Bayes Optimal Early Stopping Policies for Black-Box Optimization

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Abstract
We derive an optimal policy for adaptively restarting a randomized algorithm, based on observed features of the run-so-far, so as to minimize the expected time required for the algorithm to successfully terminate. Given a suitable Bayesian prior, this result can be used to select the optimal black-box optimization algorithm from among a large family of algorithms that includes random search, Successive Halving, and Hyperband. On CIFAR-10 and ImageNet hyperparameter tuning problems, the proposed policies offer up to a factor of 13 improvement over random search in terms of expected time to reach a given target accuracy, and up to a factor of 3 improvement over a baseline adaptive policy that terminates a run whenever its accuracy is below-median.

1. Introduction
Many real-world problems can be effectively solved using black-box optimization. Examples include hyperparameter tuning, as well as design of circuits, antennas, and other structures. In such problems, we are given a feasible set $\mathcal{F}$, and the goal is to find a point $x \in \mathcal{F}$ that maximizes an objective function $f : \mathcal{F} \rightarrow \mathbb{R}$, while evaluating $f$ as few times as possible.

In this work we consider multi-fidelity black-box optimization problems (Huang et al., 2006) where, for each point $x \in \mathcal{F}$, there is an iterative process that produces a sequence of values $\{f(x,t)\}_{t=1}^{T}$. Having observed $f(x,t)$, we can observe $f(x,t+1)$ by paying a certain evaluation cost. For example, in a hyperparameter tuning problem, $f(x,t)$ might be the validation accuracy obtained after training for $t$ epochs using hyperparameter vector $x$, and the cost of computing $f(x,t+1)$ having already computed $f(x,t)$ might be the time required to train for one epoch. The goal is now to find an $x \in \mathcal{F}$ that maximizes $f(x,T)$, while minimizing total evaluation cost (e.g., total training time). Our results also apply to the closely-related problem of maximizing $f(x,t)$ over both $x$ and $t$, a more natural goal in the context of hyperparameter tuning. Solving such problems requires addressing the usual challenges associated with black-box optimization, but also presents the opportunity to reduce cost by adaptively allocating resources across different values of $x$ based on observed partial sequences $f(x,1), f(x,2), \ldots, f(x,t)$.

Though hyperparameter tuning is perhaps the most common example of such a problem within machine learning, the multi-fidelity formulation is also relevant to more traditional experiment design problems. For example, in a circuit design problem, $f(x,1)$ might be the result of a cheap simulation, $f(x,2)$ might be the result of a more expensive one, and $f(x,3)$ might be the result of a physical experiment involving the proposed circuit (e.g., see (Huang et al., 2006)).

In this work, we focus on the resource allocation aspect of multi-fidelity black-box optimization. To this end, we assume that points $x \in \mathcal{F}$ are sampled from a fixed distribution (which could be uniform or learned), which in turn induces a distribution over sequences $\{f(x,t)\}_{t=1}^{T}$. We present theoretical results in a Bayesian setting, where the induced distribution over sequences is given as a prior. Given the prior, our job is to adaptively determine when to sample new $x$ values and how to allocate effort among them. Experimentally, we show that a simple explore-exploit algorithm can be used to effectively estimate the prior on-the-fly.

On the surface, the resource allocation aspect of black-box optimization may seem less interesting than the geometric aspect (i.e., deciding which $x \in \mathcal{F}$ to consider next), on which most previous work has focused. However, recent work has shown that in many cases, a simple resource allocation policy applied to random search can outperform sophisticated Bayesian optimization algorithms (Li et al., 2017). Thus, even in the restricted setting we consider, improved resource allocation has significant potential benefit.

The contributions of this paper are twofold. First, we formulate an abstract problem in which one may sample sequences (e.g., accuracy curves) from a known distribution,
and observe prefixes of those sequences by paying a certain cost (e.g., training time). For this problem, we derive a policy that is optimal in terms of expected time to reach a success condition (e.g., suitably high accuracy). This policy has many potential uses beyond the ones already mentioned. For example, it can be used to adaptively restart a randomized algorithm (e.g., a SAT solver) based on observed features of the run-so-far, so as to minimize its expected running time (e.g., see (Gomes et al., 1998)).

Second, we show empirically that this policy can provide order-of-magnitude improvements over random restart and Hyperband on CIFAR-10 and ImageNet hyperparameter tuning problems, when provided with an accurate prior. Though we do not achieve comparable results without such a prior, our experiments demonstrate significant headroom which we hope will motivate future work on this problem.

