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

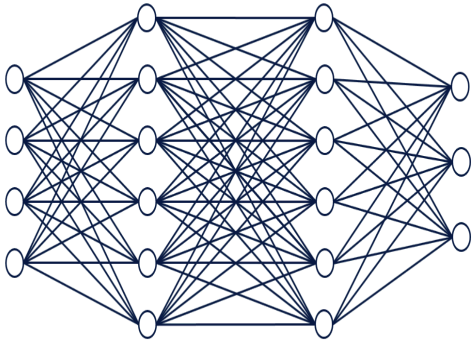
Peter Frazier

Ziv Scully

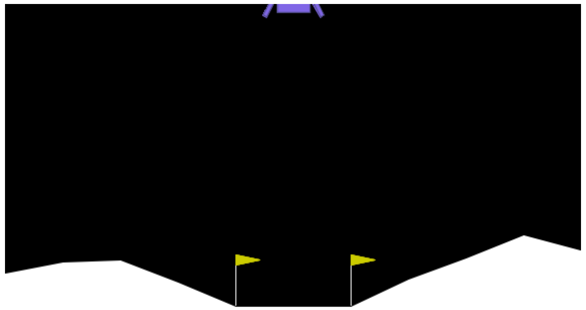
Alexander Terenin

World of Parameter Optimization

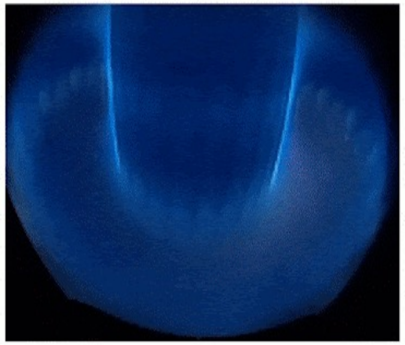
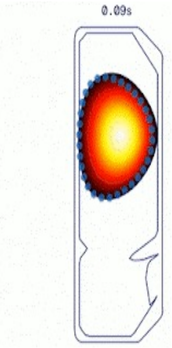
Hyperparameter tuning:

Training parameters →  → Accuracy

Control optimization:

Control parameters →  → Reward

Plasma physics:

Reactor parameters →  

→ Stability

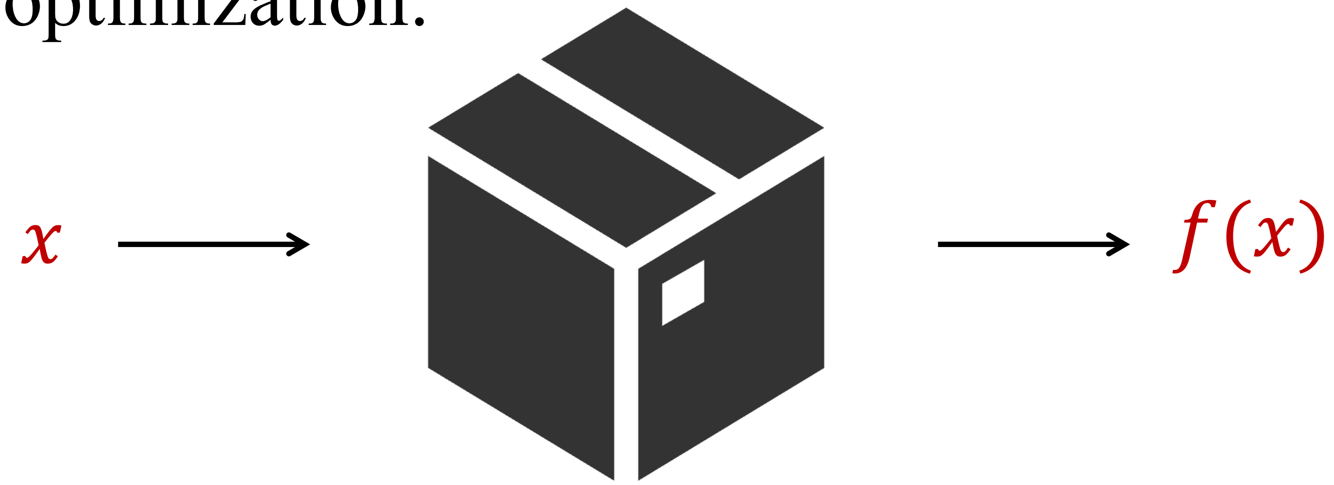
World of Parameter Optimization

Black-box optimization:

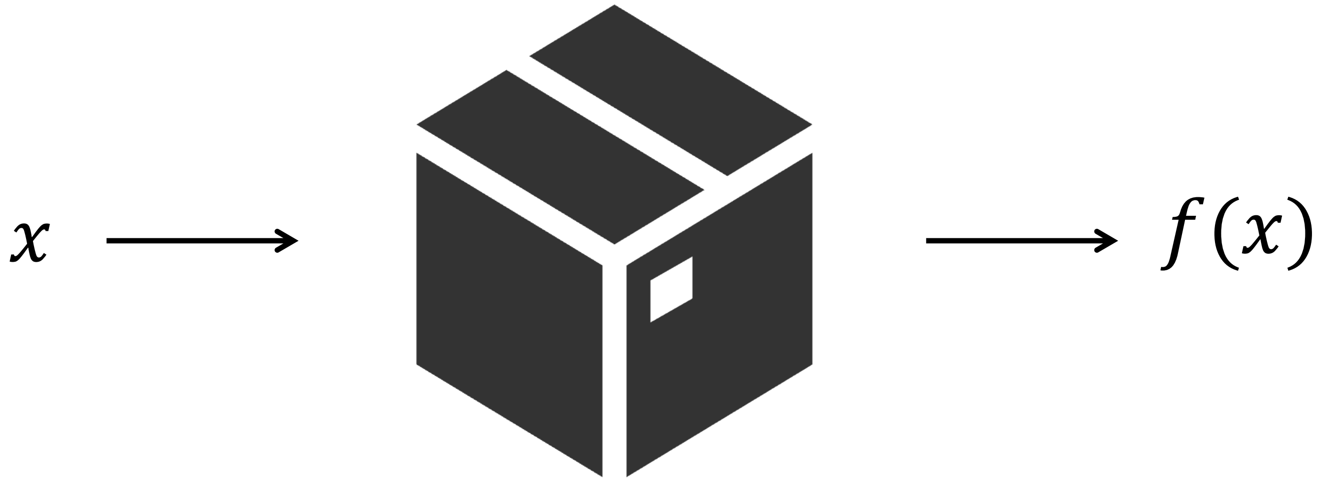
Input parameters →  → Performance metrics

World of Parameter Optimization

Black-box optimization:



Optimizing Black-box Functions



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

Optimizing Black-box Functions

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

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

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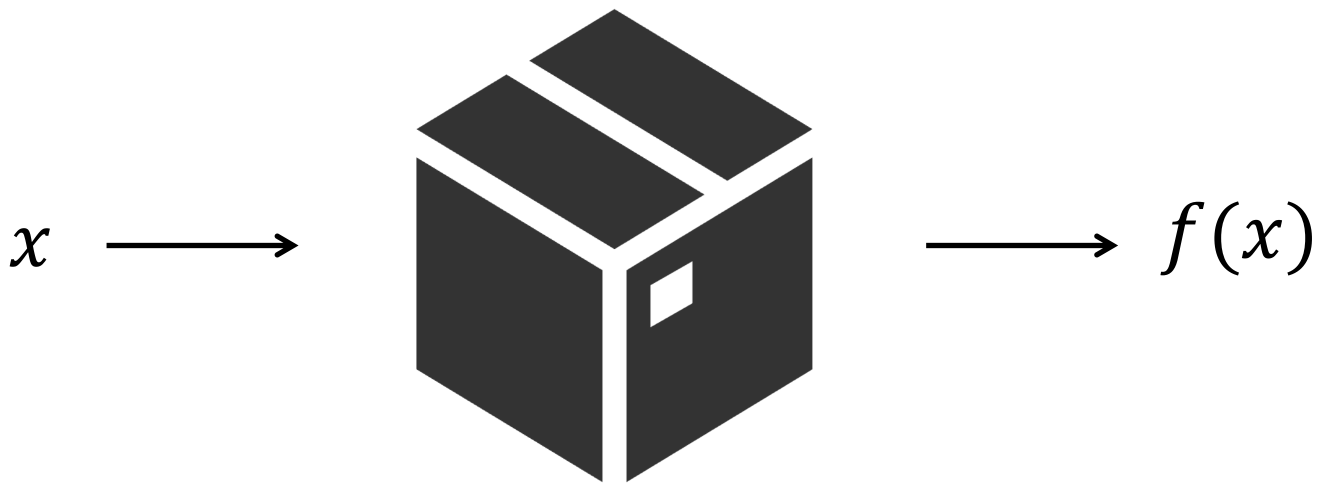
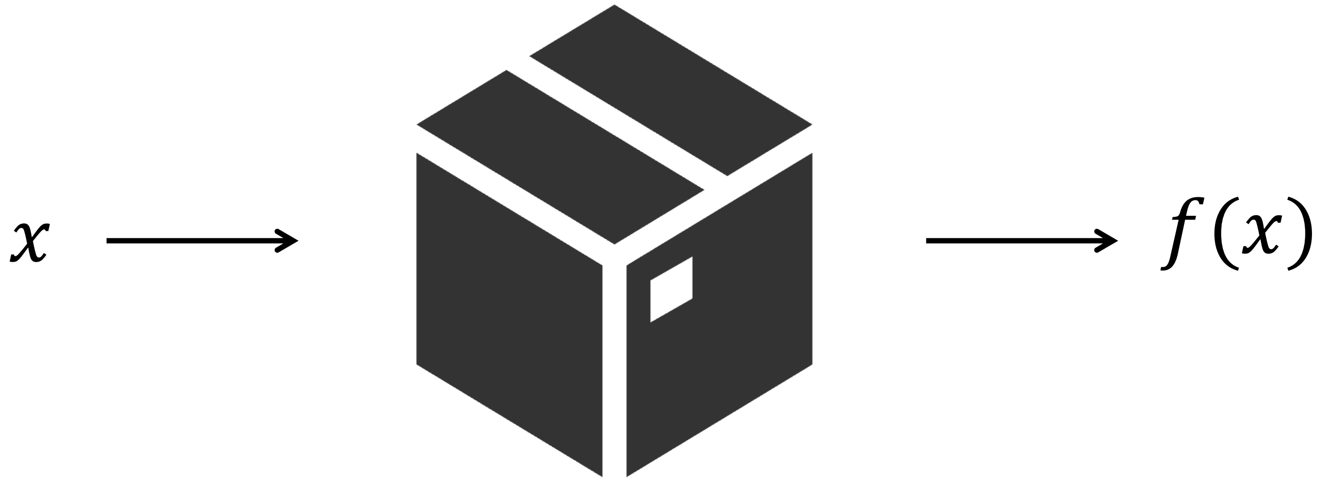
Optimizing Black-box Functions



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

Optimizing Black-box Functions



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

$f \sim$Gaussian Process

Bayesian Optimization

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

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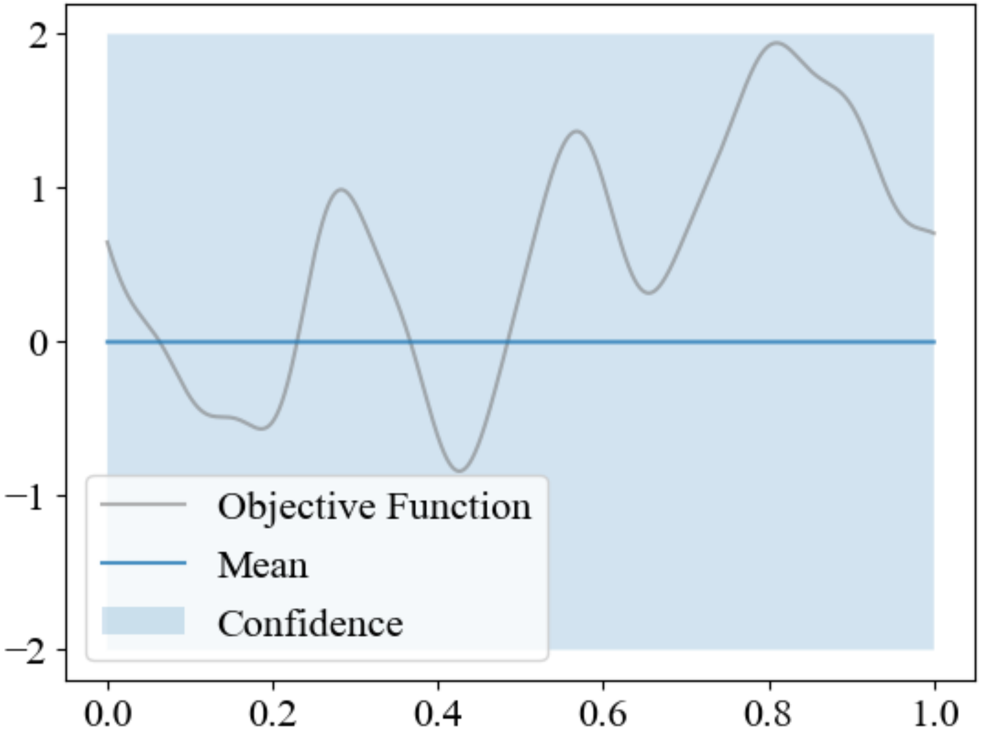

