

# Cost-aware Stopping for Bayesian Optimization

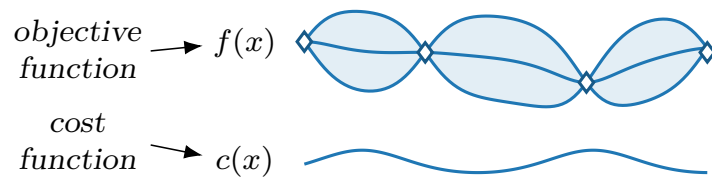
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## Abstract

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

**Goal:** *Adaptively* select evaluations  $x_1, x_2, \dots$  and stop at time  $\tau$  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 probabilistic confidence), e.g., UCB-LCB (Markarova et al., 2022).

## PBGI/LogEIPC Stopping Rule

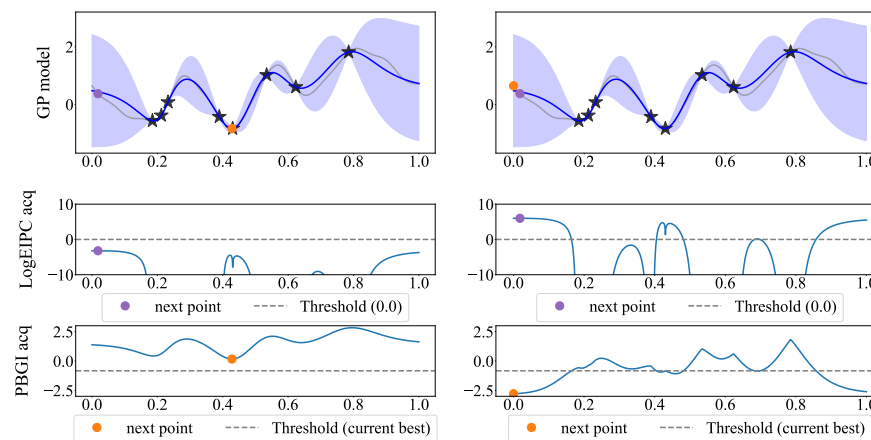
**EI stopping rule:** (Nguyen et al., 2017) Stop when the expected improvement is no longer worth the unit cost:  $\alpha_t^{\text{EI}}(x; y_{1:t}^*) \leq c$ .

**Our PBGI/LogEIPC stopping rule:** Stop when the Gittins index at *every* unevaluated point is at least the current best observed value:

$$\min_{x \in X \setminus \{x_1, \dots, x_t\}} \alpha_t^{\text{PBGI}}(x) \geq y_{1:t}^* \Leftrightarrow \max_{x \in X \setminus \{x_1, \dots, x_t\}} \alpha_t^{\text{LogEIPC}}(x; y_{1:t}^*) \leq 0.$$

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

## Behavior Illustration



## Theoretical Guarantee

**Theorem 1** (Upper Bound on Cost up to Stopping)

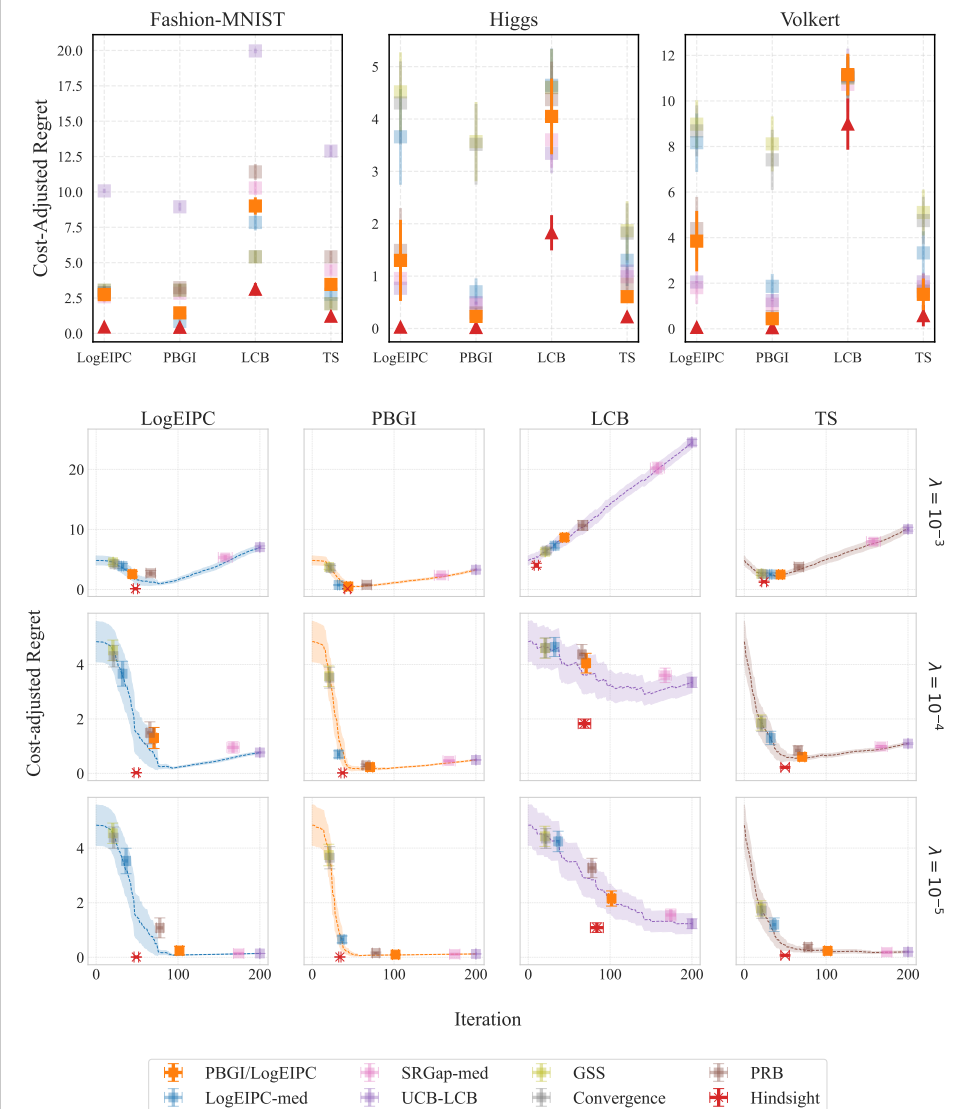
For optimizing a random function  $f$  with constant mean  $\mu$ , using PBGI or LogEIPC acquisition function with our stopping rule, the expected cumulative cost up to stopping is bounded by

$$\mathbb{E} \left[ \sum_{t=2}^{\tau} c(x_t) \right] \leq \mu - \mathbb{E} \left[ \min_{x \in X} f(x) \right]. \quad (1)$$

**Key insight:** Using our stopping rule, both PBGI and LogEIPC are guaranteed to evaluate only points where their evaluation cost  $\leq$  the one-step expected improvement before stopping.

**Benefit:** Avoid excessive cost spending, unlike many existing cost-unaware stopping rules.

## Performance



## Computation Time