2. Related Work

As a speedup technique for black-box optimization, our work is most closely related to early stopping methods. Various methods for early stopping have been proposed, based on both parametric and non-parametric models (Domhan et al., 2015; Golovin et al., 2017). Recent work on model-free algorithms such as Successive Halving (Jamieson & Talwalkar, 2016) and Hyperband (Li et al., 2017) has shown that algorithms that apply early stopping to random search can be competitive with Bayesian optimization.

Outside of optimization, earlier work demonstrated the potential of restarts to speed up randomized algorithms such as SAT solvers (Gomes et al., 1998). In this setting, significant speedups can be obtained even without adaptivity, using a fixed sequence of restart thresholds. The problem of choosing such a sequence has been addressed in worst-case, online, and average-case settings (Luby et al., 1993; Gagliolo & Schmidhuber, 2007; Streeter et al., 2007). Our work presents adaptive policies that can be applied to the same problem, offering additional potential speedups.

Finally, our optimal policy is related to Gittins index policies (Gittins, 1979), as discussed in §3.3.

3. Theoretical Results

We now formalize the resource allocation problem introduced in §1, define types of policies that can be used to solve it, derive Bayes-optimal policies, and present algorithms for efficiently computing near-optimal policies.

3.1. Problem Definition

The problem we consider is defined by a tuple \( (\mathcal{F}, \mathcal{D}, \mathcal{O}, g) \), where

- \( \mathcal{F} \) is a set of seeds,
- \( \mathcal{D} \) is a probability distribution over \( \mathcal{F} \),
- \( \mathcal{O} \) is a set of possible observations, and
- \( g : \mathcal{F} \times \mathbb{Z}_+ \rightarrow \mathcal{O} \) is an observation function: \( g(x, t) \) is what we observe after spending time \( t \) on seed \( x \).

We will consider policies that have the ability to sample a seed \( x \sim \mathcal{D} \), and to observe \( g(x, 1) \) by paying a unit cost. Once a policy has already observed \( g(x, t) \) for some \( x \) and \( t \), it may observe \( g(x, t + 1) \) by paying unit cost. The goal is to minimize the time required to observe the special symbol \(* \in \mathcal{O} \), which indicates that some success condition has been met.

To simplify the presentation, we have assumed unit observation costs. However, our results can be readily extended to costs that depend on \( t \) or even on \( x \), as discussed at the end of §3.2.

For hyperparameter tuning problems, \( x \) represents a randomly-sampled hyperparameter vector, \( g(x, t) \) might represent the resulting validation accuracy after training for \( t \) epochs, and \(* \) might represent validation accuracy above some predetermined threshold. In the context of speeding up a randomized SAT solver, \( x \) represents the seed used for the pseudo-random number generator, \( g(x, t) \) might contain features based on the solver’s internal state after it has run for \( t \) time steps with random seed \( x \), and \(* \) represents the solver having terminated successfully.

We consider several types of policies, defined in the next section. In all cases, executing a policy \( \pi \) produces a sequence of observations, denoted \( \text{trace}(\pi) \). This sequence is random due to the sampling of \( \text{trace}(\pi) \). This sequence is random due to the sampling of seeds from \( \mathcal{D} \), and its distribution is a function of \( \pi \). Let the random variable \( C_\pi(\pi) \) denote the length of the shortest prefix of \( \text{trace}(\pi) \) that contains \(* \). An optimal policy is one that minimizes the expected cost incurred before observing \(* \):

\[
c_\pi(\pi) \equiv \mathbb{E}[C_\pi(\pi)] .
\]

3.1.1. Types of Policies

We consider multiple types of policies for solving the above problem.

The simplest type of policy is one that repeatedly samples a seed, then performs a run whose length depends on the observations according to a fixed adaptive stopping rule.

**Definition 1.** A stopping rule is a function \( \tau : \mathcal{O}^* \rightarrow \{0, 1\} \) which takes an observation sequence as input, and returns a boolean indicating whether to stop making observations.
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Executing $\tau$ with seed $x$ yields the sequence of observations $obs(\tau, x) \equiv \{o_t\}_{t=1}^{t_{\text{stop}}}$, where $o_t = g(x, t)$, and $t_{\text{stop}}$ is defined by

$$\tau(o_{1:t}) = \begin{cases} 0 & \text{if } t < t_{\text{stop}} \\ 1 & \text{if } t = t_{\text{stop}} \end{cases}.$$  

In the context of hyperparameter tuning, the observations might be accuracy values, and a possible stopping rule is: stop if accuracy has not improved in the last 10 time steps.

We also consider randomized stopping rules, which return a probability rather than a boolean.