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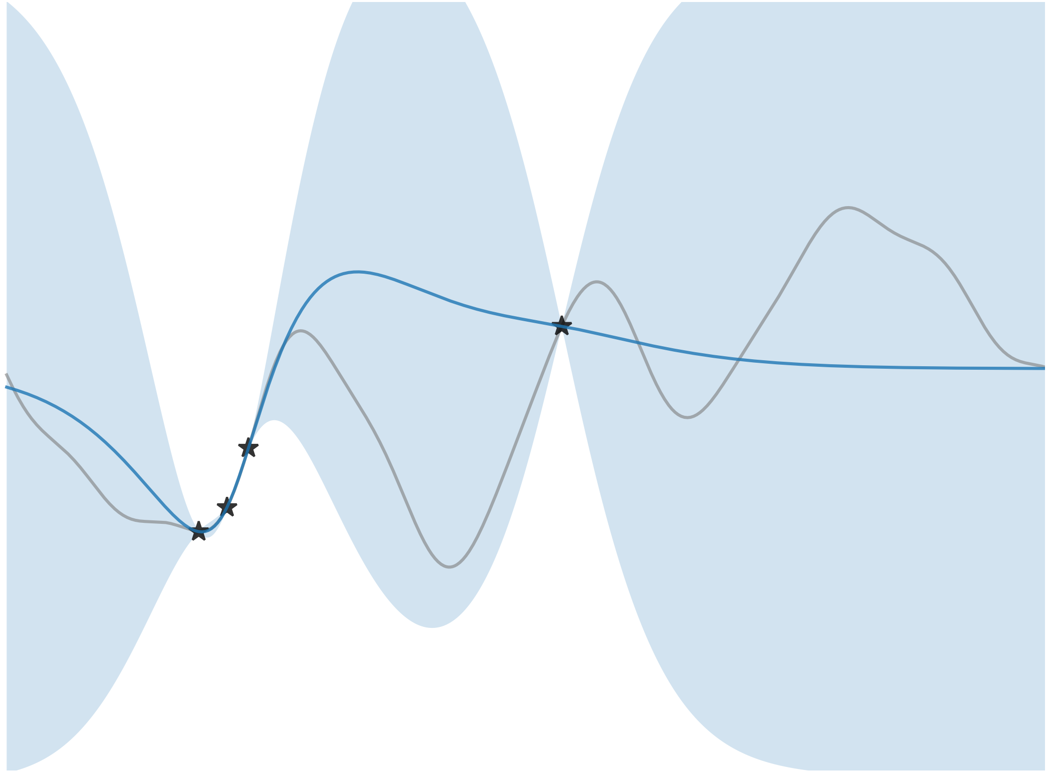

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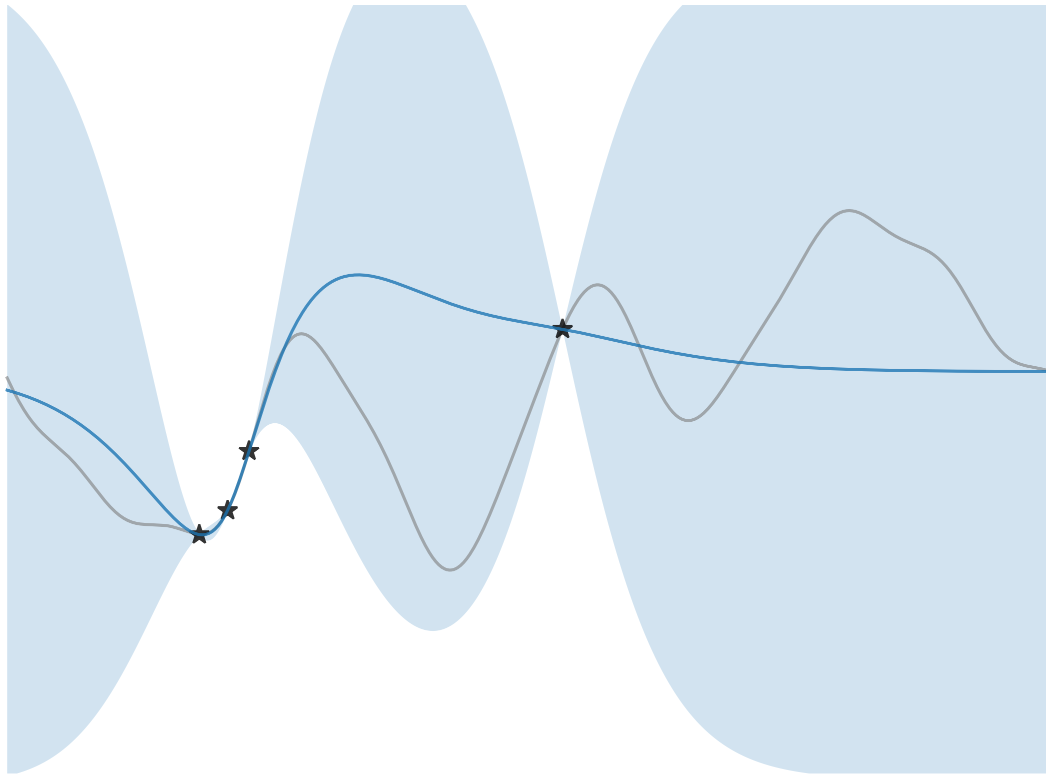
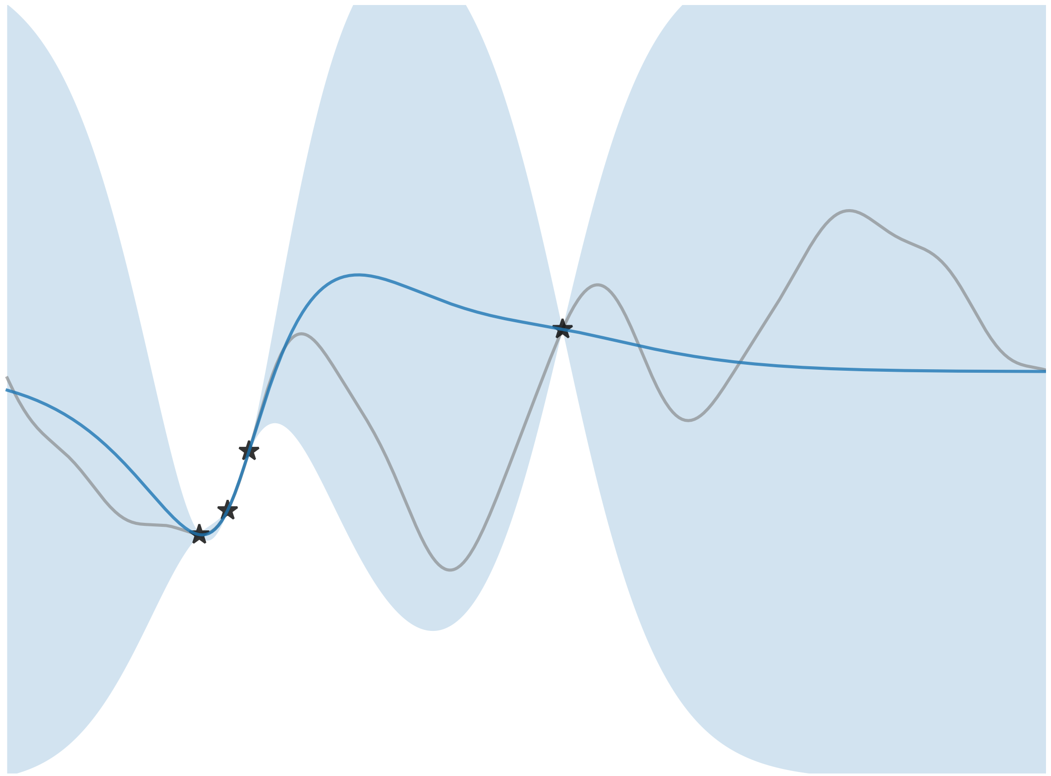


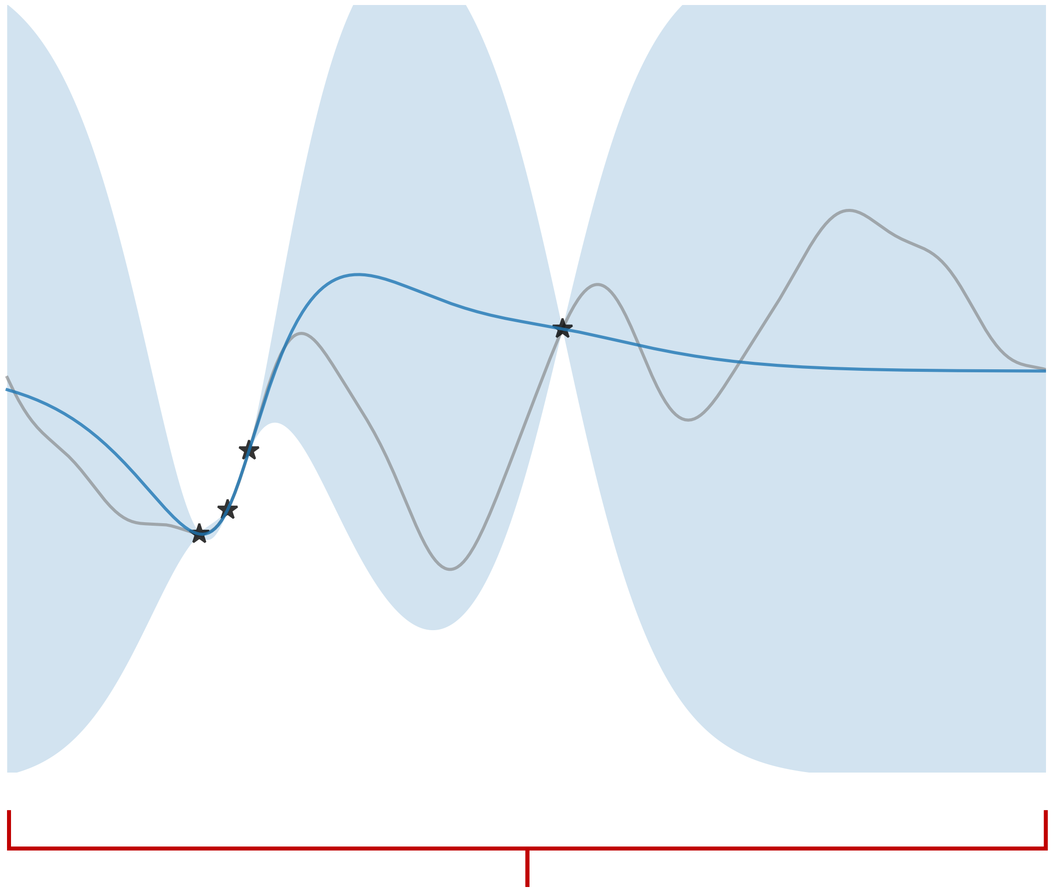
What to evaluate next?

Bayesian Optimization



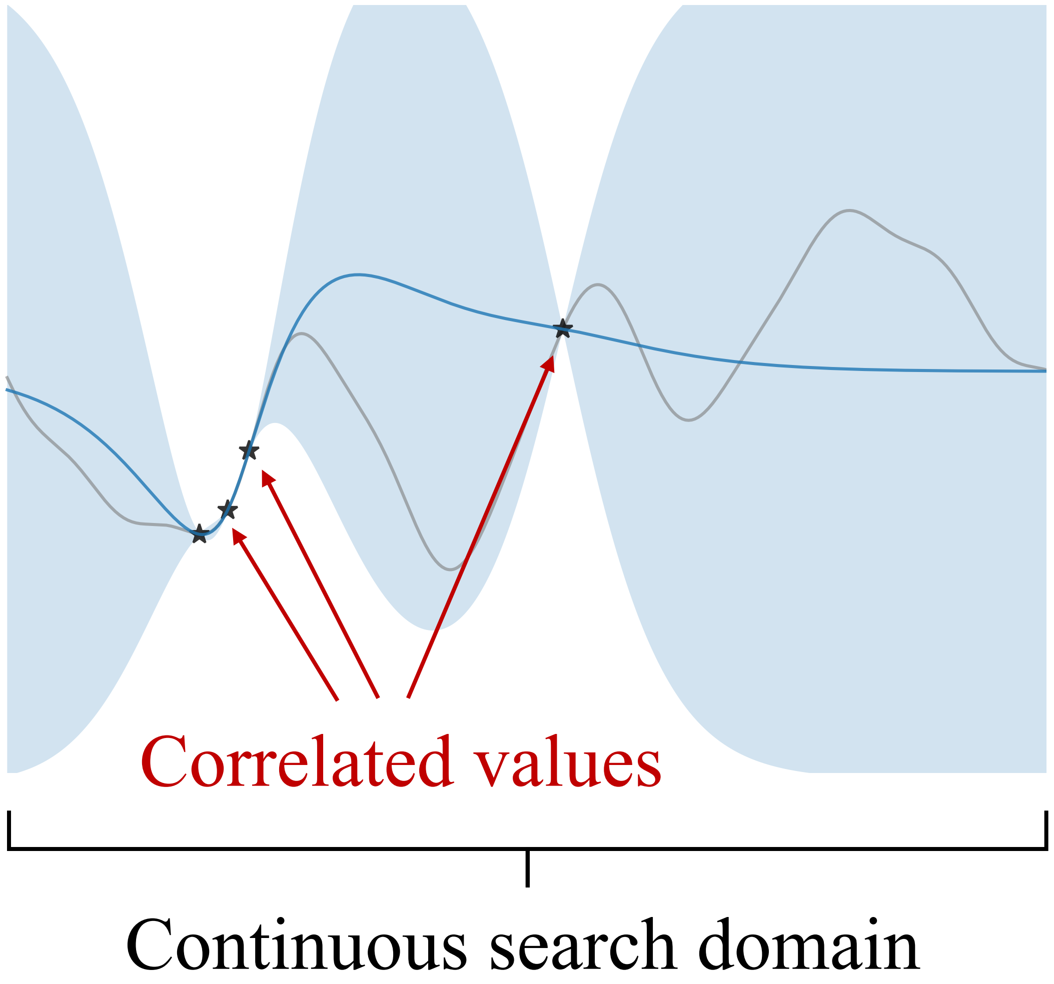
Optimal policy?

