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

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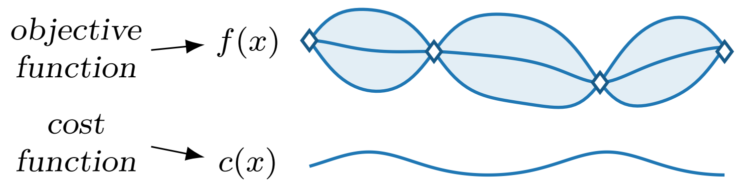
Abstract

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.

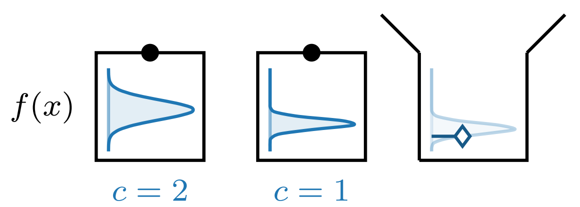
Cost-aware Bayesian Optimization



Expected-budget-constrained (EBC) Bayesian optimization:

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

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

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

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

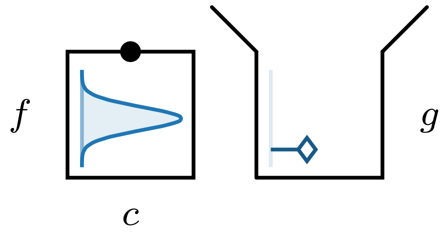
$$\alpha_t^{\mathrm{PBGI}}(x) = g \qquad \text{where } g \text{ solves} \qquad \mathrm{EI}_{f\mid x_{1:t},y_{1:t}}(x;g) = \lambda c(x)$$

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?

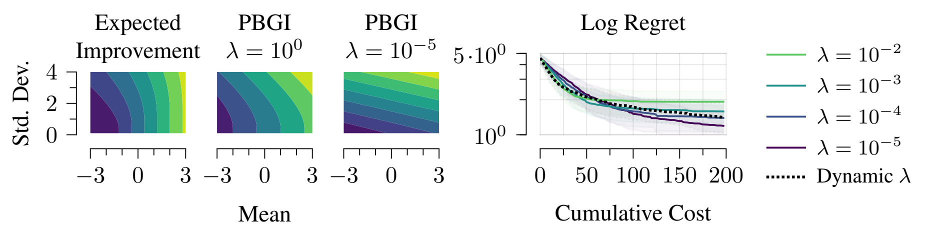
Simplified problem: one closed and one open box

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

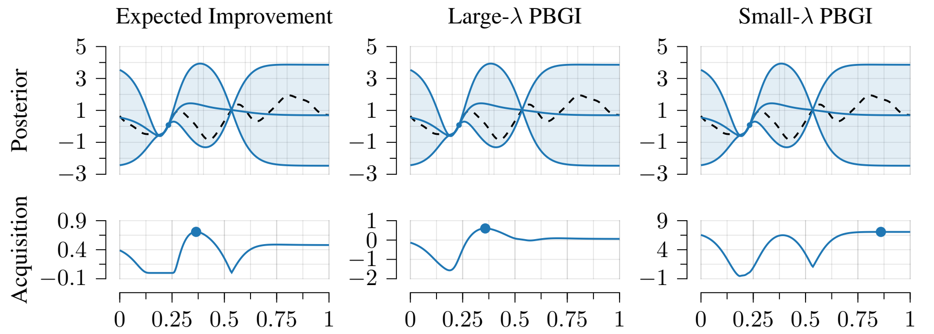


Should one open the closed box? Depends on the observed value g!
If *both* opening and not opening are optimal: g is a *fair value*
α_t^{PBGI}: pick points according to their fair values

