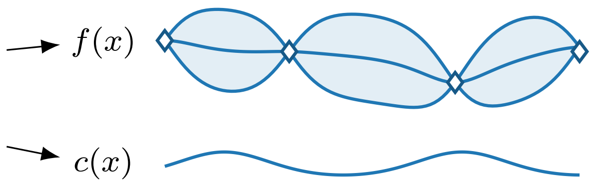
Cost-aware Bayesian Optimization via the Pandora's Box Gittins Index

Qian Xie,[1] Raul Astudillo,[2] Peter Frazier,[1] Ziv Scully,[1] and Alexander Terenin[1]
[1]Cornell University [2]Caltech

Abstract

Bayesian optimization is a technique for efficient global optimization of black-box unknown functions. In many practical settings, it is desirable to explicitly incorporate function evaluation costs into acquisition functions used for Bayesian optimization. To do so, we develop a connection between cost-aware Bayesian optimization and *Pandora's Box*, a decision problem from economics. The Pandora's Box problem admits a Bayesian-optimal solution based on an expression called the *Gittins index*, which can be reinterpreted as an acquisition function. We demonstrate empirically that this acquisition function performs well on cost-aware Bayesian optimization, particularly in medium-high dimensions. We further show that this performance carries over to classical Bayesian optimization without explicit evaluation costs. Our work constitutes a first step towards integrating techniques from Gittins index theory into Bayesian optimization.

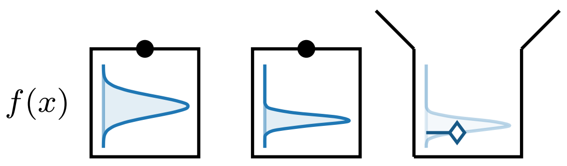
Cost-aware Bayesian Optimization



Expected-budget-constrained (EBC) Bayesian optimization:

$$\mathbb{E} \sup_{x \in X} f(x) - \mathbb{E} \max_{1 \le t \le T} f(x_t) \quad \text{subject to } \mathbb{E} \textstyle\sum_{t=1}^{T} c(x_t) \le B$$

Pandora's Box



Cost-per-sample (CPS) objective: $\mathbb{E} \max_{1 \le t \le T} f(x_t) - \mathbb{E} \sum_{t=1}^{T} c(x_t)$

Optimal policy (notation: $\mathrm{EI}_\psi(x; y) = \mathbb{E} \max(0, \psi(x) - y)$):

$\alpha^\star(x) = g$ where g solves $\mathrm{EI}_f(x; g) = c(x)$

Our work: EBC and CPS problems are equivalent
(extends prior work on generalized Pandora's boxes to continuous rewards)

Key difference from Bayesian optimization: no correlations

Pandora's Box Gittins Index: a new acquisition function

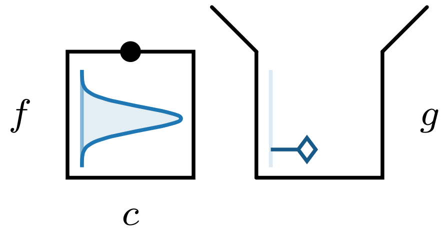
$\alpha_t^{\mathrm{PBGI}}(x) = g$ where g solves $\mathrm{EI}_{f \mid x_{1:t}, y_{1:t}}(x; g) = \lambda c(x)$

Idea: extend $\alpha^\star$ by plugging posterior in for f
λ: cost scaling factor from budget-constraint Lagrangian duality
Computation: one-dimensional convex optimization

Where does α_t^{PBGI} come from?

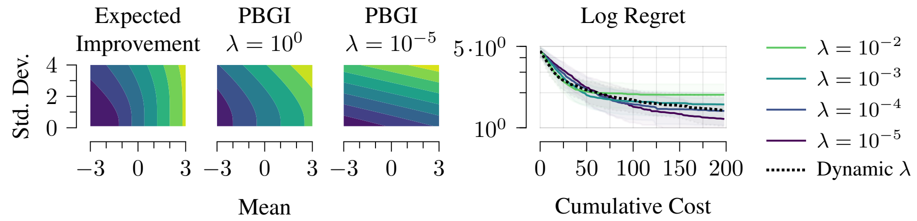
Simplified problem: one closed and one open box

