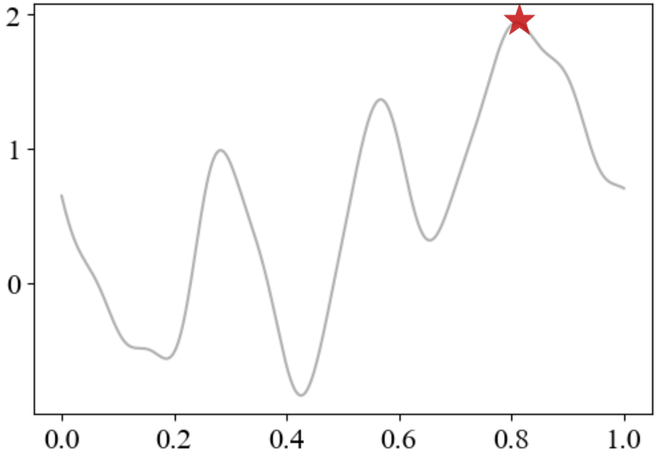


Bayesian Optimization

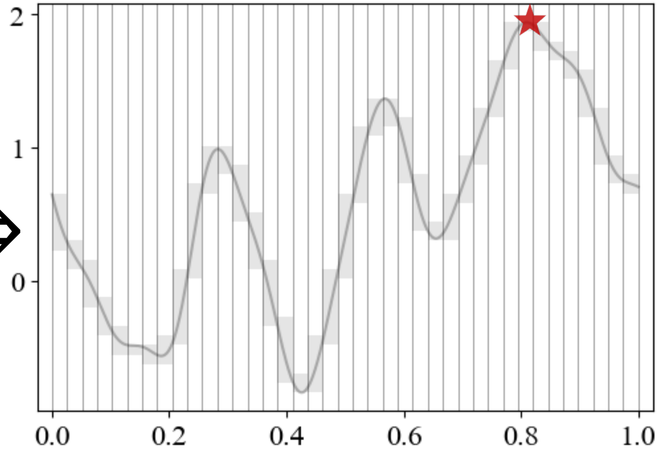
Continuous ⟹ Discrete

Correlated

Our Approach: Spatial Simplification



$\Longrightarrow$

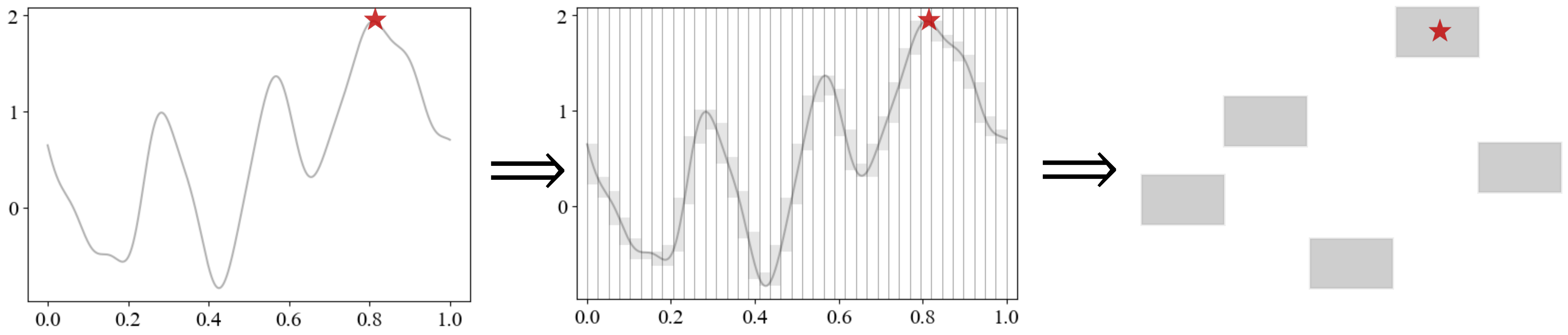


Bayesian Optimization

Continuous $\Longrightarrow$ Discrete

Correlated

Our Approach: Spatial Simplification

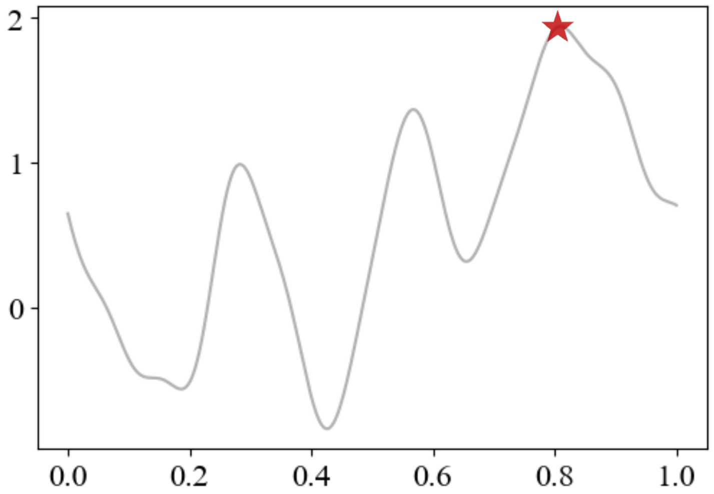


Bayesian Optimization

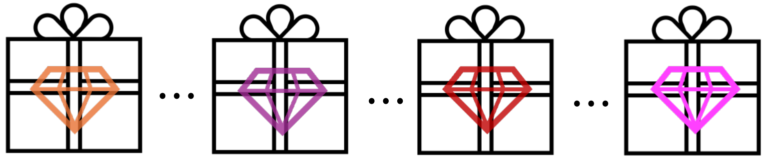