Challenges of Bayesian optimization

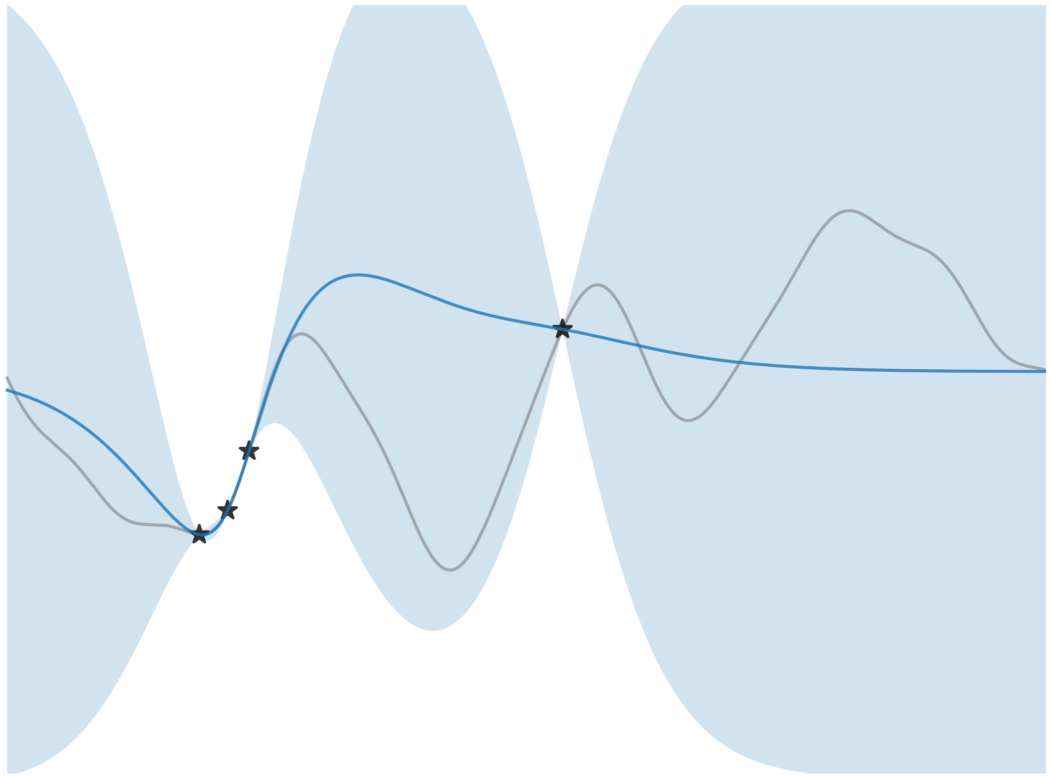


Continuous search domain

Challenges of Bayesian optimization

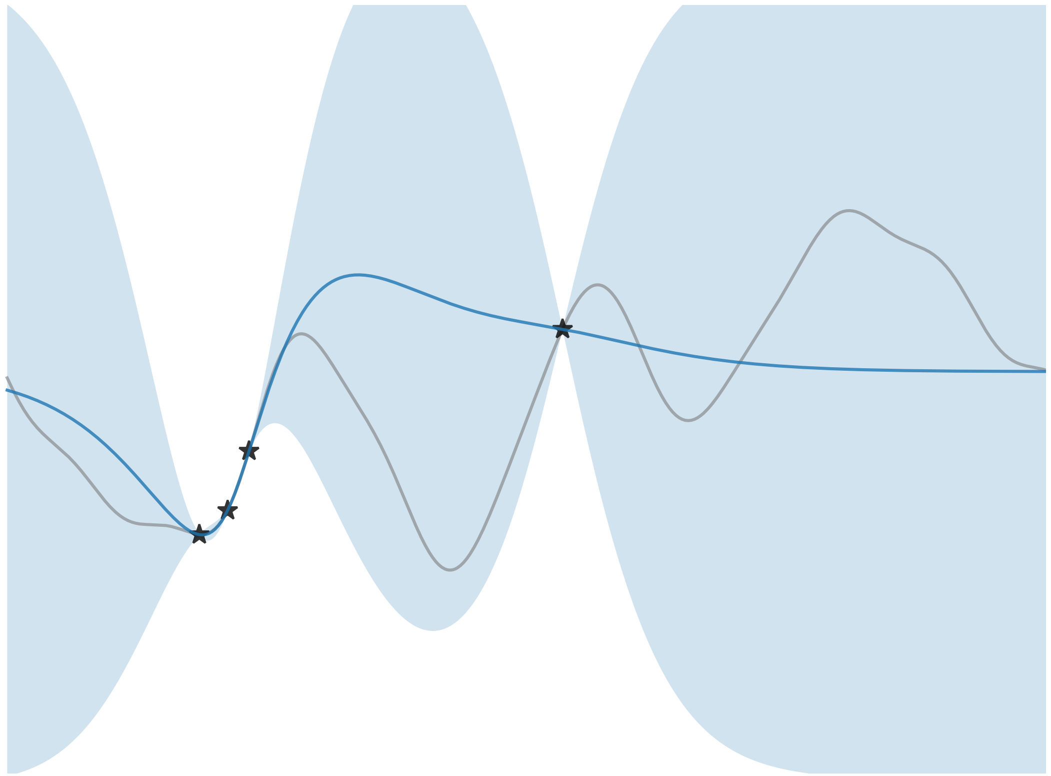


Challenges of Bayesian Optimization



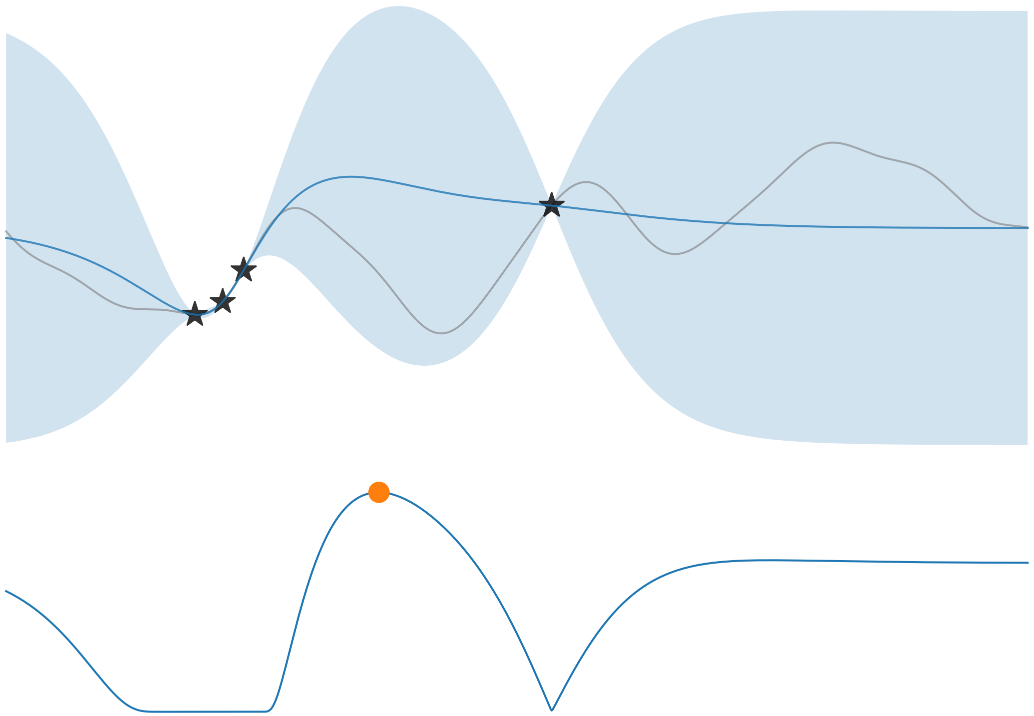
Correlation & continuity $\Longrightarrow$ Intractable MDP

Challenges of Bayesian Optimization



Intractable MDP $\Longrightarrow$ Optimal policy unknown

Popular Policy: Expected Improvement

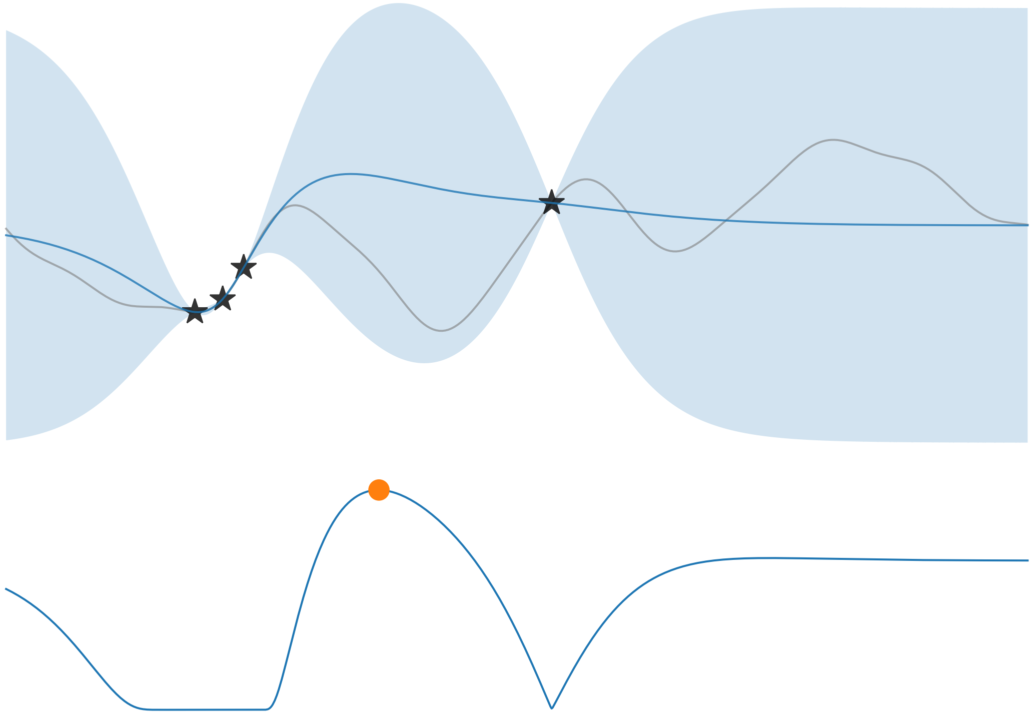


current best observed

data

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

Popular Policy: Expected Improvement



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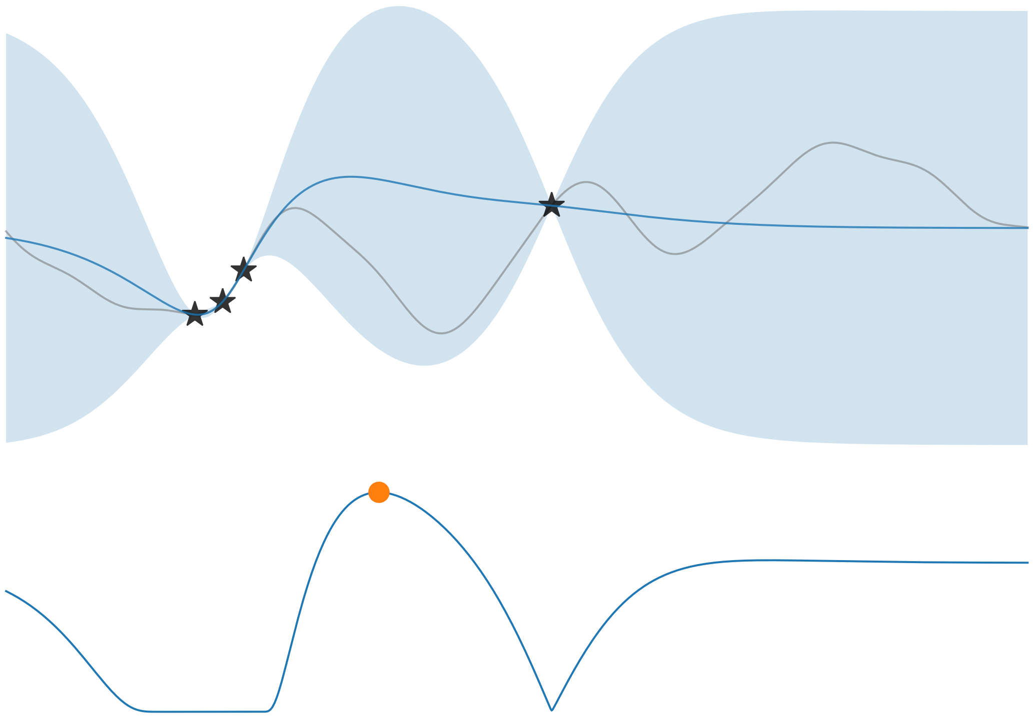
$$\max_x \mathrm{EI}_{f|D}(x; y_{\text{best}})$$