**Definition 2.** For any stopping rule $\tau$, the static restart policy $\pi_{\text{static}}(\tau)$ repeatedly executes $\tau$ with independently sampled seeds, yielding the observation sequence

$$\text{trace}(\pi_{\text{static}}(\tau)) \equiv \text{obs}(\tau, x_1) \sim \text{obs}(\tau, x_2) \sim \ldots$$

where $x_i \sim D \forall i$, and $\sim$ is the concatenation operator.

At the opposite extreme, we consider run-switching policies, which have the ability to suspend and resume individual runs adaptively using an arbitrary rule. In the context of hyperparameter tuning, an example might be: perform two runs of length $t = 10$, each using a random hyperparameter vector, then discard the run with lower accuracy and continue the remaining run indefinitely. The recently-developed Hyperband and Successive Halving algorithms can both be expressed as run-switching policies.

**Definition 3.** A run-switching policy $\pi : (\mathcal{O}^*)^\infty \rightarrow \mathbb{Z}_{\geq 0}$ takes as input an infinite sequence $L$, where $L_i$ is the (possibly empty) sequence of observations for seed $x_i$, and returns the index of the seed to use for the next observation.

Executing $\pi$ yields a random sequence of observations $\text{trace}(\pi) \equiv \{o_i\}_{i=1}^\infty$. Letting $L^t_i$ denote the input to $\pi$ on time step $t$, and letting $x_i \sim D$ be the $i$th sampled seed, $o_i$ and $L^t_i$ are defined as follows.

1. For all $i$, $L^t_i$ is the empty sequence.
2. $o_i = g(x_i, s + 1)$, where $i = \pi(L^t_i)$ and $s = |L^t_i|$.
3. For all $t$, $L^{t+1}_i = L^t_i \sim \langle o_i \rangle$, where $i = \pi(L^t_i)$, and $L^{t+1}_j = L^t_j$ for $j \neq i$ ($\sim$ denotes concatenation).

### 3.2. Optimal Policies

We now derive an optimal run-switching policy. Specifically, we will prove Theorem 1, which shows that the Bayes-optimal run-switching policy is a static restart policy, and that this restart policy repeatedly runs the stopping rule $\tau^*$ that maximizes a certain benefit to cost ratio.

We adopt the following notation. For any stopping rule $\tau$,

- $q(\tau) = \mathbb{P}_{x \sim D}[\ast \in \text{obs}(\tau, x)]$ is the probability that a run of $\tau$ succeeds, and
- $c(\tau) = \mathbb{E}_{x \sim D}[|\text{obs}(\tau, x)|]$ is the expected cost of a single run under $\tau$.

$\mathcal{T}$ is the set of all (possibly randomized) stopping rules.

**Theorem 1.** The static restart policy $\pi^* \equiv \pi_{\text{static}}(\tau^*)$ is an optimal run-switching policy (i.e., for any run-switching policy $\pi$, $c_*(\pi) \geq c_*(\pi^*)$), where

$$\tau^* = \arg\max_{\tau \in \mathcal{T}} \left\{ \frac{q(\tau)}{c(\tau)} \right\}.$$  

In the context of hyperparameter tuning, Theorem 1 means that once the optimal policy starts a new training run it will never revisit a previous one, meaning that it is not necessary to store multiple checkpoints or resume a previously paused run in order to execute the policy. This also means that the optimal run-switching policy is easy to parallelize, a significant advantage in practice.

The proof of Theorem 1 consists of two parts. Letting $r^* = \frac{q(\tau^*)}{c(\tau^*)}$, we first show that the static restart policy $\pi_0 = \pi_{\text{static}}(\tau^*)$ has $c_*(\pi_0) = \frac{1}{r^*}$. We then prove a matching lower bound, showing that any run-switching policy $\pi$ has $c_*(\pi) \geq \frac{1}{r^*}$.

The first part of the proof is a corollary of the following lemma, which gives the expected time-to-success of any static restart policy. The proof mirrors the proof of Lemma 1 of Luby et al. (1993), which considers non-adaptive stopping rules defined by an integer time limit.

**Lemma 1.** For any stopping rule $\tau$, the static restart policy $\pi = \pi_{\text{static}}(\tau)$ has expected time-to-success $c_*(\pi) = \frac{q(\tau)}{r(\tau)}$.