Continuous ⟹ Discrete

Correlated ⟹ Independent

Our Approach: Spatial Simplification



⟹



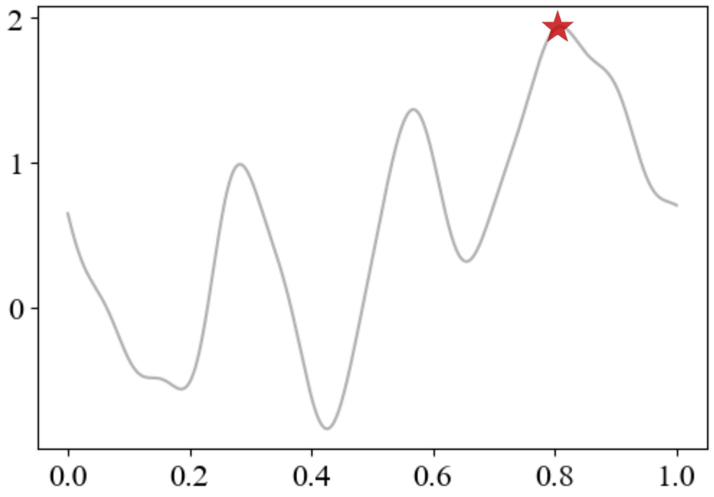
Bayesian Optimization

Pandora's Box [Weitzman'79]

Continuous ⟹ Discrete

Correlated ⟹ Independent

Our Approach: Spatial Simplification



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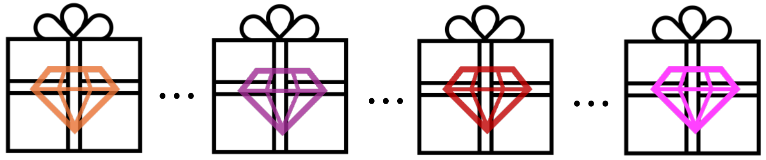


Bayesian Optimization

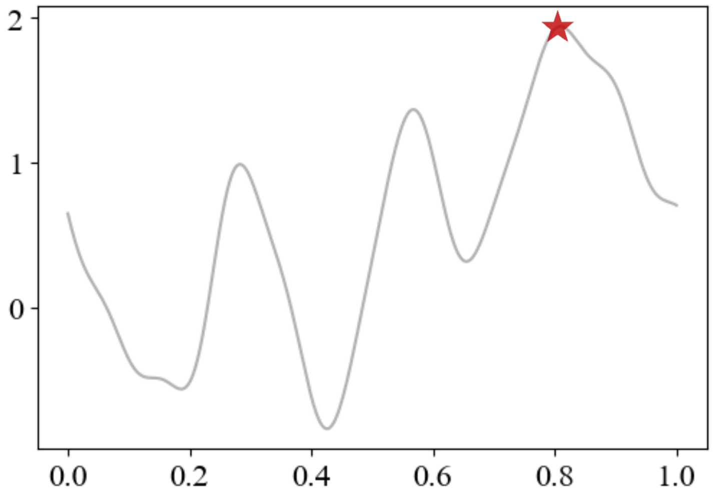
Pandora's Box [Weitzman'79]