Popular Policy: Expected Improvement



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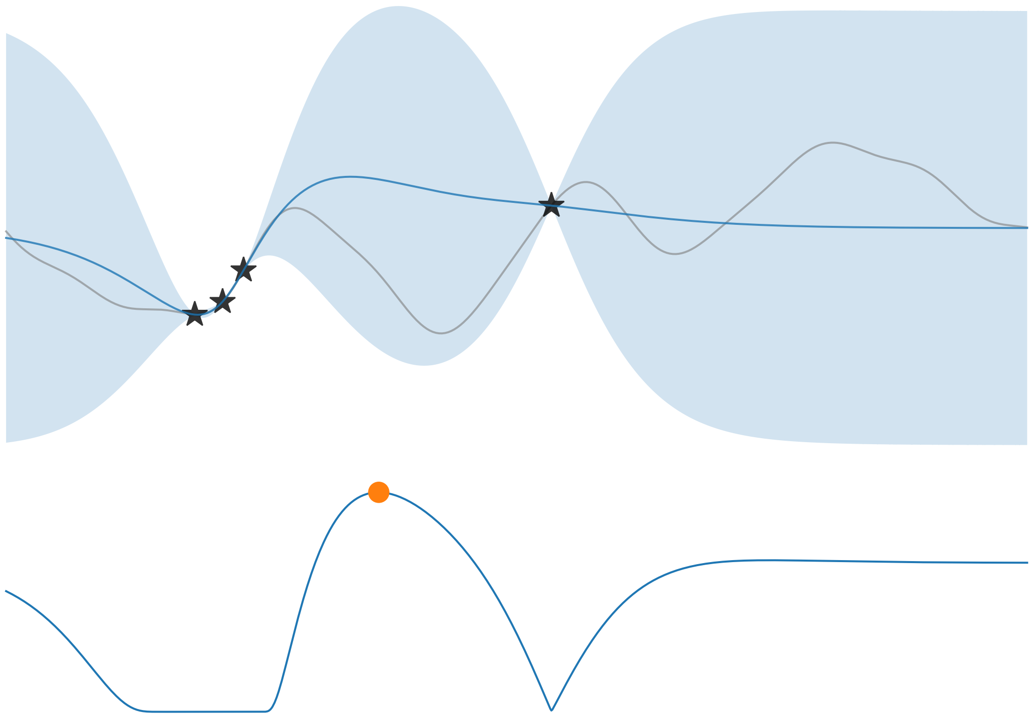
One-step approximation to MDP

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

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  - Max-value Entropy Search
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Approaches to Bayesian Optimization

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- Our work: Gittins Index

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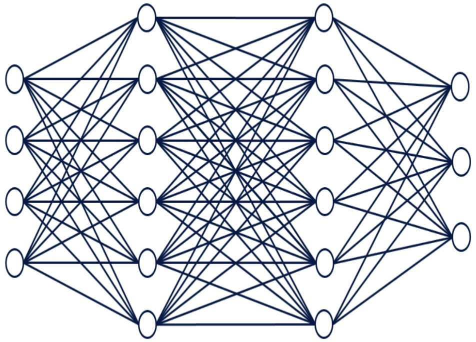
Why another approach?

Challenge: Varying Evaluation Costs

Hyperparameter tuning:

Training parameters →  → Accuracy

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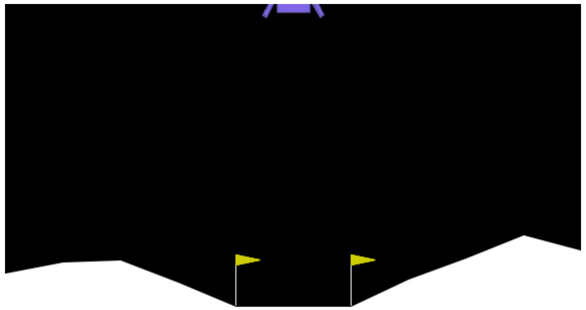
Control parameters →  → Reward

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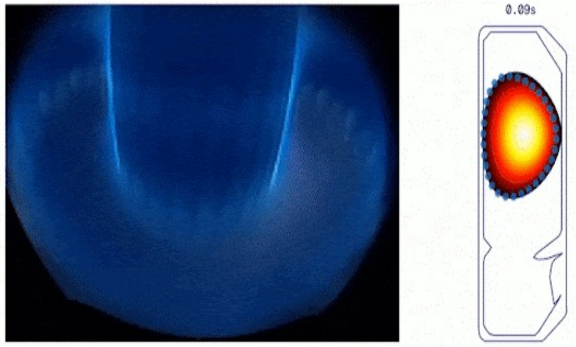
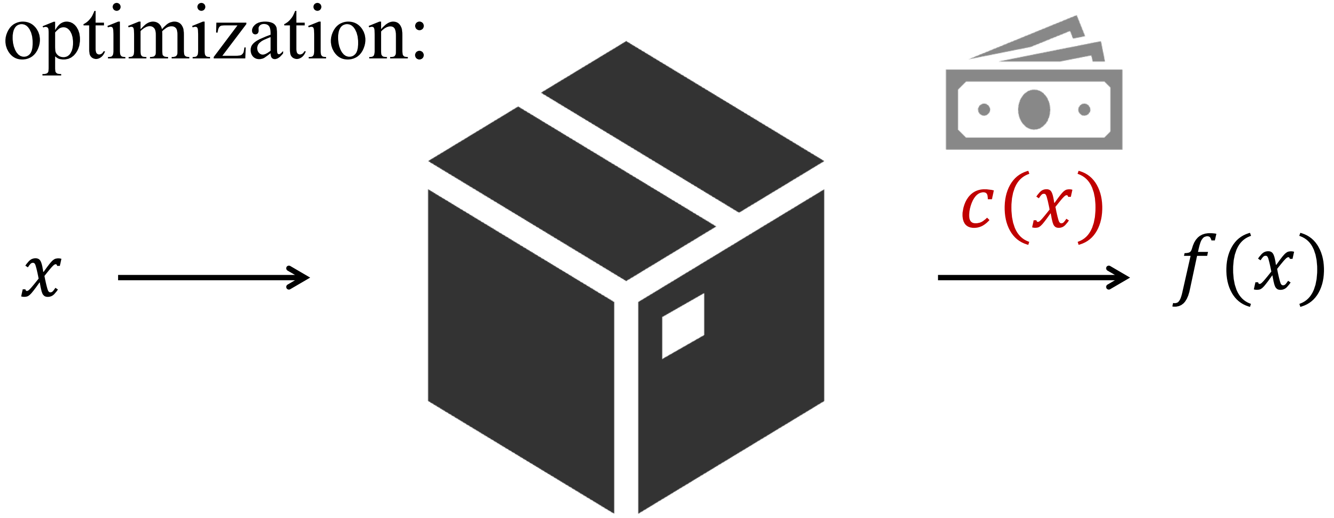
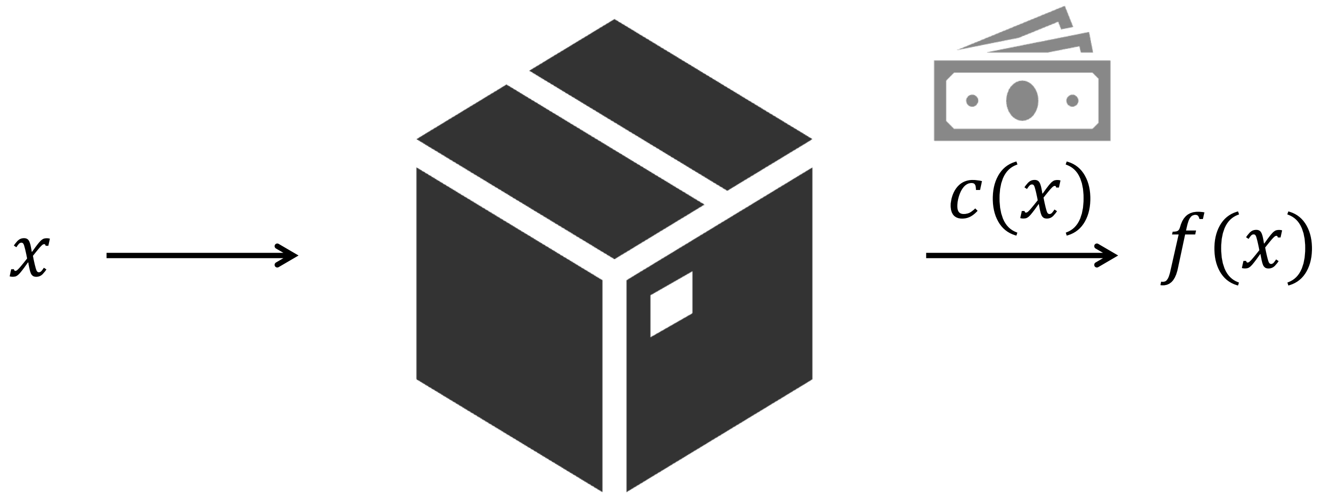
Reactor parameters →  → Stability

Challenge: Varying Evaluation Costs

Black-box optimization:



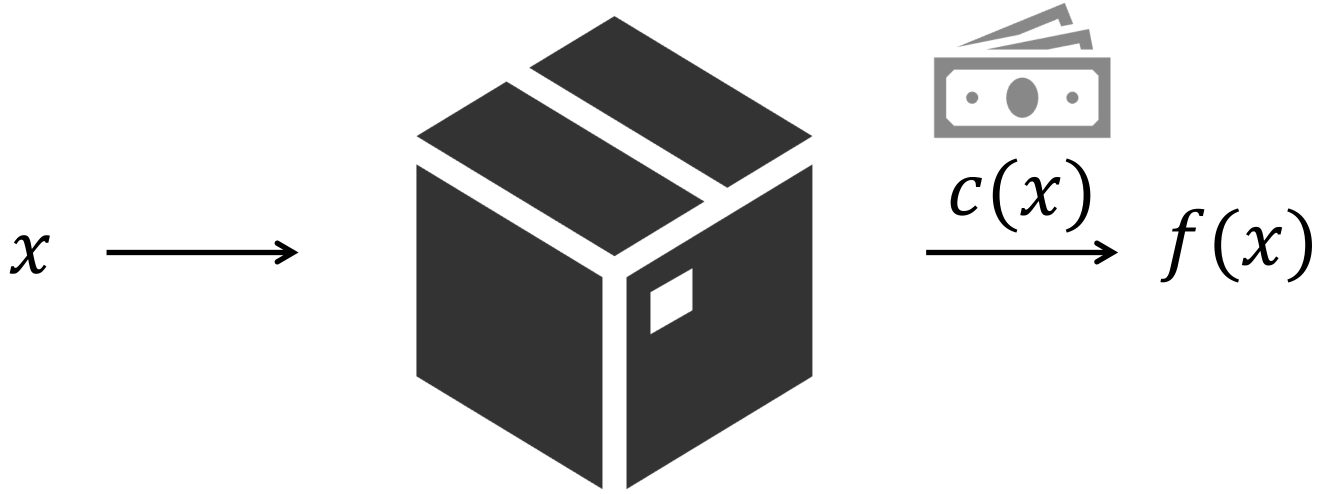
Challenge: Varying Evaluation Costs



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

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

Cost-aware Bayesian Optimization



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[Lee, Perrone, Archambeau, Seeger'21]

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

Cost-aware Bayesian Optimization

Uniform costs

Expected improvement

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

Varying costs

Cost-aware Bayesian Optimization

Uniform costs

Expected improvement

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

Varying costs

Expected improvement per cost

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

Cost-aware Bayesian Optimization

Uniform costs

Expected improvement

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

Varying costs

Expected improvement per cost

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Why divide?

Cost-aware Bayesian Optimization

Uniform costs

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Varying costs

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

Why divide?

Our view: lack of a guidance to incorporate costs

Cost-aware Bayesian Optimization

Uniform costs	Varying costs
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

Expected improvement

Multi-step Lookahead EI

Varying costs

Expected improvement per cost

Budgeted Multi-step Lookahead EI

slow

Cost-aware Bayesian Optimization

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

Cost-aware Bayesian Optimization

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

New design principle: Gittins Index

Cost-aware Bayesian Optimization

Uniform costs	Varying costs
Expected improvement	Expected improvement per cost
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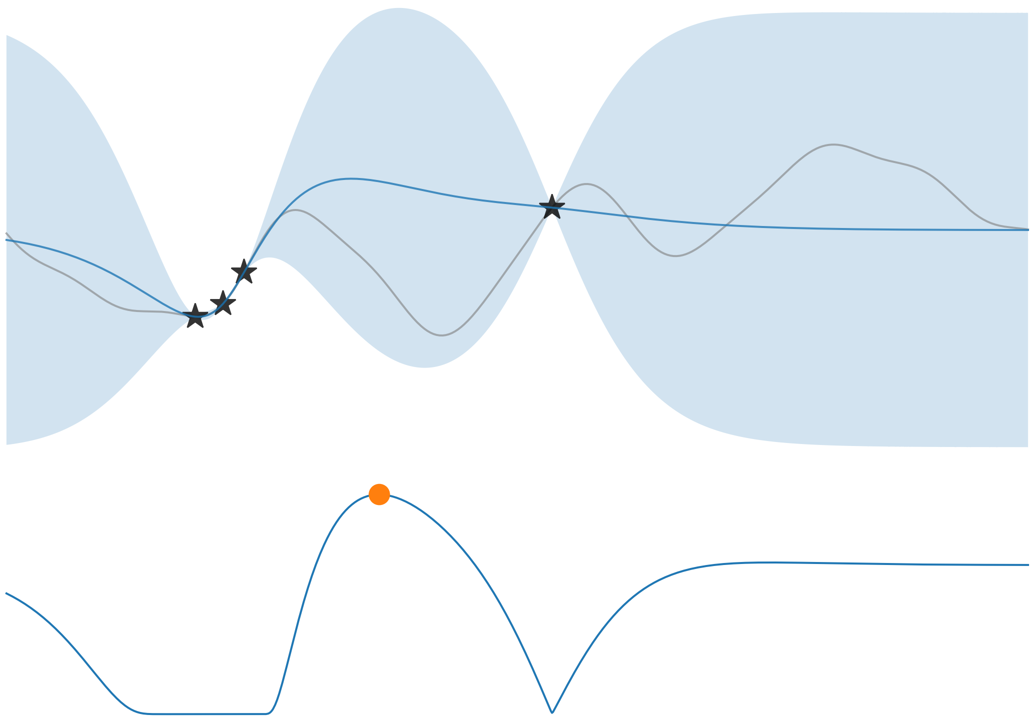
⋮	⋮