**Proof.** Let $x_1 \sim D$ be the seed used for the first run of $\tau$, let $C_1 = |\text{obs}(\tau, x_1)|$ be the cost of the first run, and let $S$ be the event that the first run succeeds (i.e., $\ast \in \text{obs}(\tau, x_1)$). The first run succeeds with probability $q = q(\tau)$. Conditioned on the first run failing, the expected remaining time-to-success is $c_*(\pi)$. Thus, letting $K = c_*(\pi)$, $K$ satisfies the recurrence

$$K = q\mathbb{E}[C_1 | S] + (1 - q)\mathbb{E}[|C_1| \sim S] + K.$$  

Subtracting $K(1 - q)$ from both sides,

$$K \cdot q = q\mathbb{E}[C_1 | S] + (1 - q)\mathbb{E}[|C_1| \sim S] = \mathbb{E}[C_1].$$  

Thus, $K = \frac{\mathbb{E}[C_1]}{q} = \frac{r(\tau)}{q(\tau)}$, as claimed. \qed

Because maximizing $\frac{q(\tau)}{r(\tau)}$ is equivalent to minimizing $\frac{c(\tau)}{q(\tau)}$,

Lemma 1 immediately implies that the policy given by Theorem 1 is optimal among static restart policies. To show
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that \( \pi_{\text{static}}(\tau^*) \) is also an optimal run-switching policy, we now prove the lower bound: \( c_s(\pi) \geq \frac{1}{\tau^*} \). This is shown in Lemma 3, the proof of which requires the following lemma.

**Lemma 2.** For any run-switching policy \( \pi \), there exists a sequence \( \{ \tau_j \} \) of (randomized) stopping rules such that \( c_s(\pi) = \sum_j c(\tau_j) \) and \( q_\pi = \sum_j q(\tau_j) \), where \( q_\pi \) is the probability that \( \pi \) succeeds (i.e., \( \tau^* \in \text{trace}(\pi) \)).

**Proof.** To define the sequence of stopping rules, suppose we execute \( \pi \), stopping when it succeeds (if ever). Let \( L_j \) be the resulting observation sequence for seed \( x_j \). Let \( o_j \) be the truncated observation sequence that results from executing \( \tau_j \). We will define \( \tau_j \) in such a way that the random variables \( o_j \) and \( L_j \) have exactly the same distribution.

Assuming \( o_j \) and \( L_j \) have the same distribution,

\[
c(\tau_j) = \mathbb{E}[|o_j|] = \mathbb{E}[|L_j|] .
\]

Because the cost of running \( \pi \) until it succeeds is \( \sum_j |L_j| \), we have \( c(\pi) = \mathbb{E} \left[ \sum_j |L_j| \right] = \sum_j \mathbb{E}[|L_j|] = \sum_j c(\tau_j) \).

A similar argument can be used to prove the analogous equation for \( q \). Let \( S_j \) be the event that \( L_j \) contains the success token \( \tau^* \). Because the success token can appear at most once in \( L \), the events \( \{ S_j \} \) are mutually exclusive, and

\[
q_\pi = \sum_j \mathbb{P}[S_j] .
\]

Then, because \( L_j \) and \( o_j \) have the same distribution, \( q(\tau_j) = \mathbb{P}[S_j] \), so \( q_\pi = \sum_j q(\tau_j) \).

To define \( \tau_j \) formally, for any observation sequence \( o \) let \( E_o^j \) be the event that \( o \) is a prefix of \( L_j \). Define

\[
\tau_j(o) = \mathbb{P}[|L_j| > |o| \mid E_o^j] .
\]

It then follows inductively that for any \( o \), \( \mathbb{P}[o_j = o] = \mathbb{P}[L_j = o] \), so \( o_j \) and \( L_j \) have the same distribution. \( \square \)

**Lemma 3.** Any run-switching policy \( \pi \) has \( c_s(\pi) \geq \frac{1}{\tau^*} \).

**Proof.** By Lemma 2, there exists a sequence \( \{ \tau_j \} \) of stopping rules such that \( c_s(\pi) = \sum_j c(\tau_j) \) and \( q_\pi = \sum_j q(\tau_j) \), where \( q_\pi \) is the probability that \( \pi \) succeeds when run forever. For any stopping rule \( \tau \), \( q(\tau) \leq r^* c(\tau) \). Thus,

\[
q_\pi = \sum_j q(\tau_j) \leq r^* \sum_j c(\tau_j) = r^* c_s(\pi) .
\]

If \( q_\pi = 1 \), this implies \( c_s(\pi) \geq \frac{1}{\tau^*} \), as required. If \( q_\pi < 1 \), \( c_s(\pi) = \infty \) and the lemma holds trivially. \( \square \)

The results of this section can be easily generalized to the case where observing \( g(x, t + 1) \) given \( g(x, t) \) has a cost that depends on \( t \) and \( x \). After redefining \( \text{trace}(\pi) \) as a sequence of (observation, cost) pairs, and redefining \( c \) and \( c_s \) appropriately, the proof of Lemma 2 requires only minor changes, while the remaining proofs go through as-is.