Continuous $\Longrightarrow$ Discrete

Correlated $\Longrightarrow$ Independent

Optimal policy: Gittins index

Our Approach: Spatial Simplification



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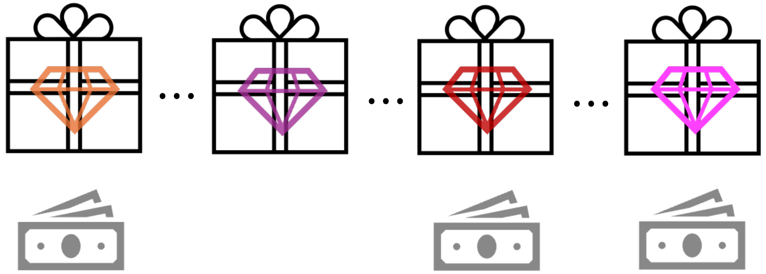


Bayesian Optimization

Pandora's Box [Weitzman'79]

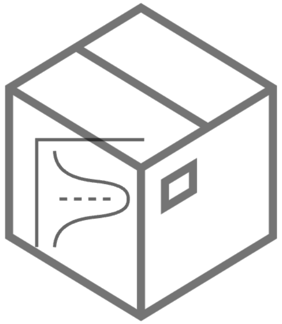
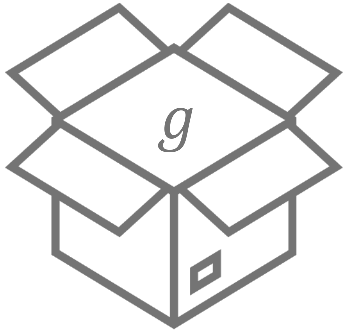
Continuous $\Longrightarrow$ Discrete

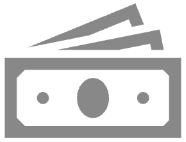
allow varying costs

Correlated $\Longrightarrow$ Independent

Optimal policy: Gittins index

Intuition Behind Pandora's Box Gittins Index

$f(x)$  vs. 

$c(x)$ 

Gittins index

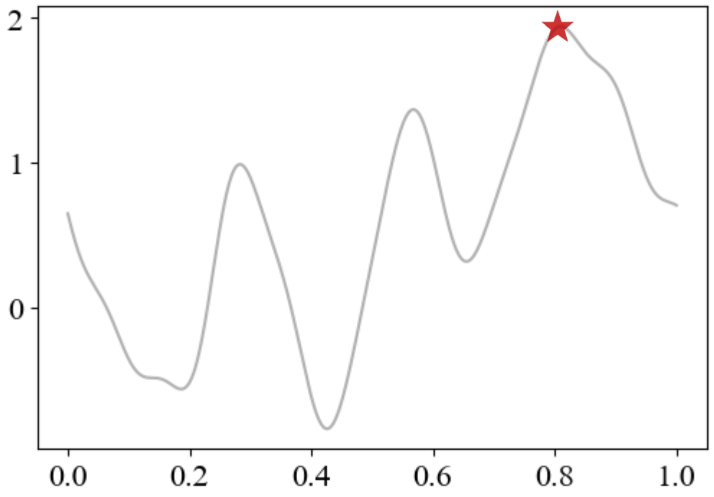
Open closed box $\mathrm{GI}(x)$ Take opened box