New design principle: Gittins Index

Cost-aware

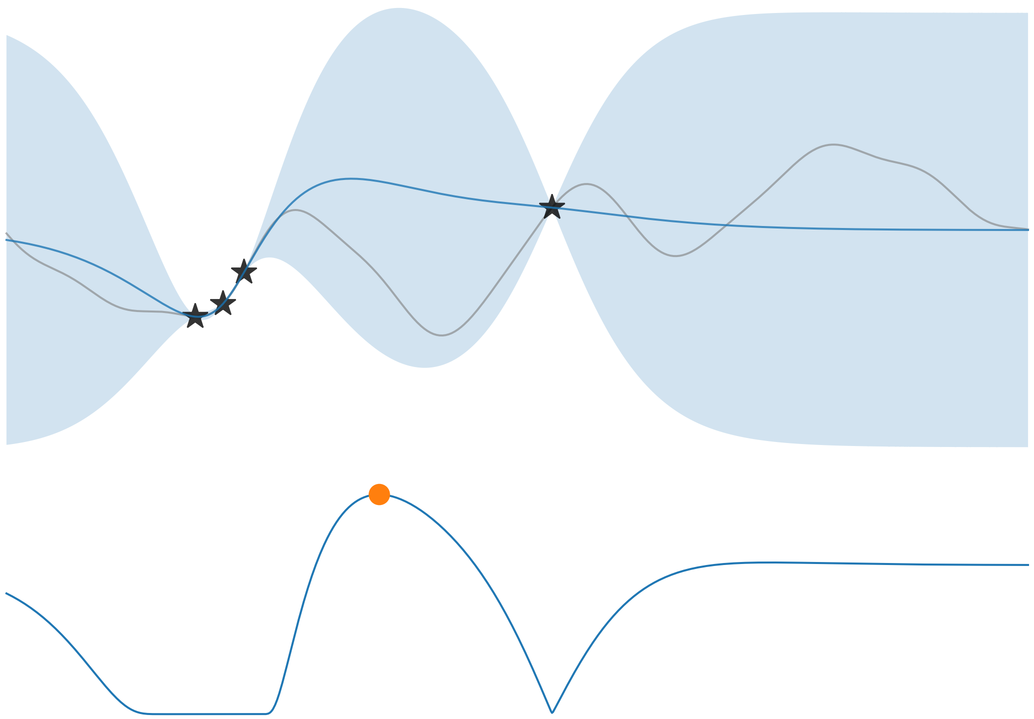
Expected Improvement



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

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

Expected Improvement



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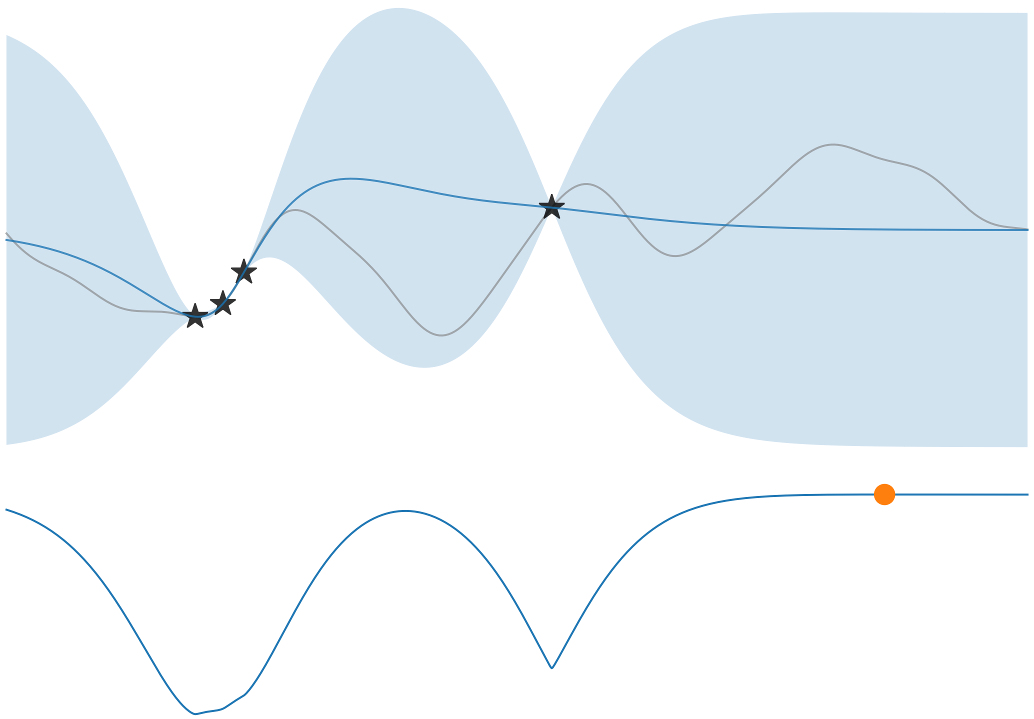
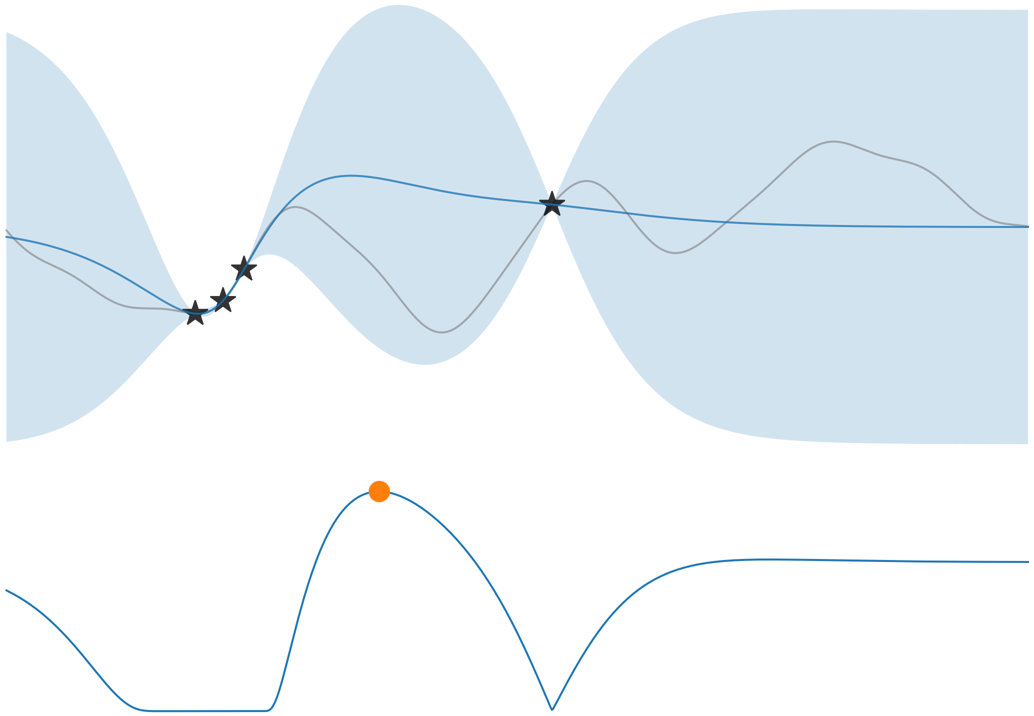
Gittins Index



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

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

Expected Improvement



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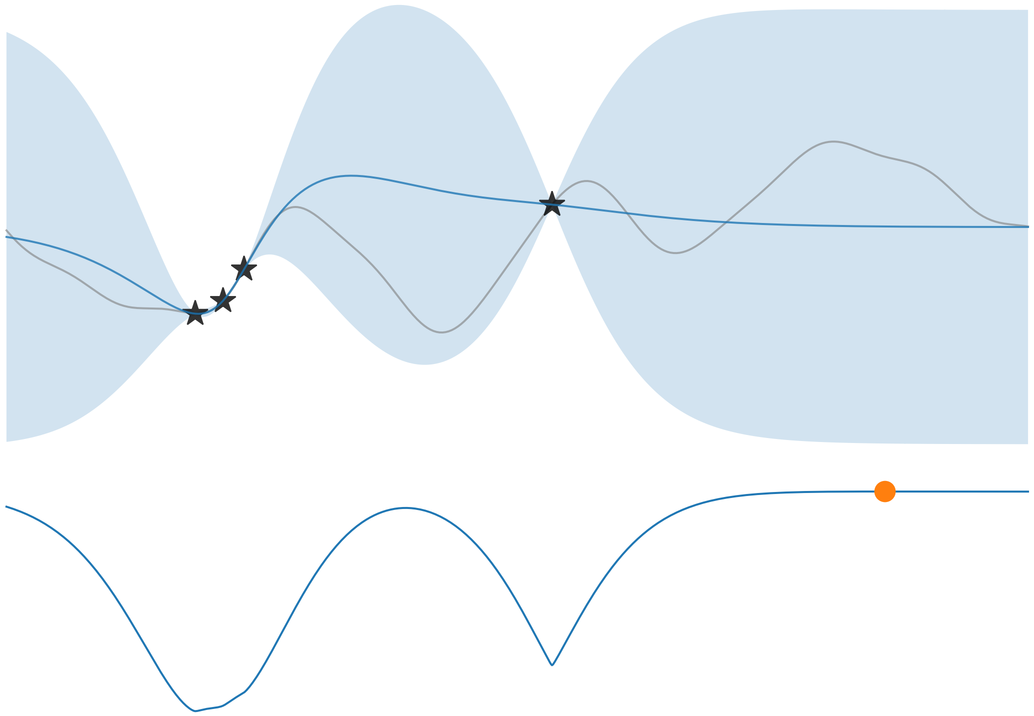
One-step approximation to MDP

Gittins Index



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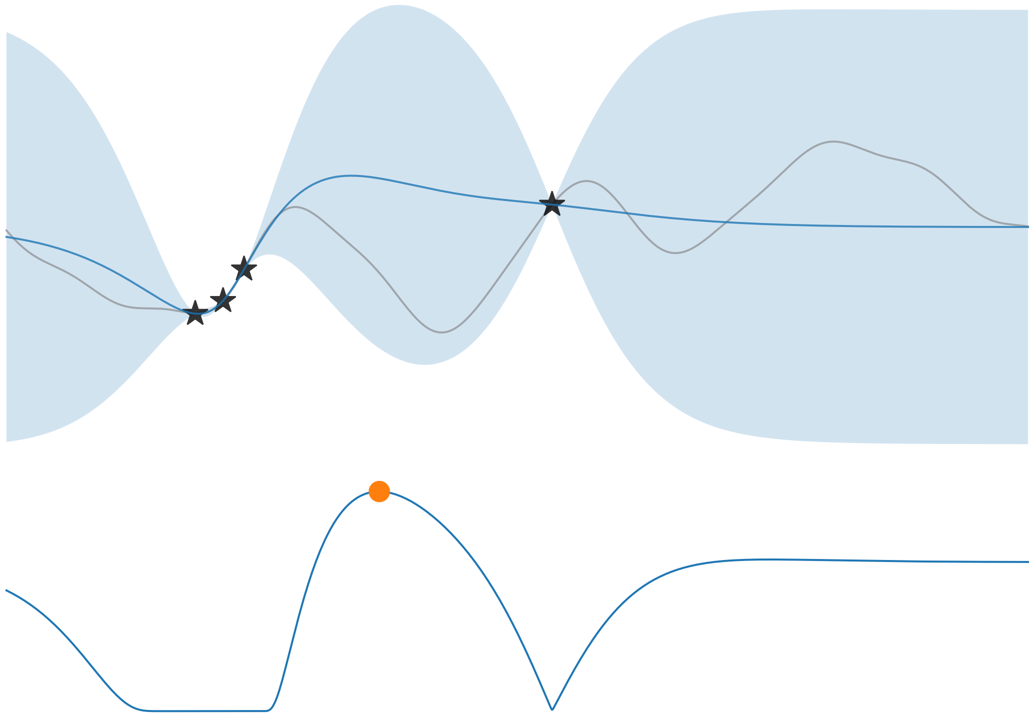

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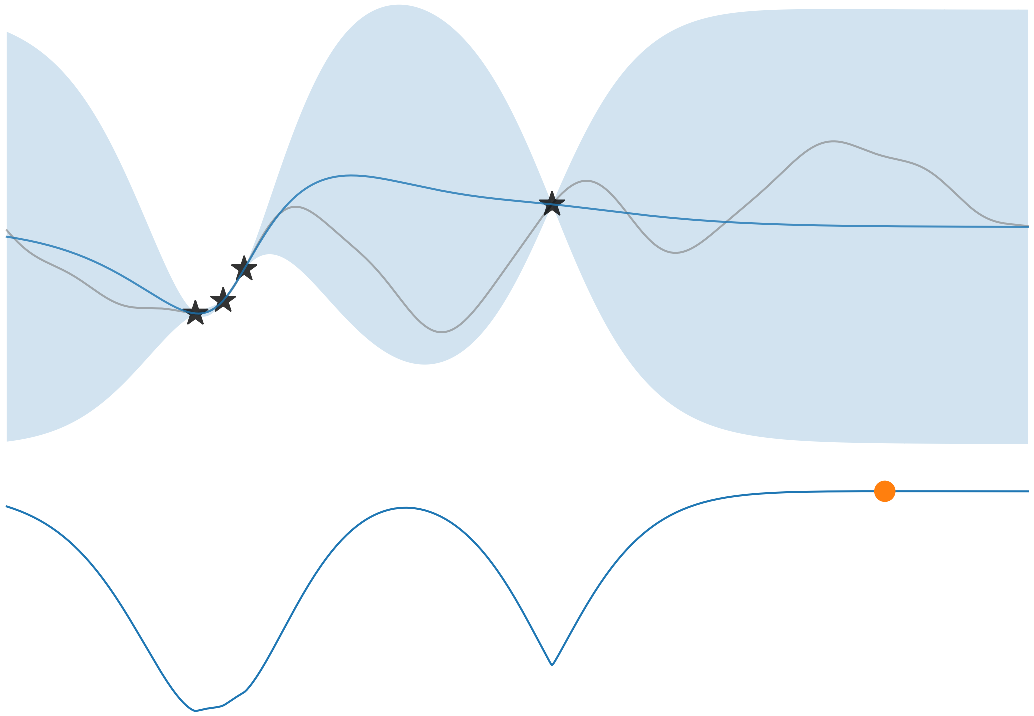
Temporal simplification to MDP