Policy	Value
Open box	$\mathbb{E} \max(f, g) - c$
Don't open	g

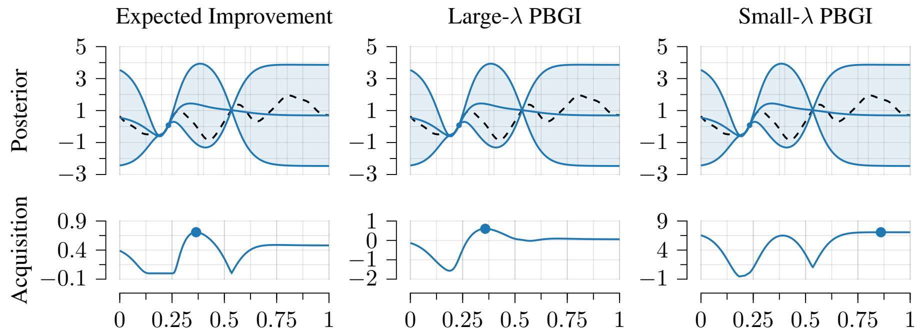


Should one open the closed box? Depends on g!
If *both* opening and not opening is optimal: g is a *fair value*
α_t^{PBGI}: pick points according to their fair values

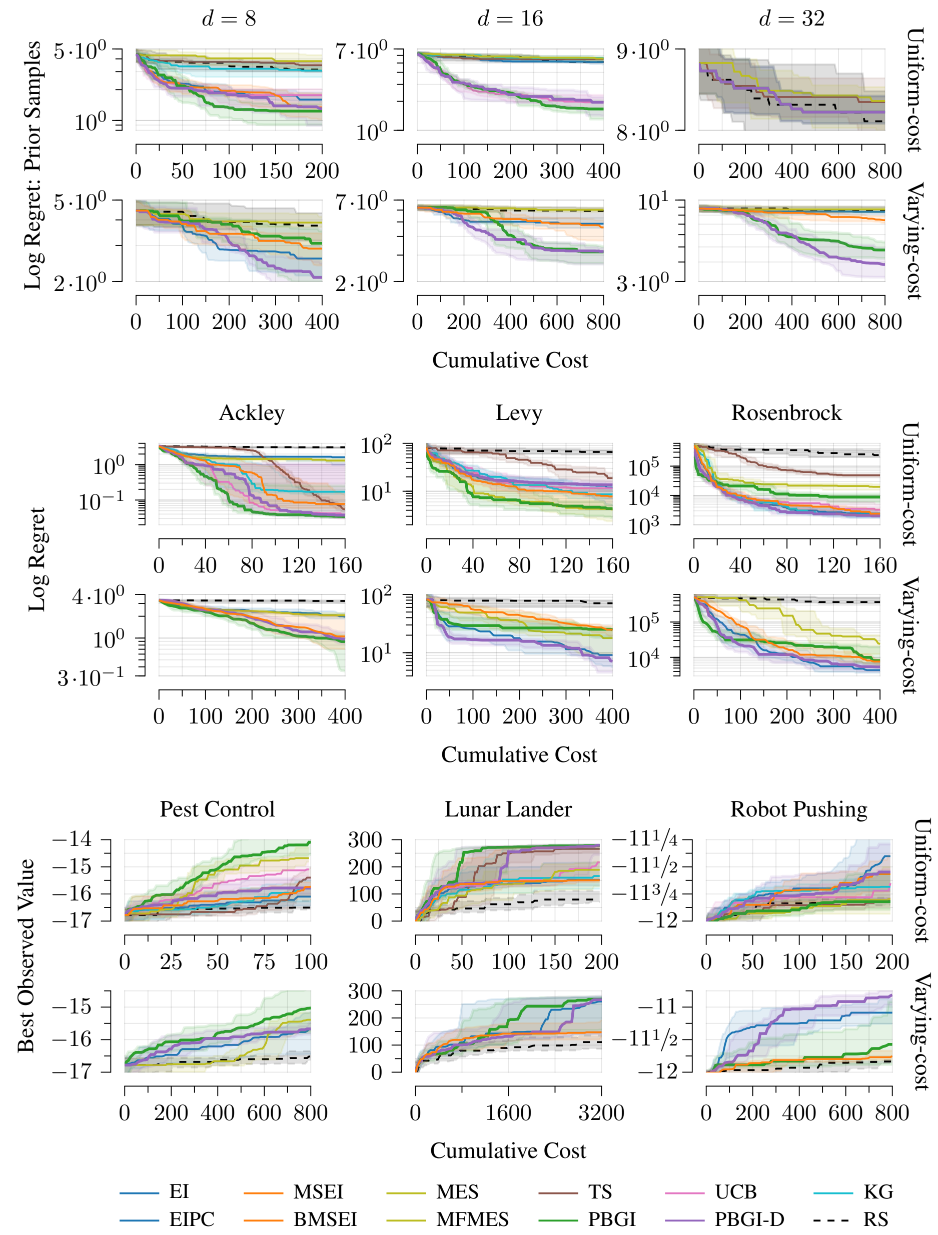
Behavior and Comparisons



Large λ: similar to α_t^{EI} Small λ: similar to α_t^{UCB}



Performance



Computation Time