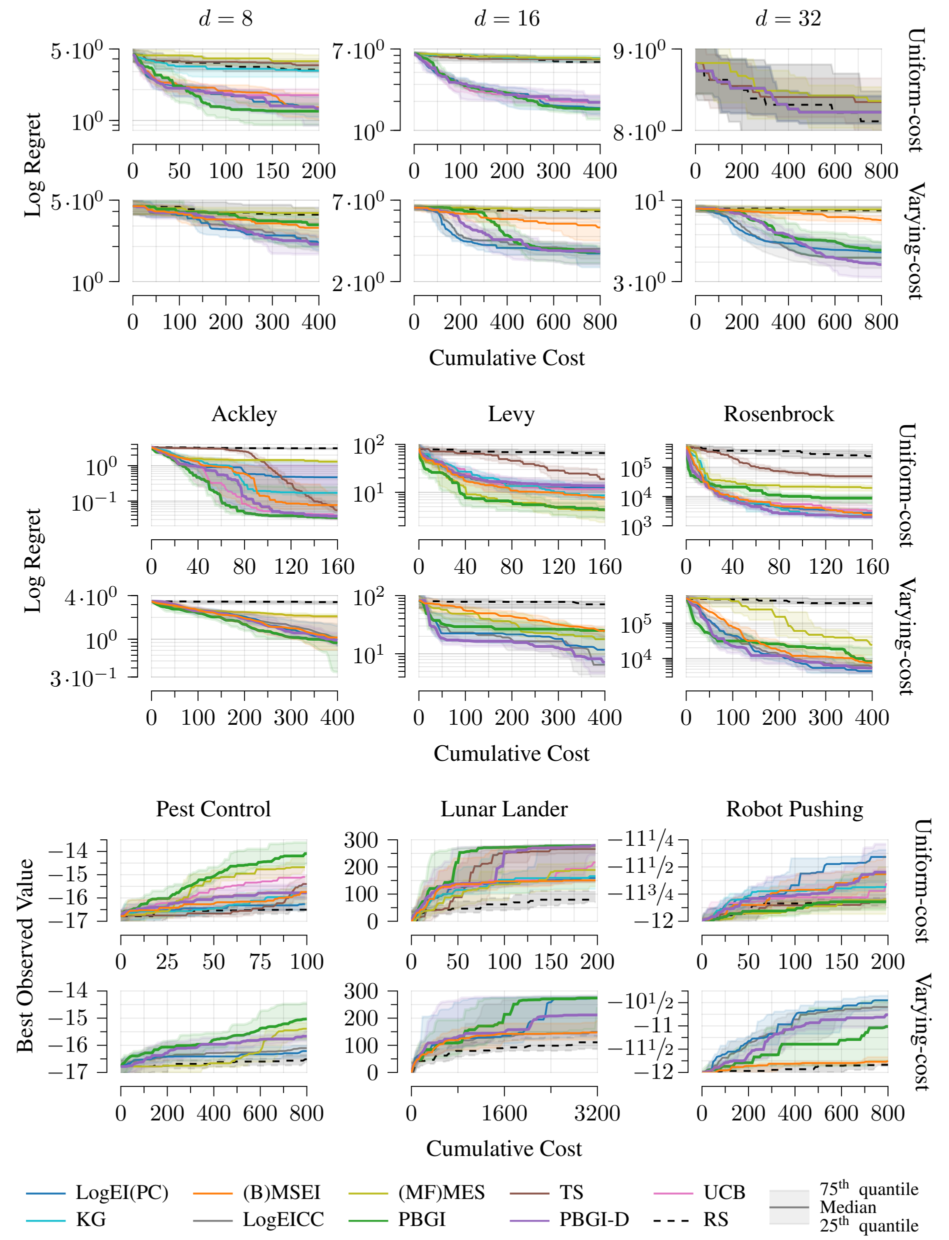
Behavior and Comparisons



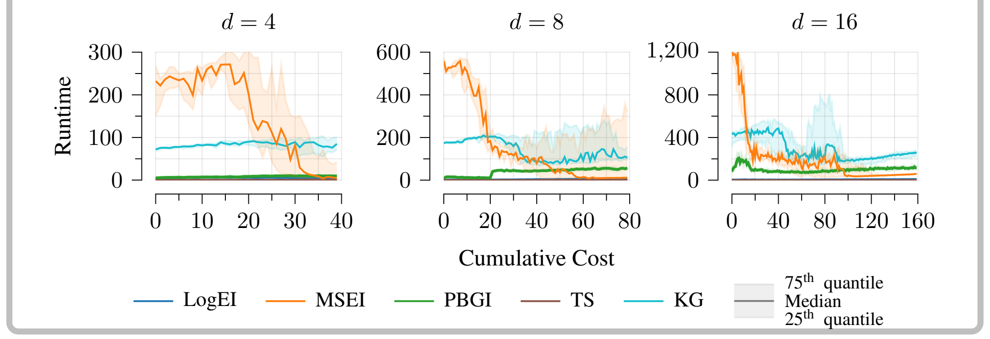
Large λ: similar to α_t^{EI} Small λ: similar to α_t^{UCB}