Gittins Index



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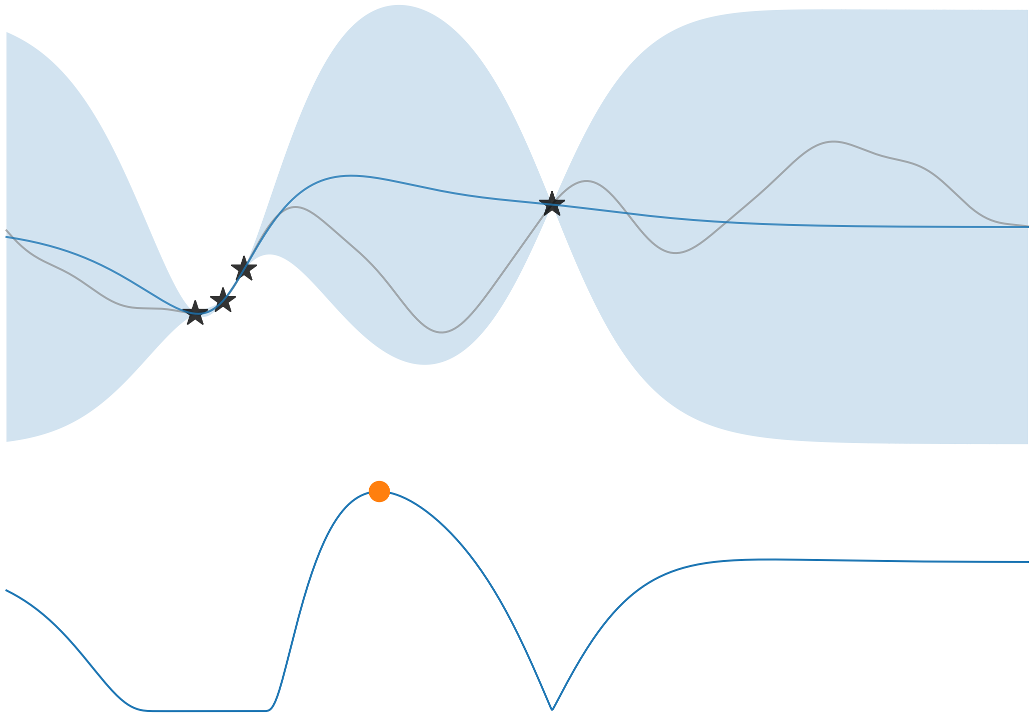
Expected Improvement



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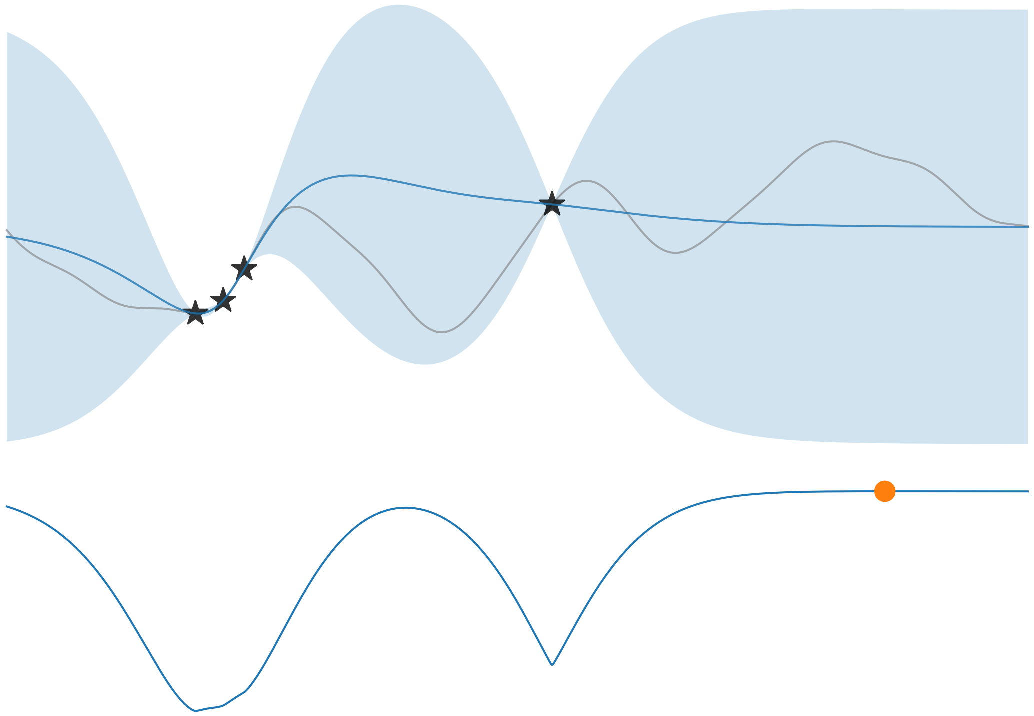
Temporal simplification to MDP

Gittins Index

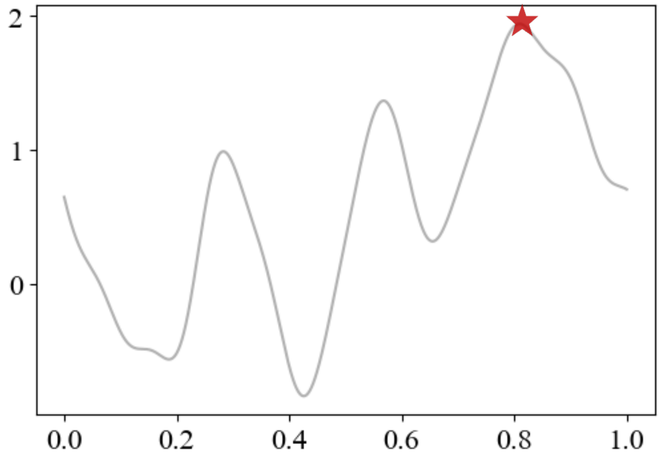


$$\mathrm{GI}_{f|D}(x) = g \text{ s.t. } \mathrm{EI}_{f|D}(x; g) = c(x)$$

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

Spatial simplification to MDP

Our Approach: Spatial Simplification

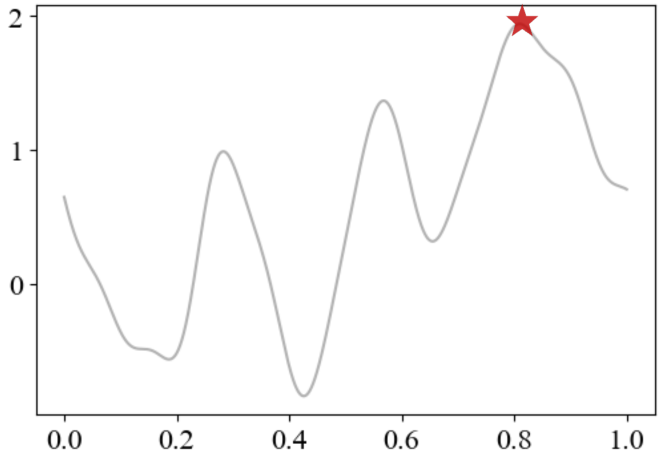


Bayesian Optimization

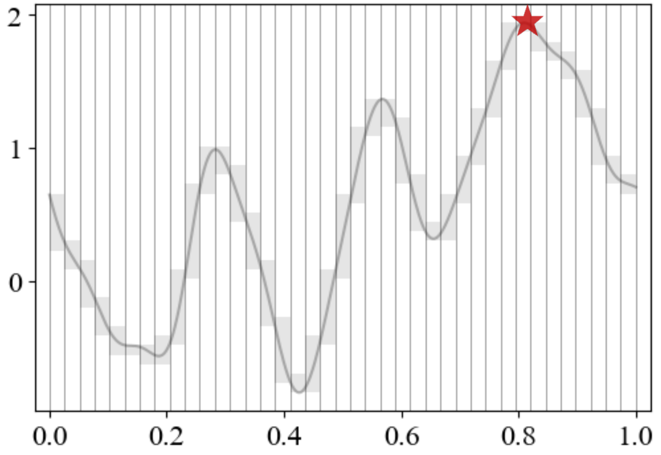
Continuous

Correlated

Our Approach: Spatial Simplification



$\Longrightarrow$

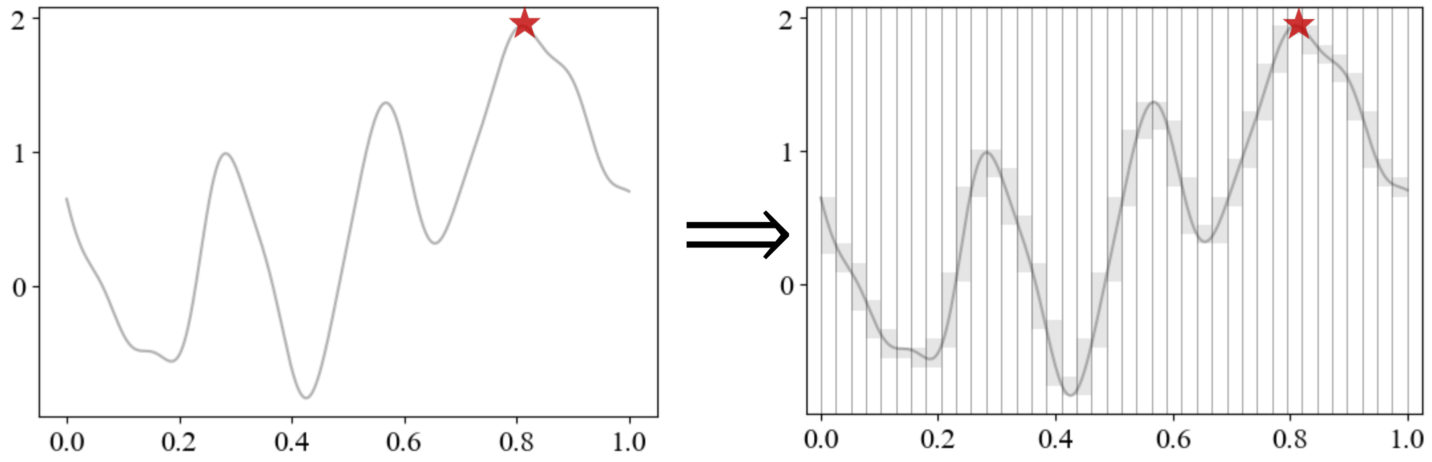


Bayesian Optimization

Continuous $\Longrightarrow$ Discrete

Correlated

Our Approach: Spatial Simplification



Bayesian Optimization

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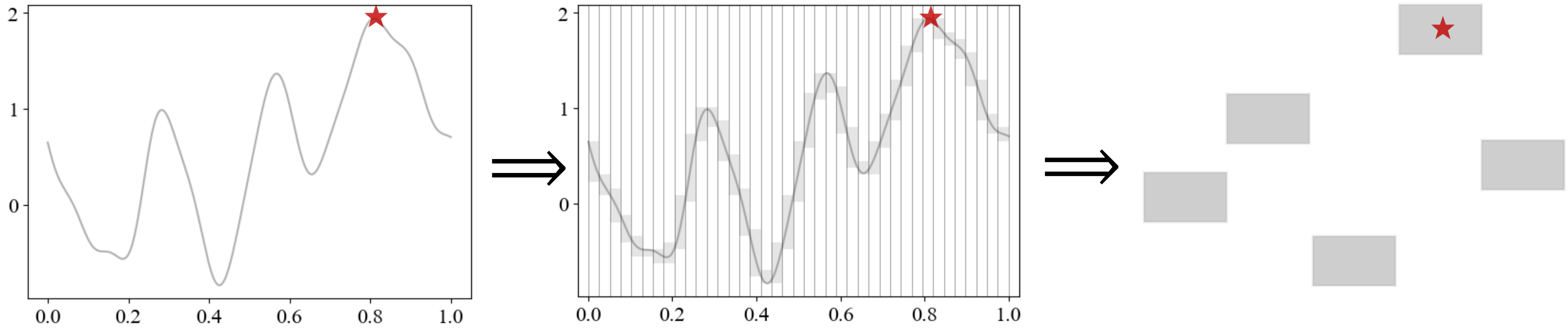
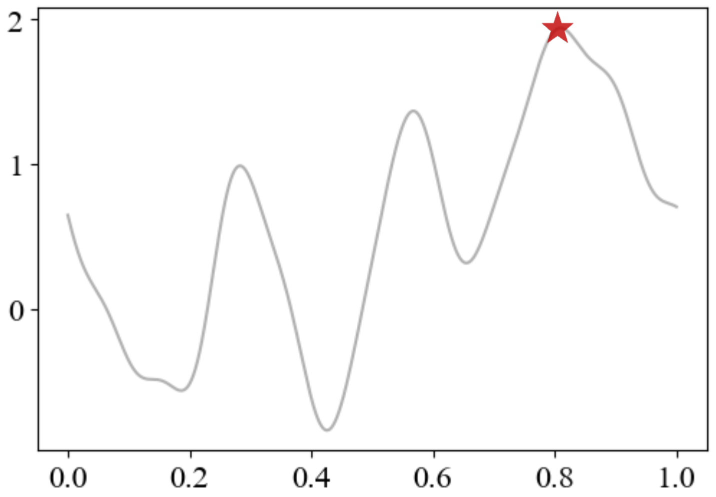