**3.3. Relationship to Gittins Indices**

The optimal policy derived in Theorem 1 is in fact the Gittins index policy for a particular instance of the Bayesian multi-armed bandit problem. Establishing this connection shows that, in addition to minimizing expected time-to-success, the policy of Theorem 1 maximizes an exponentially-discounted count of the number of times the success token is observed.

In the Bayesian multi-armed bandit problem, we are given a set of \( k \) “arms”, each of which is a Markov chain with known initial state and transition probabilities. At each time step \( t \), a policy selects the index \( i_t \) of the arm to pull. This causes Markov chain \( i_t \) to transition to a new state, and the player receives a corresponding reward \( r_t \), drawn from a known distribution which depends on the current state of arm \( i \). The goal is to maximize the discounted reward, \( \sum_t \beta^t r_t \), for discount factor \( \beta \). The Gittins index theorem (Gittins, 1979) shows that, if each arm \( i \) is currently in state \( z_i \), the optimal policy selects arm \( \text{argmax}_i \{ G_i(z_i) \} \), where \( G_i(z) \) is the Gittins index associated with arm \( i \) when it is in state \( z \). To define the Gittins index, let \( t_{\text{Stop}}(\tau) \) be a random variable equal to the number of steps taken by stopping rule \( \tau \). As discussed by (Weber, 1992), the Gittins index can be defined as

\[
G_i(z) = \sup_{\tau \in \mathcal{T}} \left\{ \frac{\mathbb{E}[\sum_{t=1}^{t_{\text{Stop}}(\tau)} \beta^t r_t(i, z, \tau)]}{\mathbb{E}[\sum_{t=1}^{t_{\text{Stop}}(\tau)} \beta^t]} \right\} . \tag{1}
\]

To relate this to Theorem 1, suppose we have an infinite number of arms, where arm \( i \) corresponds to the \( i \)th sampled seed. Each arm has the same Markov chain, which has a state for every observation sequence that does not include the success token \( \tau^* \). Additionally, there is an absorbing state that is entered once the success token is observed. A reward of 1 is obtained when first entering the absorbing state, and the reward is 0 otherwise.

For \( \beta = 1 \), the denominator of (1) is \( c(\tau) \) and the numerator is \( q(\tau) \), so the stopping rule that obtains the supremum in (1) is the \( \tau^* \) defined in Theorem 1. With additional work, it can be shown that the Gittins index policy is equivalent to \( \pi_{\text{static}}(\tau^*) \). The Gittins index theorem then shows that, in addition to minimizing expected time-to-success, \( \pi_{\text{static}}(\tau^*) \) maximizes discounted cumulative reward when the discount factor is sufficiently close to 1.

**3.4. Computing an Optimal Policy**

As shown in Theorem 1, the problem of computing an optimal run-switching policy can be reduced to the
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simpler problem of computing the stopping rule \( \tau^* = \arg \max_{r \in T} \{ \frac{g(r)}{c(r)} \} \). We now show that \( \tau^* \) can be computed efficiently using binary search.

Let \( r^* = \max_{r \in T} \{ \frac{g(r)}{c(r)} \} \). Each iteration of the binary search algorithm will guess a value \( r \), and check whether \( r < r^* \) by solving the maximization problem:

\[
\Delta(r) = \max_{\tau \in T} \{ q(\tau) - r \cdot c(\tau) \}
\]

This is sufficient to determine whether \( r < r^* \), as shown by the following lemma.

**Lemma 4.** \( \Delta(r) > 0 \) if and only if \( r < r^* \).

**Proof.** \( \Delta(r) > 0 \) iff. there exists a stopping rule \( \tau \) with \( q(\tau) - r \cdot c(\tau) > 0 \), or equivalently \( \frac{g(r)}{c(\tau)} > r \). By definition, such a rule exists iff. \( r < r^* \). \( \square \)

**Algorithm 1** FindStoppingRule

**Parameters:** \( \epsilon > 0 \).

Initialize \( L \leftarrow 0, U \leftarrow 1 \).

while \( U > (1+\epsilon)L \) do

Set \( r \leftarrow \frac{U+L}{2} \).
Set \( \delta \leftarrow \Delta(r) \) (see equation (2)).

If \( \delta > 0 \) set \( L \leftarrow r \), otherwise set \( U \leftarrow r \).