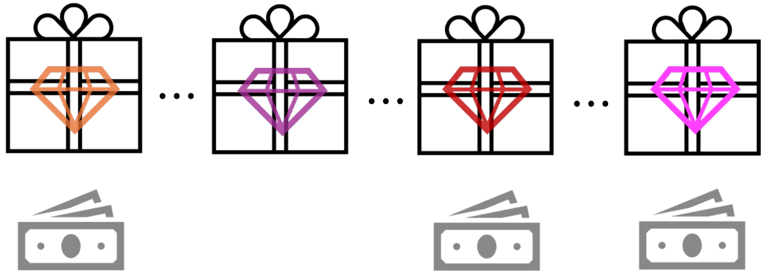
g

Profit: $\mathbb{E}[\max(f(x), g)] - c(x)$ Profit: g

$\mathrm{GI}(x)$: solution g to $\mathbb{E}[\max(f(x), g)] - c(x) = g$

How to translate Gittins index?





Bayesian Optimization

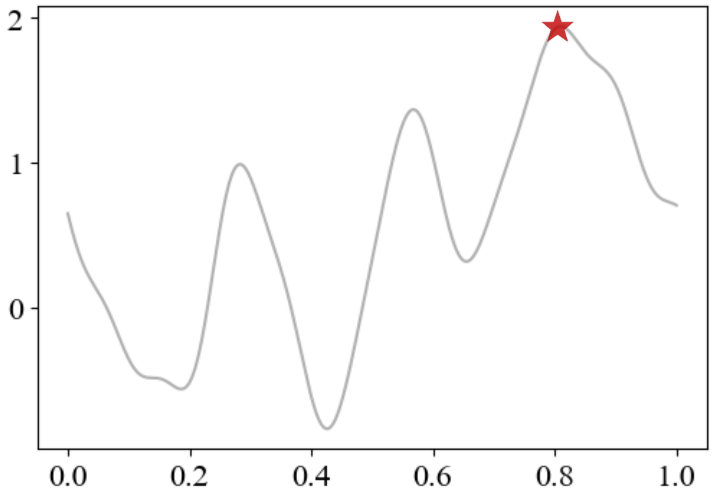
Pandora's Box [Weitzman'79]

Continuous	$\Longrightarrow$	Discrete
Correlated	$\Longrightarrow$	Independent

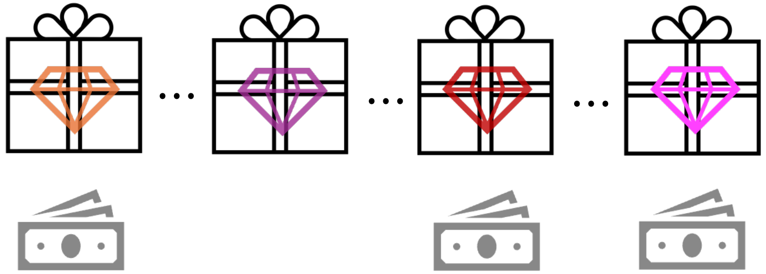
How to translate?

$\Longleftarrow$ Optimal policy: Gittins index

How to translate Gittins index?



Bayesian Optimization



Pandora's Box [Weitzman'79]

Continuous $\Longrightarrow$ Discrete

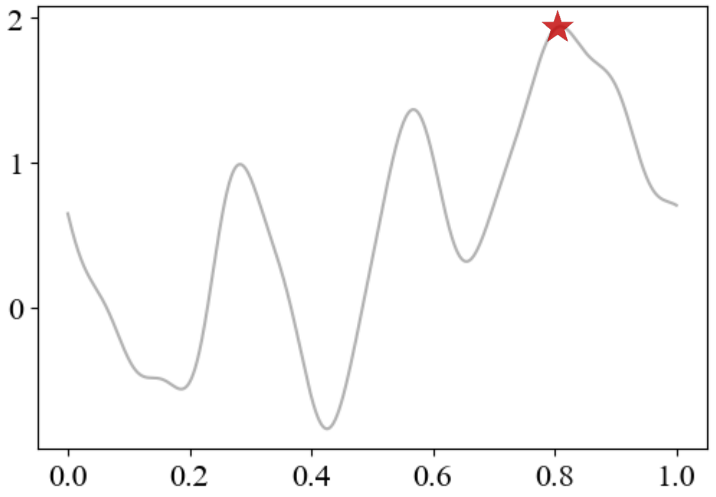
Correlated $\Longrightarrow$ Independent