Bayesian Optimization

Continuous ⟹ Discrete

Correlated ⟹ Independent

Our Approach: Spatial Simplification



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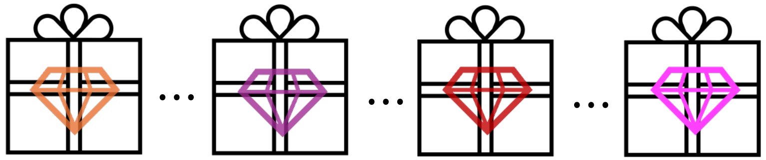


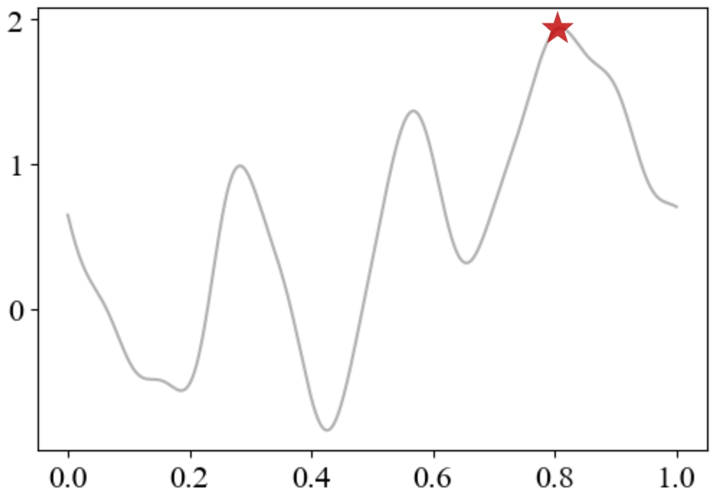
Bayesian Optimization

Pandora's Box [Weitzman'79]

Continuous $\Longrightarrow$ Discrete

Correlated $\Longrightarrow$ Independent

Our Approach: Spatial Simplification



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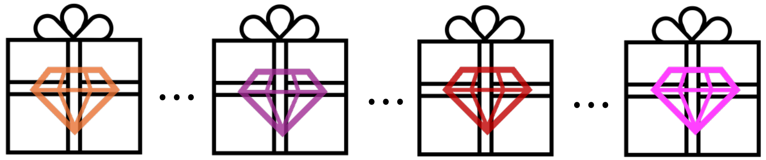


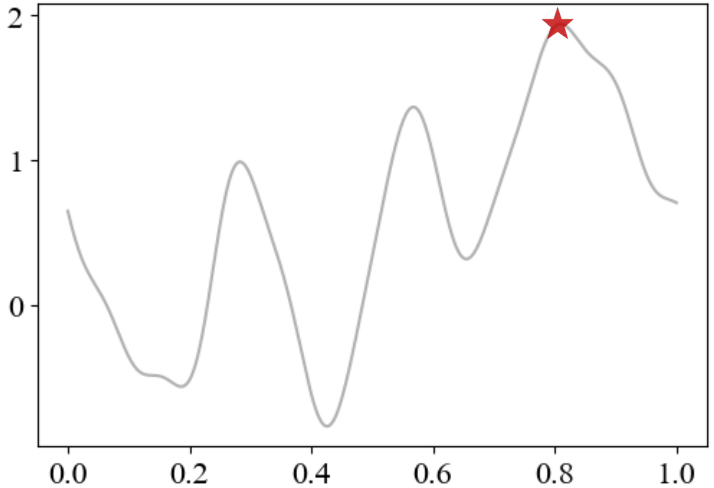
Bayesian Optimization

Pandora's Box [Weitzman'79]

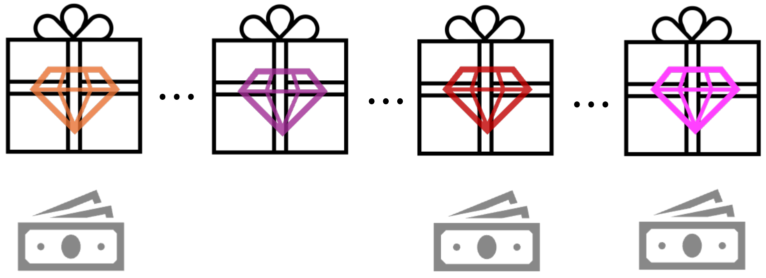
Continuous	$\Longrightarrow$	Discrete
Correlated	$\Longrightarrow$	Independent

Optimal policy: Gittins index

Our Approach: Spatial Simplification



⟹



Bayesian Optimization | Pandora's Box

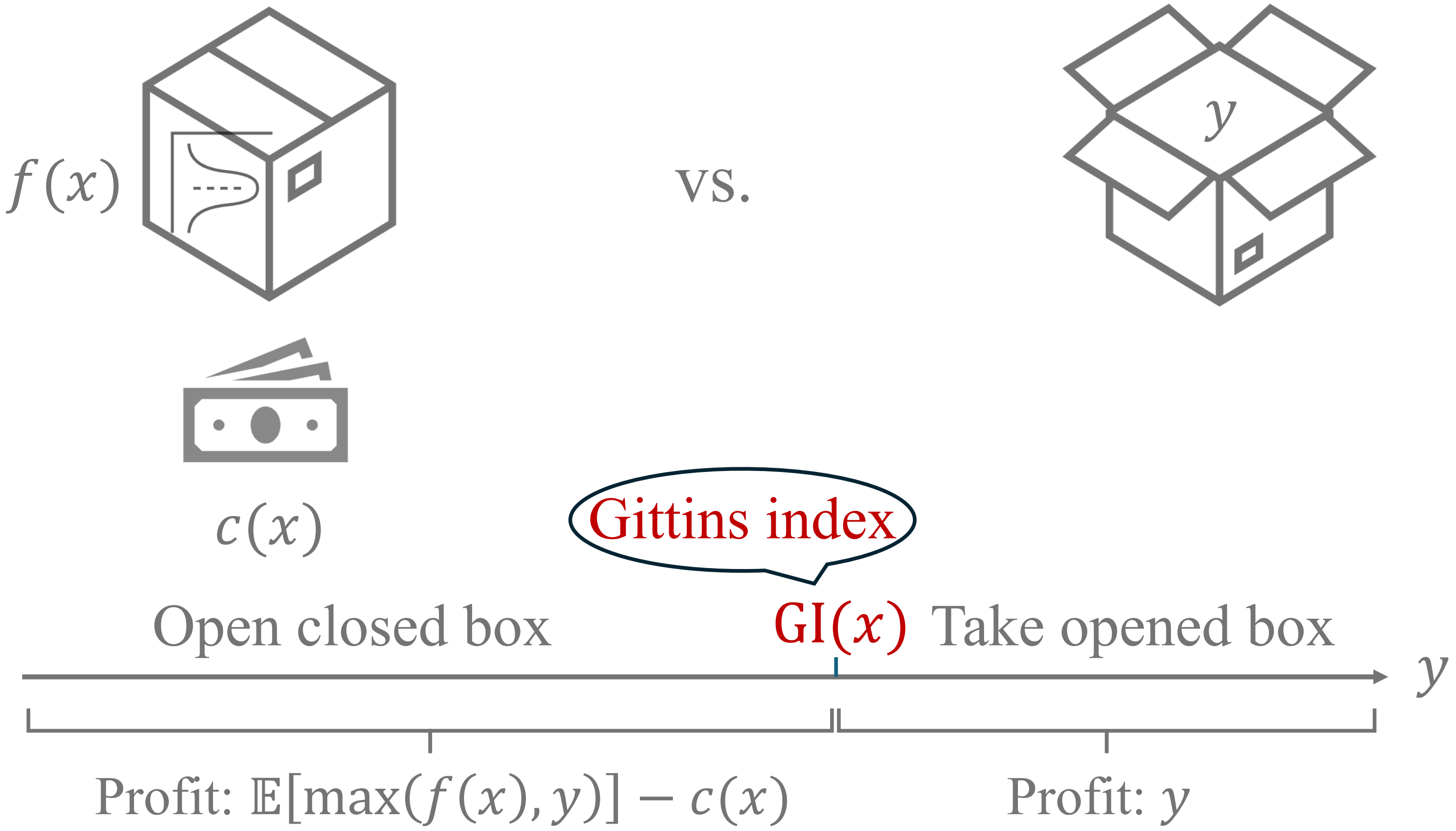
Continuous ⟹ Discrete

allow varying costs

Correlated ⟹ Independent

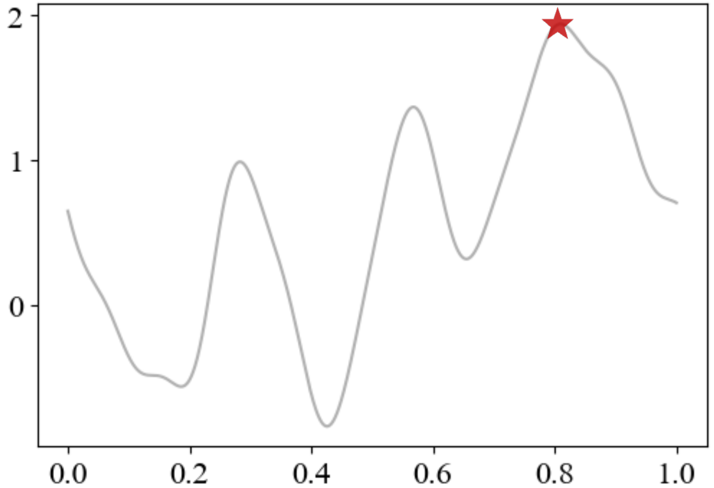
Optimal policy: Gittins index

Intuition Behind Pandora's Box Gittins Index

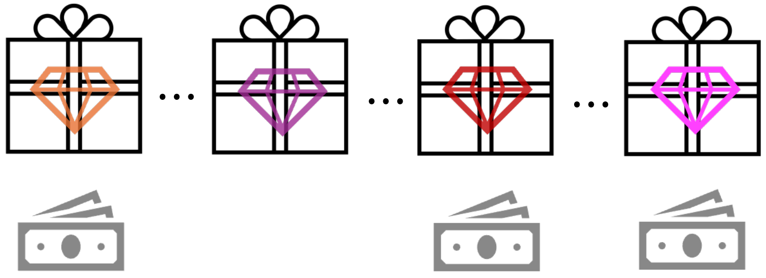


$\mathrm{GI}(x)$: solution y to $\mathbb{E}[\max(f(x), y)] - c(x) = y$

How to translate Gittins index?



$\Longrightarrow$



Bayesian Optimization | Pandora's Box

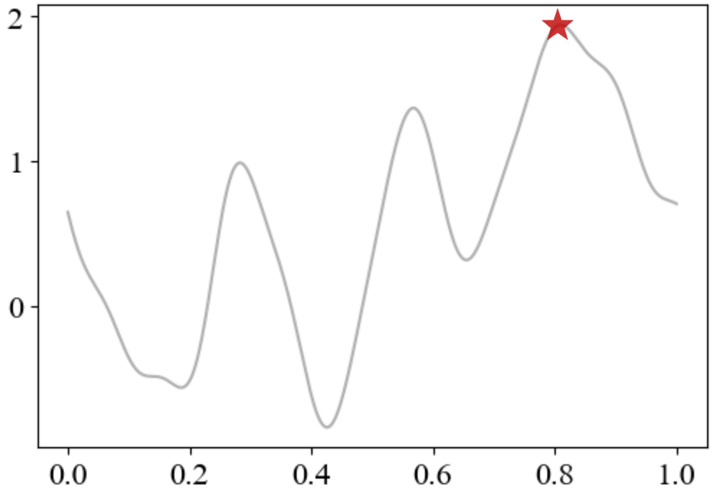
Continuous $\Longrightarrow$ Discrete

Correlated $\Longrightarrow$ Independent

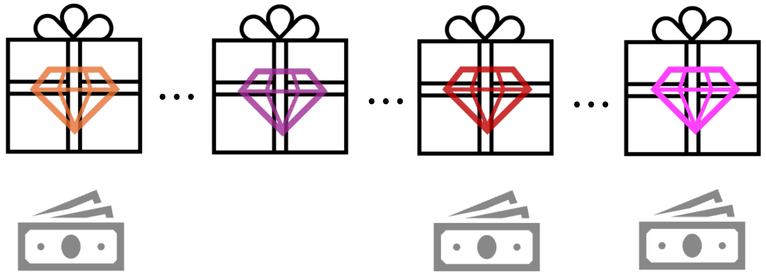
How to translate?

$\Longleftarrow$ Optimal policy: Gittins index

How to translate Gittins index?