Performance



Computation Time



Cost-aware Stopping for Bayesian Optimization

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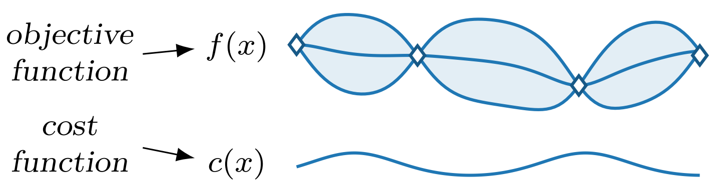
Abstract

In automated machine learning, scientific discovery, and other applications of Bayesian optimization, deciding when to stop evaluating expensive black-box functions is an important practical consideration. While several adaptive stopping rules have been proposed, in the cost-aware setting they lack guarantees ensuring they stop before incurring excessive function evaluation costs. We propose a *cost-aware stopping rule* for Bayesian optimization that adapts to varying evaluation costs and is free of heuristic tuning. Our rule is grounded in a theoretical connection to state-of-the-art cost-aware acquisition functions, namely the Pandora's Box Gittins Index (PBGI) and log expected improvement per cost. We prove a theoretical guarantee bounding the expected cumulative evaluation cost incurred by our stopping rule when paired with these two acquisition functions. In experiments on synthetic and empirical tasks, including hyperparameter optimization and neural architecture size search, we show that combining our stopping rule with the PBGI acquisition function consistently matches or outperforms other acquisition-function–stopping-rule pairs in terms of *cost-adjusted simple regret*, a metric capturing trade-offs between solution quality and cumulative evaluation cost.

Cost-aware Bayesian Optimization



Cost-adjusted simple regret: $\underbrace{\min_{1\le t\le\tau} f(x_t) - \inf_{x\in X} f(x)}_{\text{simple regret}} + \underbrace{\sum_{t=1}^{\tau} c(x_t)}_{\text{cumulative cost}}$

Goal: *Adaptively* select evaluations $x_1, x_2, \dots$ and stop at time τ to minimize the expected cost-adjusted simple regret.

Existing Adaptive Stopping Rules

Simple heuristics: stop when the best observed value remains unchanged or improvement is not statistically significant.

Acquisition-based: stop when PI, EI or KG falls below a threshold.

Regret-based: stop when regret bounds drop below a threshold (with some probability) such as in UCB-LCB.

PBGI/LogEIPC Stopping Rule

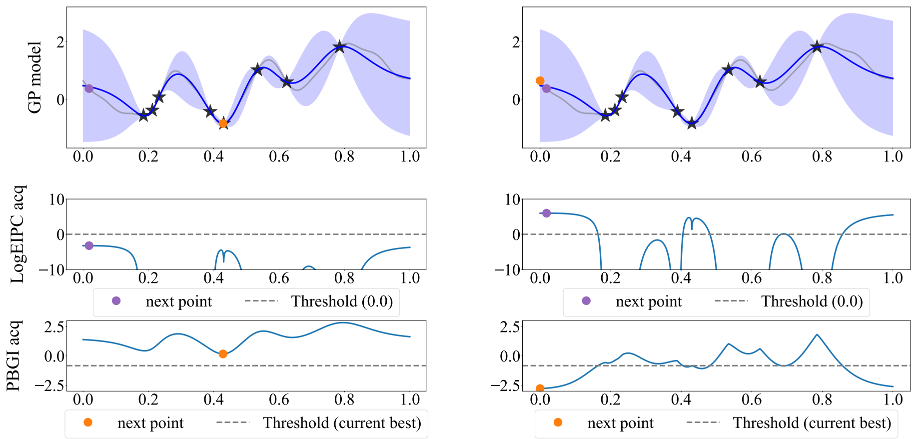
EI stopping rule. Stop when the expected improvement is no longer worth the unit cost: $\alpha_t^{\mathrm{EI}}(x; y^*_{1:t}) \le c$.

PBGI/LogEIPC stopping rule (this work). Stop when the Gittins index at *every* unevaluated point is at least the current best observed value:

$$\min_{x\in X\setminus\{x_1,\dots,x_t\}} \alpha_t^{\mathrm{PBGI}}(x) \ge y^*_{1:t} \quad \Leftrightarrow \quad \max_{x\in X\setminus\{x_1,\dots,x_t\}} \alpha_t^{\mathrm{LogEIPC}}(x; y^*_{1:t}) \le 0.$$

Result (Weitzman, 1979). Under the *independent-value* setting, it is *Bayesian-optimal* when paired with the PBGI acquisition function.