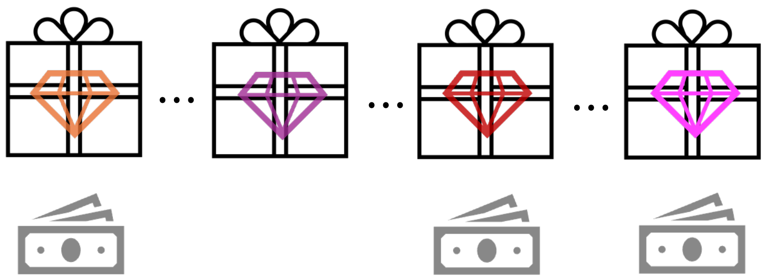
incorporate posterior

Our policy $\Longleftarrow$ Optimal policy: Gittins index

$\max_x \mathrm{GI}_{f|D}(x)$ $\max_x \mathrm{GI}(x)$

Is Gittins good in Bayesian Optimization?





Bayesian Optimization

Pandora's Box [Weitzman'79]

Continuous $\Longrightarrow$ Discrete

Correlated $\Longrightarrow$ Independent

incorporate posterior

Is Gittins index good? $\Longleftarrow$ Gittins index is optimal

$\max_x \mathrm{GI}_{f|D}(x)$ $\qquad$ $\max_x \mathrm{GI}(x)$

Experiment Setup: Objective Functions

Samples from prior

Synthetic

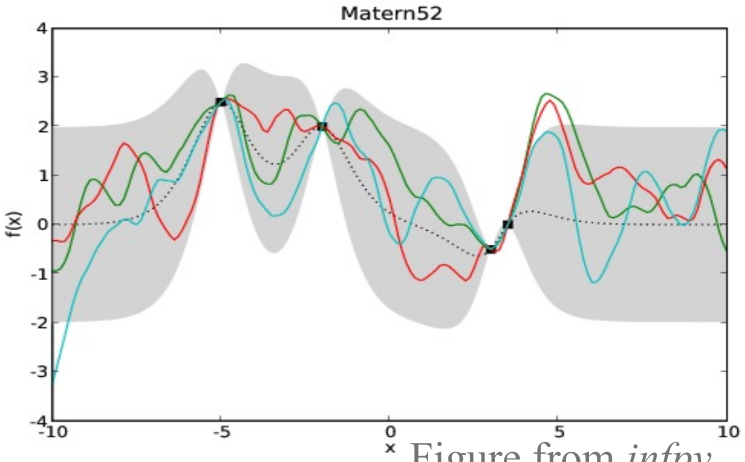


Figure from *infpy*

Ackley function

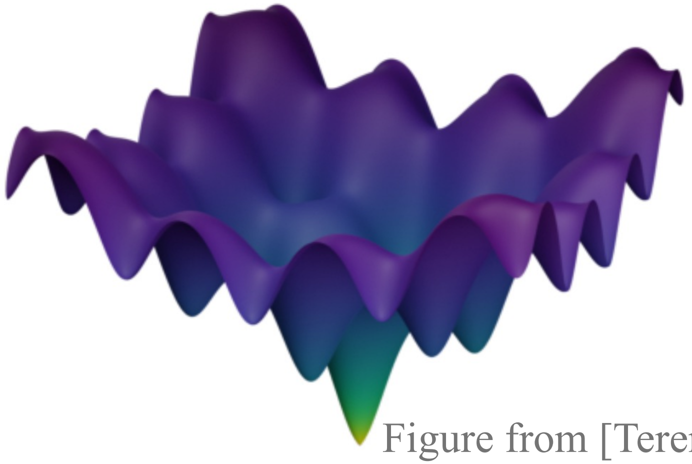


Figure from [Terenin'22]