Return \( \hat{\tau} = \arg \max_{\tau \in T} \{ q(\tau) - L \cdot c(\tau) \} \)

Pseudocode for the binary search algorithm is given in Algorithm 1. Assuming it takes cost at least 1 to make an observation, we have \( r^* \leq 1 \). Thus, the inequality \( L < r^* \leq U \) holds initially. By Lemma 4, this invariant is maintained whenever the algorithm updates \( L \) or \( U \). This, together with the fact that the algorithm only terminates once \( U \leq (1+\epsilon)L \), can be used to show that the algorithm returns a stopping rule \( \hat{\tau} \) with \( \frac{g(\hat{\tau})}{c(\tau)} \geq \frac{1}{r^*} \). Together with Lemmas 1 and 3, this implies \( r_{\text{static}}(\hat{\tau}) \) has expected time-to-success within a factor \( 1 + \epsilon \) of optimal. With additional work, it can be shown that Algorithm 1 terminates in \( O(\log(\frac{1}{\epsilon r^*})) \) iterations.

Each iteration of binary search requires evaluating \( \Delta(r) \) for some \( r \). The best way of doing this depends on how the Bayesian prior over observation sequences is represented. In the typical case of a uniform distribution over a collection of sequences collected as training data, \( \Delta(r) \) can be computed in time linear in the total number of observations, as described in the next section.

### 3.4.1. Stopping Rules as Trees

Any deterministic stopping rule can be represented as a rooted tree whose edges are labeled with observations. Any path through the tree corresponds to a possible observation sequence, and the tree has a path for every sequence for which the rule returns 0 (i.e., does not stop). In a hyperparameter tuning problem, the edges might be labeled with discretized accuracy values, and the rule would continue training as long as the observed accuracy-curve-so-far matches some path in the tree.

Using this representation, we can compute \( \Delta(r) \) in linear time.

**Lemma 5.** Given a uniform distribution \( D \) over observation sequences \( o_1, o_2, \ldots, o_k \), \( \Delta(r) \) can be computed in time \( O(n) \) where \( n = \sum_{i=1}^k |o_i| \).

**Proof (sketch).** In terms of its behavior on these \( k \) sequences, any stopping rule can be represented as a subtree of a tree \( T \), where \( T \) has one root-to-leaf path for each of the \( k \) sequences. The vertices can be assigned weights so that the quantity \( q(\tau) - r \cdot c(\tau) \) equals the sum of the vertex weights. Computing \( \Delta(r) \) then becomes the problem of computing a maximum-weight subtree. This can be done working backwards from the leaves in \( O(n) \) time. \( \square \)

Theorem 2 summarizes the results of this section.

**Theorem 2.** Given a uniform distribution over observation sequences \( o_1, o_2, \ldots, o_k \), a run-switching policy that is provably within a factor \( 1 + \epsilon \) of optimal can be computed in time \( O(n \log(\frac{1}{\epsilon r^*})) \), where \( n = \sum_{i=1}^k |o_i| \).

### 3.5. Approximately Optimal Policies

As discussed in §3.4.1, an optimal stopping rule can be represented as a tree whose vertices represent partial observation sequences. In order for an optimal policy computed on training data to generalize well, the statistics for each vertex must be estimated based on a reasonable number of observation sequences. To achieve this, it is necessary to define the observations appropriately. For example, instead of using real-valued validation accuracies as observations, one can use bucketized accuracies. We can also prune the tree to enforce a minimum sequence count.

It is also possible to use our approach with a non-uniform prior, such as the parameter Bayesian model of Domhan et al. (2015). To make use of the algorithm described in Lemma 5, we must approximate the prior by a uniform prior over a fixed set of observation sequences, which can be done by drawing a large number of curves from the prior and discretizing them appropriately. Because the number of samples is limited only by computational constraints, as opposed to available data, the accuracy loss due to discretization can be made very small.

We can also use Algorithm 1 to compute stopping rules that are not expressed as trees. For example, the probabil-
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4. Experiments

To demonstrate the benefit of the optimal run-switching policy derived in §3, we now evaluate it on two real-world hyperparameter tuning problems. For each problem, our experiments are designed to answer the following questions:

- How much benefit do adaptive policies provide over simpler alternatives, such as starting a fresh run every \( t \) time steps, for optimally chosen \( t \)?

- How close to optimal can we get when we do not have access to the prior distribution over observation sequences? In particular, how close to optimal is the performance of model-free algorithms such as Successive Halving and Hyperband?

The two benchmark problems involve tuning the hyperparameters of image classification models for CIFAR-10 (Krizhevsky & Hinton, 2009) and ImageNet (Russakovsky et al., 2015). We use a convolutional neural network based on LeNet (LeCun et al., 1998) for CIFAR-10, and we use Inception-v3 (Szegedy et al., 2016) for ImageNet.

Both models use the same set of hyperparameters, which are given in Table 4. Each hyperparameter is sampled from either a uniform or log-uniform distribution over a certain interval. The intervals were selected to include the values used in the original Inception-v3 paper, as well as a range of other plausible values.