Behavior Illustration



(a) $c(x) \equiv 0.1$ (b) $c(x) \equiv 0.0001$

Theoretical Guarantee

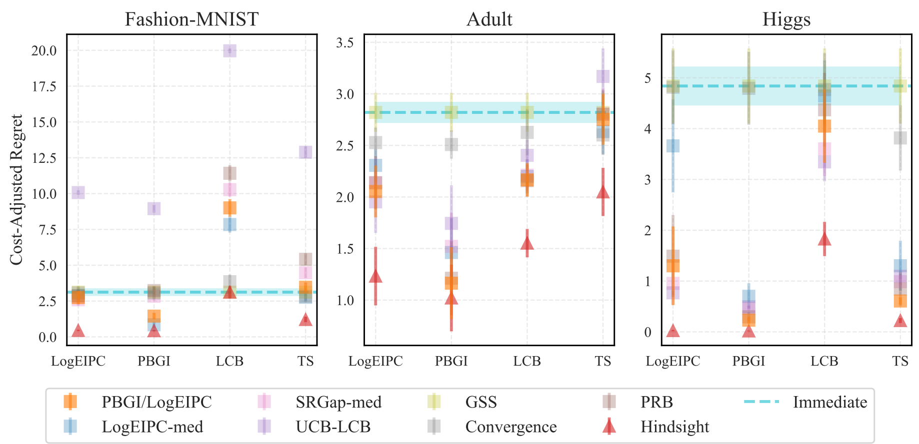
Theorem 1 (No worse than stopping-immediately)
When optimizing a random function f with a constant prior mean, our stopping rule with PBGI or EIPC achieves expected cost-adjusted regret no worse than stopping immediately after initial evaluation.

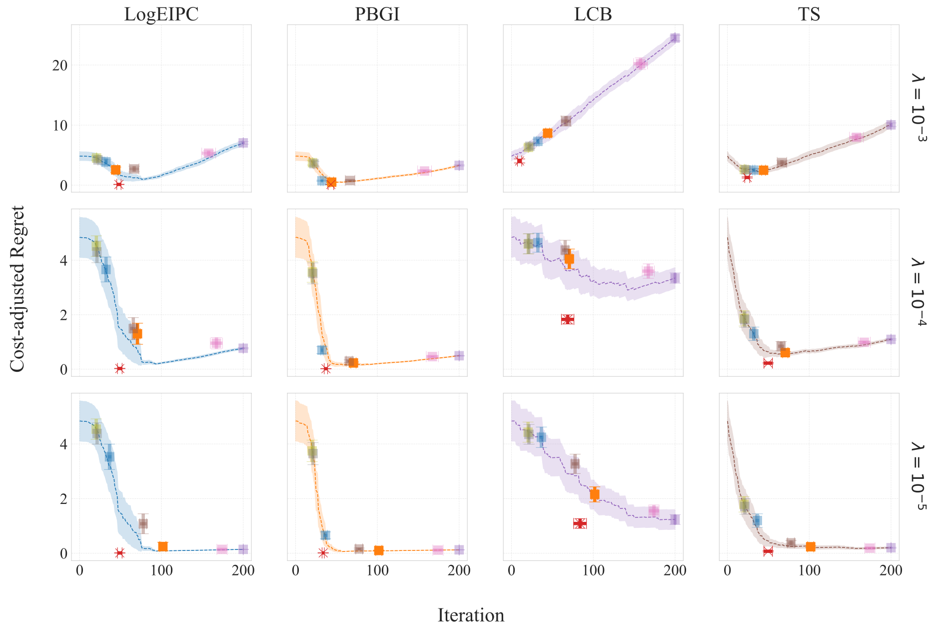
$$\mathbb{E}\left[y^*_{1:\tau} - \min_{x\in X} f(x) + \sum_{t=1}^{\tau} c(x_t)\right] \le \mathbb{E}\left[y_1 - \min_{x\in X} f(x) + c(x_1)\right].$$

Key proof idea: Using our stopping rule, both PBGI and EIPC are guaranteed to evaluate only points whose one-step expected improvement is worth the evaluation cost before stopping.

Implication: Matches the best we can hope for in the worst case, and avoids over-spending — properties many cost-unaware rules lack.

Performance





Computation Time