Pest Control

Empirical

Figure from ChatGPT

Lunar Lander

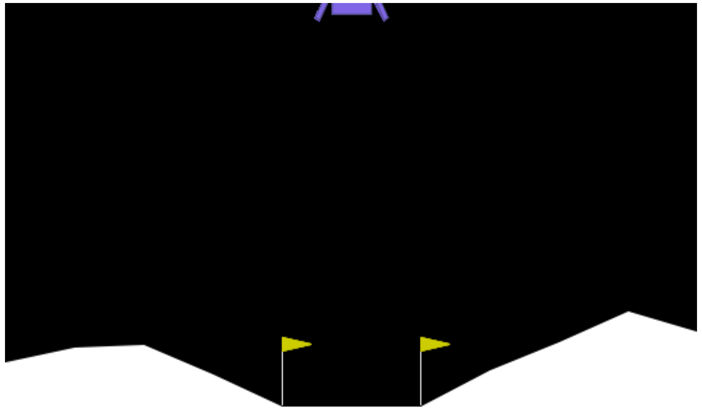
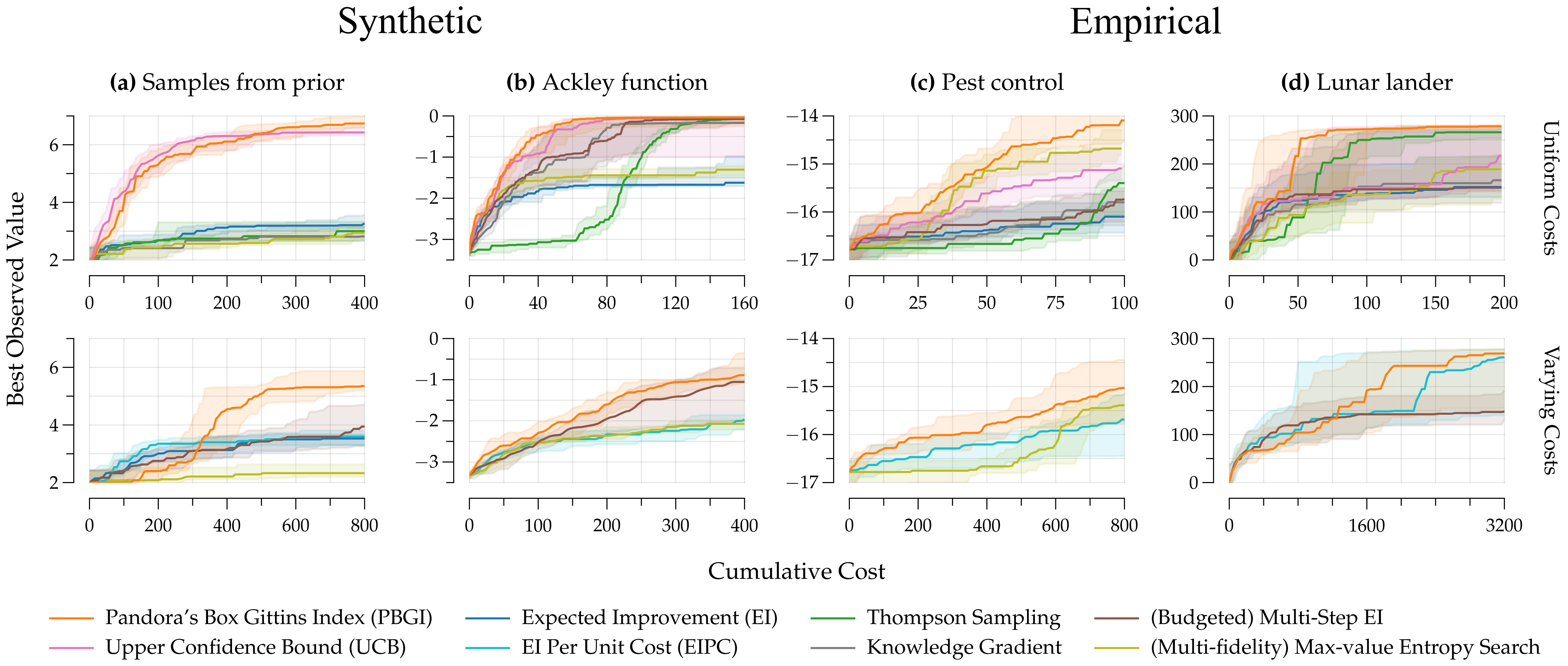


Figure from OpenAI Gym

Experiment Results



FAQ

- Easy-to-compute?