For each hyperparameter tuning problem, we sampled \( n \) hyperparameter vectors uniformly at random, and used each one to train for \( T \) update cycles, where \( n \) was as large as practically possible, and \( T \) was a rough estimate (based on a few initial runs) of the point at which most runs had achieved their maximum validation accuracy. On each update cycle, we train for 1000 gradient descent steps with a mini-batch size of 1024, and then evaluate validation accuracy on a separate held-out dataset. We used \( n = 720 \) and \( T = 100 \) for LeNet trained on CIFAR-10, and \( n = 128 \) and \( T = 200 \) for Inception-v3 trained on ImageNet.

We recorded the validation accuracy curves produced by each run, and used this data to simulate executing different policies. This approach allows for fast evaluation of new policies once the initial data has been collected, and also reduces variance due to the fact that all policies are evaluated on the same data.

To make our results easily reproducible, we have included the accuracy curves used in our experiments in the supplementary material, along with the code for our algorithms.

4.1. Non-Adaptive Restart Schedules

Before evaluating the benefit of adaptive restart policies, we first consider as a baseline the benefit of using a simple restart schedule. In particular, we consider restarting with a freshly-sampled hyperparameter vector every \( t \) update cycles, for some fixed \( t \). As shown by Luby et al. (1993), the optimal restart schedule is of this form. Figure 1 shows the expected time required to reach a given accuracy \( a \), for several different values of \( a \), as a function of the restart threshold \( t \), for the CIFAR-10 tuning problem. The chosen values of \( a \) correspond to the 50th, 90th, and 99th percentile accuracies achieved at the end of a full run.

As can be seen, choosing \( t \) too small can increase the expected time required to reach a desired accuracy by a large (or even infinite) factor, while choosing \( t \) optimally reduces expected time by a comparatively small but still non-trivial factor (e.g., roughly a factor of 2 to reach 99th percentile accuracy).

4.2. Adaptive Run-Switching Policies

We now evaluate the benefit of adaptive run-switching policies over simple restart schedules. As discussed in §3, it suffices to consider restart policies that repeatedly execute a stopping rule. We consider stopping rules that, after having performed a run of length \( t \), observe \( o_t \in \{1, 2, \ldots, K\} \), where \( o_t \) is the run’s current accuracy quantile (relative to

![Figure 1. Expected time to reach a given target accuracy as a function of restart threshold \( t \), when training LeNet on CIFAR-10 and restarting training every \( t \) update cycles using fresh random hyperparameters.](image-url)
other runs of length $t$ with the same observation prefix), discretized into one of $K$ buckets. If $K = 2$, the stopping rule makes decisions based on whether accuracy is above or below the (conditional) median.

As discussed in §3.5, we reduce overfitting by pruning the policy tree, ensuring that each leaf node is reached by at least 4 runs in the training dataset. We also considered policies that only branch when the time so far is a power of 2, but found this provided no additional benefit over pruning.

Figure 2 shows the improvement over random search that can be obtained using various schedules and policies. We plot the improvement from the best oblivious restart schedule (choosing the best restart threshold $t$), as well as the improvement from the best quantile-based policy, optimizing over all $K \in \{2, 3, 4\}$. As a baseline, we also show the performance of the above-median stopping rule, which stops a run at time $t$ if its current accuracy is below the population median. For all policies that are learned from data, we estimate the improvement over random search using cross-validation. To reduce noise when cross-validating on small dataset, we use a carefully constructed low-variance estimate described in Appendix A.

As shown in Figure 2, the best quantile-based policy offers large improvements over random search, and consistently outperforms both the optimal restart schedule and the above-median policy. Depending on the accuracy target, the improvement over random search is up to a factor of 13 for the LeNet model, and up to a factor of 5 for Inception-v3. In terms of the expected time to find a 95th-percentile-accuracy hyperparameter vector for Inception-v3, the best quantile-based policy outperforms the above-median rule by roughly a factor of 2.5, and outperforms the optimal restart schedule by more than a factor of 5.

4.3. Black-Box Optimization Algorithms

So far we have evaluated the benefit of adaptive policies that were computed using accuracy curves drawn from the distribution of interest (and evaluated using cross-validation). In practice, when facing a new black-box optimization problem we do not know the distribution over accuracy curves, and instead must estimate it on-the-fly.

In this section we compare the performance of four black-box optimization algorithms. As baselines, we consider Hyperband (Li et al., 2017), as well as the universal restart schedule of Luby et al. (1993). We also consider two new algorithms, both of which spend half their time collecting data via random search, and the other half exploiting a policy computed based on that data. For the above-median algorithm, the policy is the above-median policy described in the previous section. For the explore-exploit algorithm, the policy is the best quantile-based policy, optimizing over $K \in \{2, 3, 4\}$ as in §4.2 and determining the best policy using cross-validation (over the data collected via random search). We compute this policy using an an accuracy target
equal to the 90th percentile accuracy obtained during exploration.