$\Longrightarrow$



Bayesian Optimization

Pandora's Box

Continuous $\Longrightarrow$ Discrete

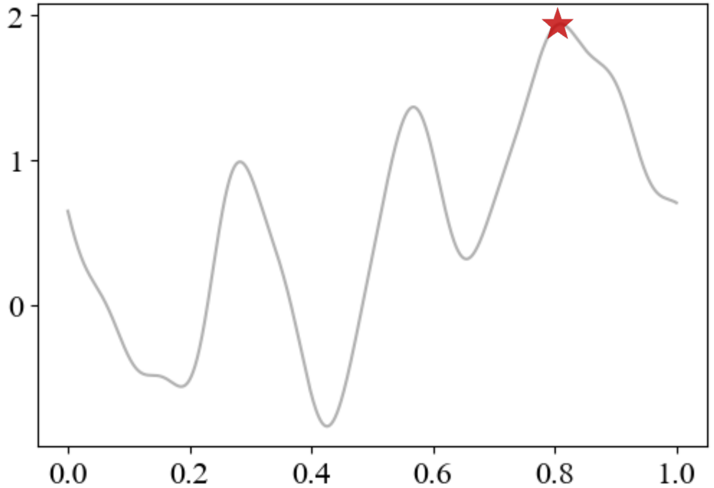
Correlated $\Longrightarrow$ Independent

incorporate posterior

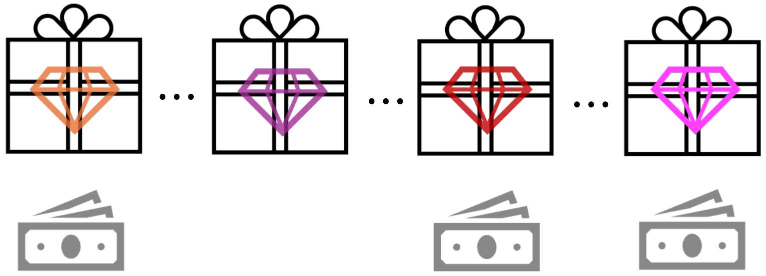
Our policy $\Longleftarrow$ Optimal policy: Gittins index

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

Is Gittins good in Bayesian optimization?



$\Longrightarrow$



Bayesian Optimization		Pandora's Box [Weitzman'79]
Continuous	$\Longrightarrow$	Discrete
Correlated	$\Longrightarrow$	Independent
Is Gittins index good? $\max_x \mathrm{GI}_{f\mid D}(x)$	$\Longleftarrow$	Gittins index is optimal $\max_x \mathrm{GI}(x)$

Experiment Setup: Objective Functions

Synthetic

Samples from prior

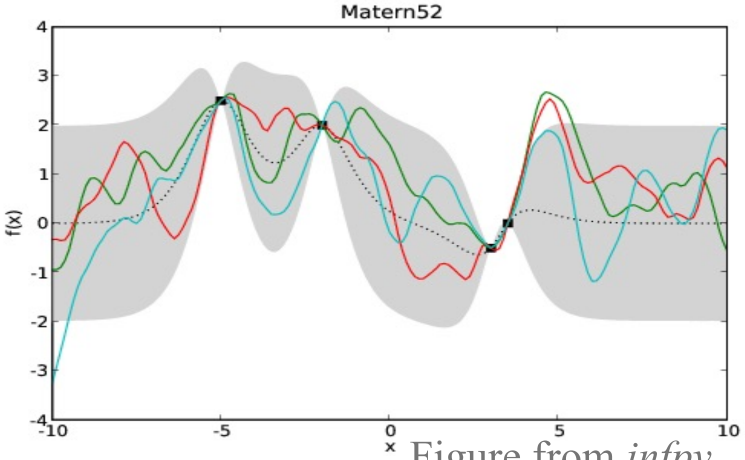


Figure from *infpy*

Ackley function

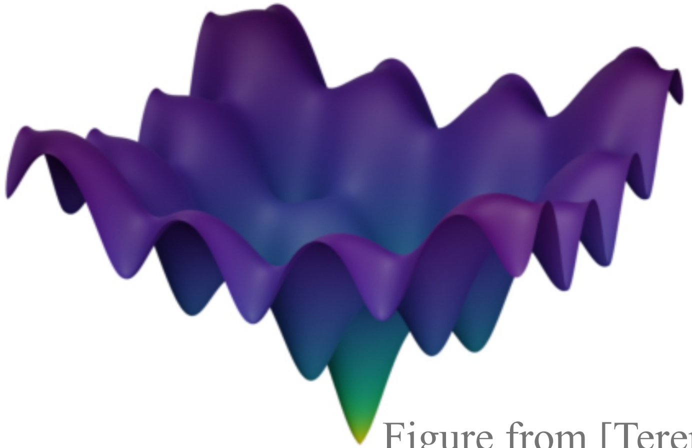


Figure from [Terenin'22]

Empirical

Pest Control

Figure from ChatGPT

Lunar Lander

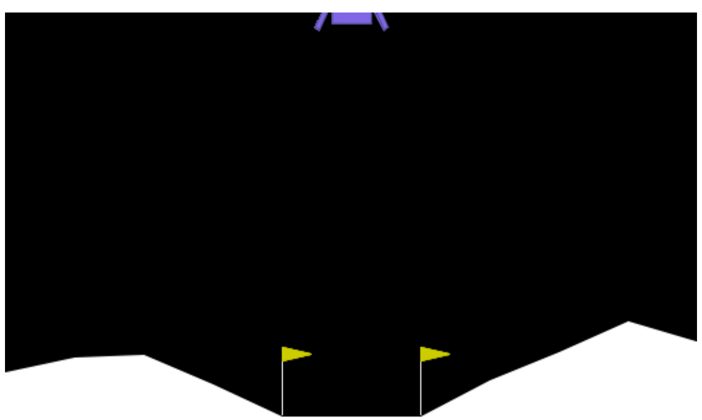
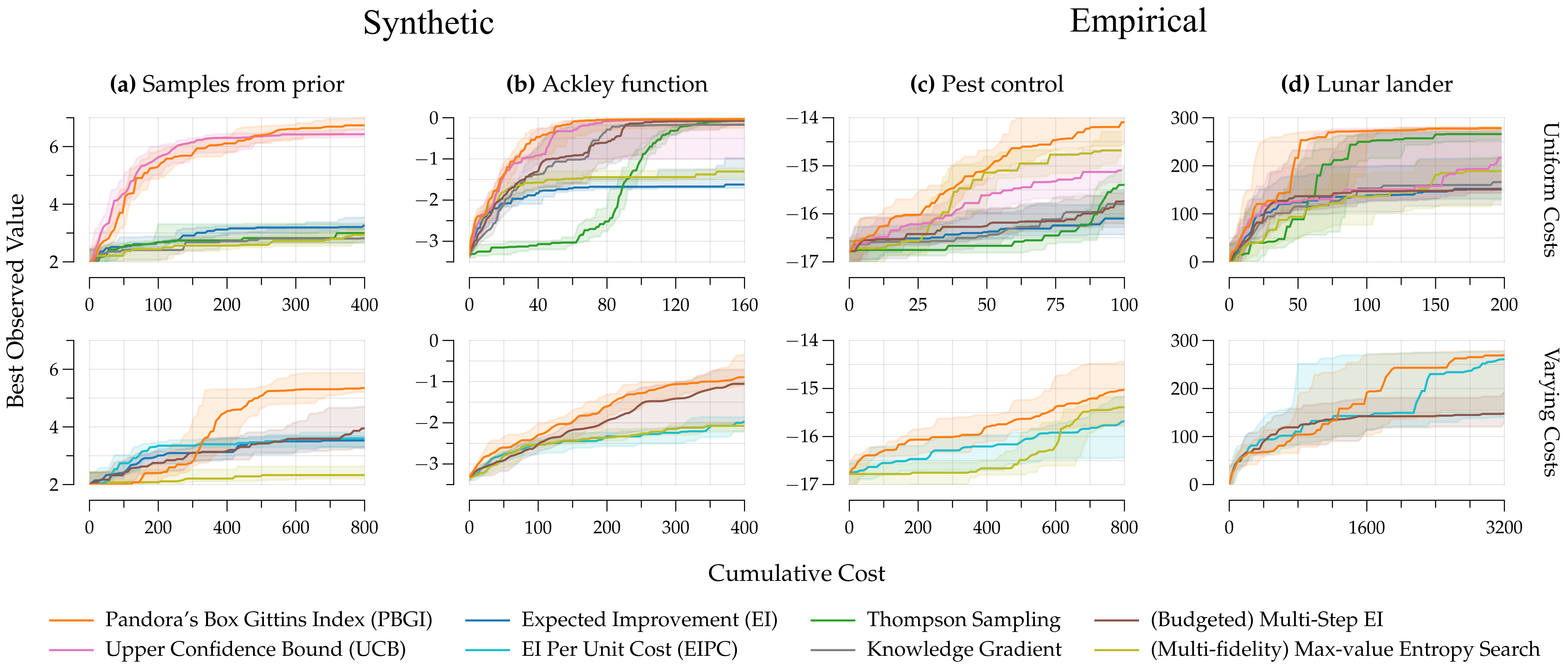


Figure from OpenAI Gym

Experiment results



FAQ

- Easy-to-compute?

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  Yes, EI + bisection

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- Any theoretical results?

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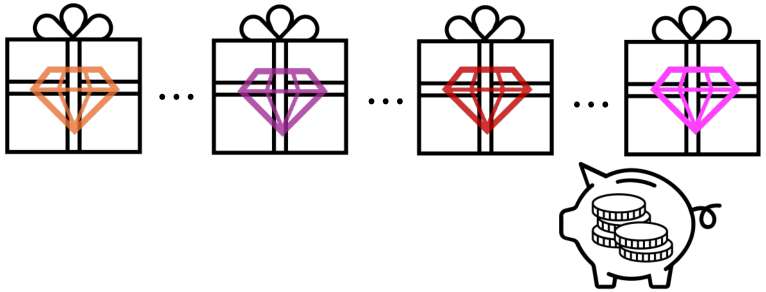
  Yes, expected-budget-constrained ≅ cost-per-sample

Theoretical Result

max best observed under budget

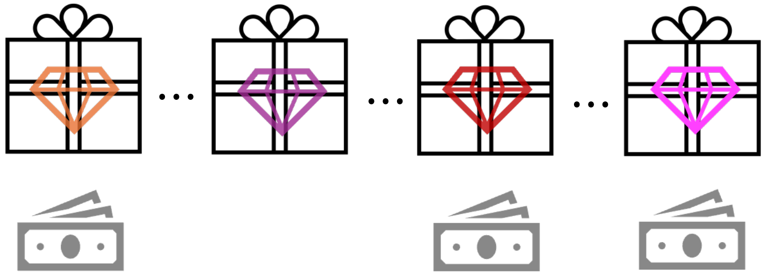


Budgeted Pandora's Box

Expected budget constraint

Optimal policy?

max (best observed – costs)



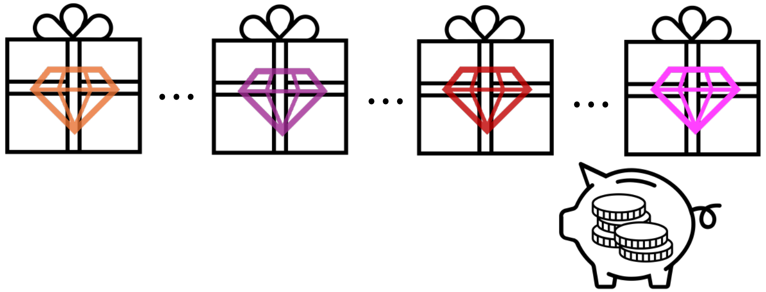
Pandora's Box

Cost per sample

Optimal policy: Gittins index

Theoretical Result

max best observed under budget



Budgeted Pandora’s Box

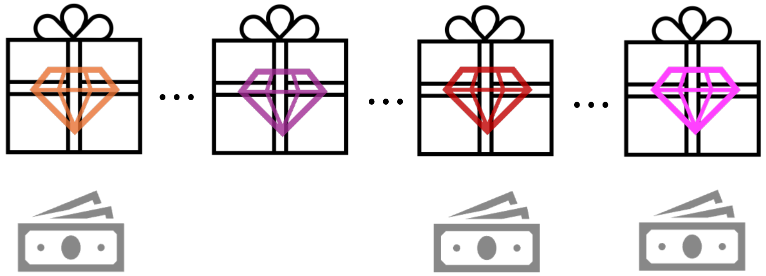
Expected budget constraint

Optimal policy ✓

extension to [Aminian, Manshadi, Niazadeh’24]

$\Longleftarrow$

max (best observed – scaled costs)



Pandora’s Box

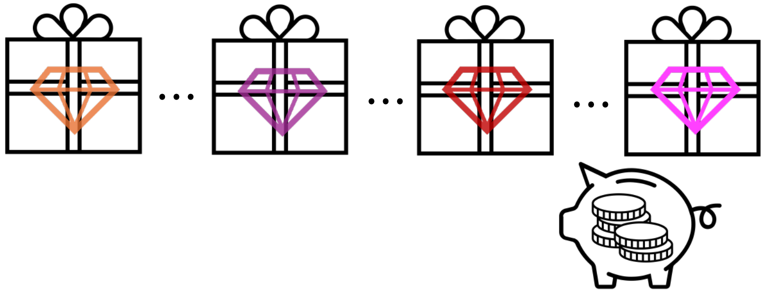
Cost per sample

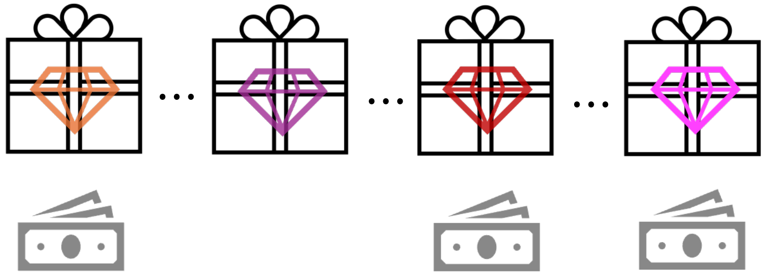
Optimal policy: Gittins index

Theoretical Result

budget-dependent

max best observed under budget ⇐ **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]

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- Easy-to-compute?

  Yes, EI + bisection

- Any theoretical results?

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- Tuning parameters?

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  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

  linked to Pandora's box and Gittins index theory
- Impact

  competitive performance
- Future potential

  multi-stage optimization with partial feedback

Check our NeurIPS'24 paper on ArXiv!