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  Yes, EI + bisection

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- Any theoretical results?

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- Easy-to-compute?

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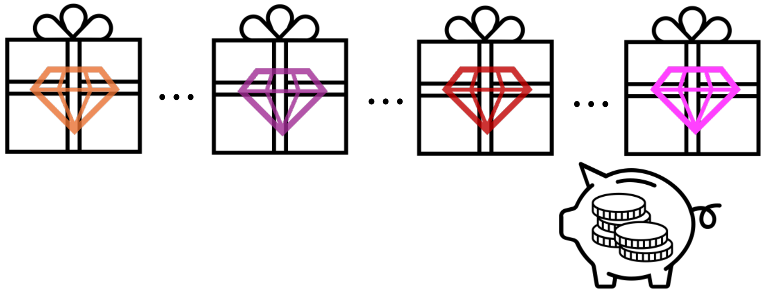
- Any theoretical results?

  Yes, expected-budget-constrained $\cong$ cost-per-sample

Theoretical Result

max best observed under budget

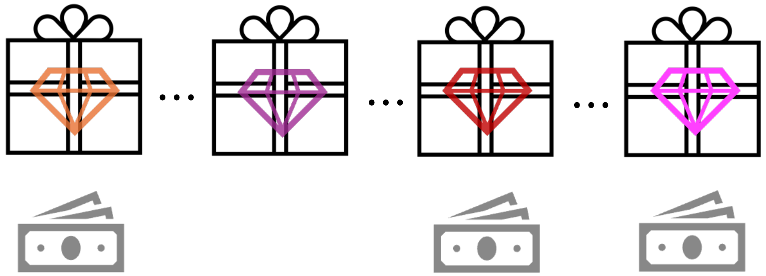


Budgeted Pandora's Box

Expected budget constraint

Optimal policy?

max (best observed – costs)



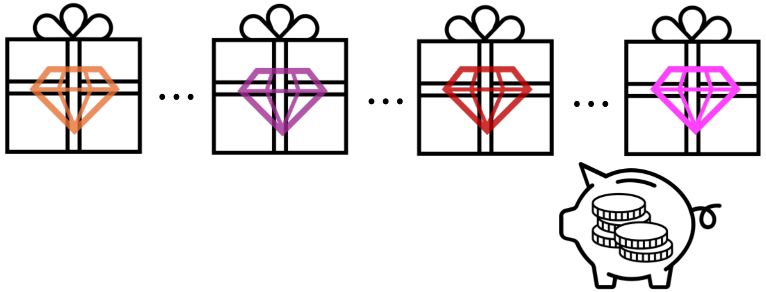
Pandora's Box

Cost per sample

Optimal policy: Gittins index

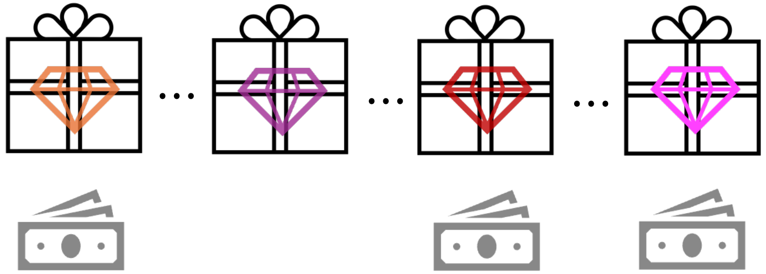
Theoretical Result

max best observed under budget



$\Longleftarrow$

max (best observed – scaled costs)



Budgeted Pandora's Box

Expected budget constraint

Optimal policy ✓

extension to [Aminian, Manshadi, Niazadeh'24]