To evaluate these algorithms, we ran each algorithm over 4000 times on each of the two benchmarks, simulating its behavior by sampling with replacement from the collection of pre-recorded accuracy curves. Compared with the alternative of actually running each algorithm on the underlying hyperparameter tuning problem, this approach allows us to reduce variance by averaging over a much larger number of runs. It also makes our results easily reproducible given the accuracy curves, which are included in the supplementary material.

Figure 3 summarizes the performance of these four algorithms relative to random search. Though Hyperband performs best when tuning the LeNet model trained on CIFAR-10, it is significantly worse than random search for tuning Inception-v3 on ImageNet. In contrast, the above-median and explore-exploit algorithms outperform random search on both problems for sufficiently high target accuracies. As might be expected, both the above-median algorithm and the explore-exploit algorithm perform better for higher accuracy targets, where the time available for exploration (and hence the amount of data available for computing a policy) is larger.

As can be seen by comparing Figures 2 and 3, all four algorithms are far from optimal when compared to policies computed from just a few hundred accuracy curves. This suggests that substantial gains could be achieved if we could estimate policies in a more sample-efficient way, for example by using transfer learning, or by using policies defined by a function approximator rather than an explicit tree. The extent to which this is possible is left as an open question for future work.

5. Conclusions

In this work have have derived optimal early stopping policies applicable to multi-fidelity black-box optimization, and have evaluated the benefit of these policies empirically on two hyperparameter tuning problems. Our main theoretical conclusions are:

- Model-free algorithms for black box optimization, such as Successive Halving and Hyperband, can be viewed as particular run-switching policies.

- The Bayes optimal run-switching policy, in terms of expected time to reach a given accuracy, is a restart policy that repeatedly executes the stopping rule that maximizes a certain benefit to cost ratio. This policy coincides with the Gittins index policy for a related (but different) reward-maximization problem.

Empirically, we have found that optimal run-switching policies can offer order-of-magnitude improvements over random search and Hyperband, and that such policies can be estimated using a fairly small number (hundreds) of observed accuracy curves. Furthermore, a simple explore-exploit algorithm based on these policies is already competitive with Hyperband on our benchmarks, although it fails to deliver the large improvements over random search that our cross-validation-based analysis shows are possible given a more accurate prior.

- In contrast to previous early stopping policies, the optimal policy does not simply stop when it is confident that the current run will not lead to success. Instead, it stops once it can no longer guarantee a benefit to cost ratio good as that obtained by starting over from scratch.
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Appendix A

We now describe the low-variance cross-validation procedure used in our experiments.

Given an algorithm \( A \) that produces a static restart policy from training data, we evaluate its performance using \( k \)-fold cross validation, combined with an important variance-reduction technique which we now describe.

Let \( X_i \) and \( Y_i \) denote the training and test datasets, respectively, for the \( i \)th split used in cross-validation, and let \( \pi_i = A(X_i) \) be the \( i \)th policy, where \( \pi_i = \pi_{\text{static}}(\tau_i^*) \). Let \( q_i(\tau_i^*) \) and \( c_i(\tau_i^*) \) be the success probability and expected cost, respectively, of \( \tau_i^* \) as measured on \( Y_i \) (both of these depend on the desired target accuracy). Cross-validation would estimate \( A \)'s expected time-to-success by taking the average expected time on test data over all splits. Using Lemma 1, it can be shown that this produces the estimate

\[
\frac{1}{k} \sum_{i=1}^{k} \frac{c_i(\tau_i^*)}{q_i(\tau_i^*)}.
\]

If there are \( n \) accuracy curves total, this estimate is asymptotically unbiased as \( \frac{n}{k} \to \infty \). However, it has high variance when \( k \) is large relative to \( n \). In the extreme case of leave-one-out cross-validation (\( k = n \)), each \( q_i(\tau_i^*) \) is estimated based on a single test run, which in general means that at least one \( q_i(\tau_i^*) \) will be 0, causing the estimate to be infinite independent of the algorithm \( A \) that is used to create the policy.

To address this problem, we instead use the estimate

\[
\frac{\sum_{i=1}^{k} c_i(\tau_i^*)}{\sum_{i=1}^{k} q_i(\tau_i^*)}.
\]

With this estimate, both the numerator and denominator are weighted sums of \( n \) data points, and the estimate has low variance so long as \( n \) is large. Moreover, the bias that remains in our estimate tends to underestimate the benefit of our adaptive policies (as can be shown formally using Jensen's inequality).