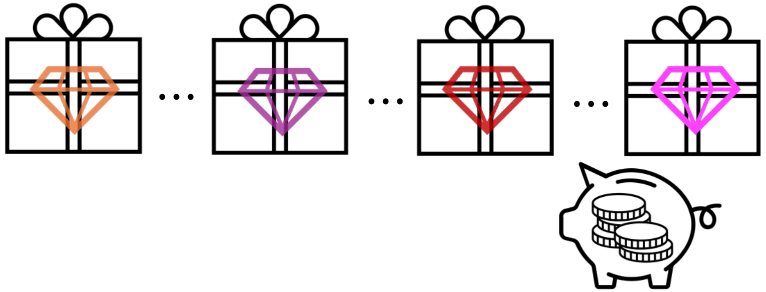
Pandora's Box

Cost per sample

Optimal policy: Gittins index

Theoretical Result

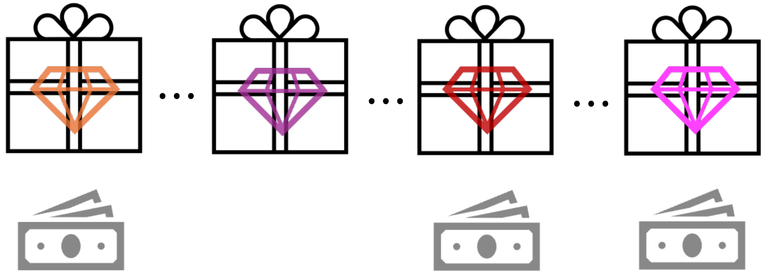
max best observed under budget



⇐

budget-dependent

max (best observed – scaled costs)



Budgeted Pandora's Box	Pandora's Box
Expected budget constraint	Cost per sample
Optimal policy ✓	Optimal policy: Gittins index

extension to [Aminian, Manshadi, Niazadeh'24]

FAQ

- Easy-to-compute?

  Yes, EI + bisection
- Any theoretical results?

  Yes, expected-budget-constrained $\cong$ cost-per-sample
- Tuning parameters?

FAQ

- Easy-to-compute?

  Yes, EI + bisection

- Any theoretical results?

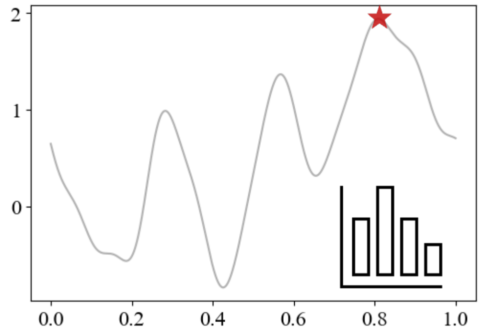
  Yes, expected-budget-constrained ≅ cost-per-sample

- Tuning parameters?

  Yes, control unit conversion

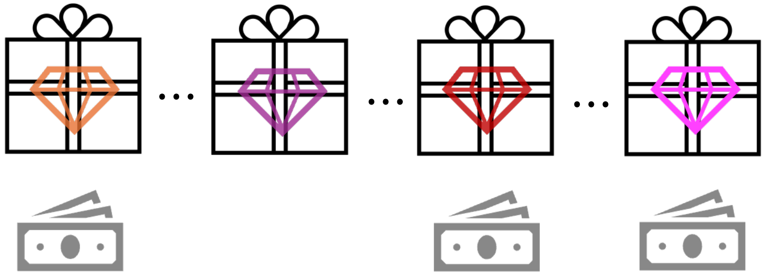
New Design Principle: Gittins Index

Problem



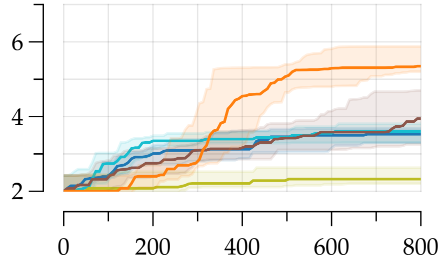
Bayesian optimization
with varying costs

Key idea



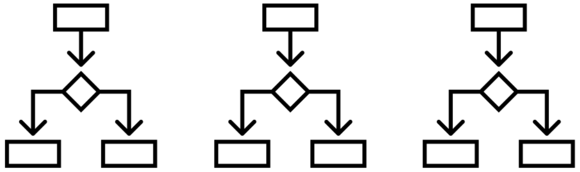
link to Pandora's box
and Gittins index theory

Impact



competitive performance

Future potential



black-box processes
with partial feedback

Check our paper on ArXiv!

"Cost-aware Bayesian Optimization via the Pandora's Box Gittins Index."