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A QUANTILE-BASED NESTED PARTITION ALGORITHM FOR BLACK-BOX FUNCTIONS ON A CONTINUOUS DOMAIN

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ABSTRACT

Simulation models commonly describe complex systems with no closed-form analytical representation. This paper proposes an algorithm for functions on continuous domains that fits into the nested partition framework and uses quantile estimation to rank regions and identify the most promising region. Additionally, we apply the optimal computational budget allocation (OCBA) method for allocating sample points using the normality property of quantile estimators. We prove that, for functions satisfying the Lipschitz condition, the algorithm converges in probability to a region that contains the true global optimum. The paper concludes with some numerical results.

1 INTRODUCTION

Currently, there is a growing demand for efficient algorithms that can solve black-box, ill-structured optimization problems. As applications for simulation optimization increase, methods that develop solutions within a given tolerance (or quantile of best solutions) and computational budget are useful. Partition-based search methods have been a popular approach to this problem (Chew et al. 2009, Shi and Ólafsson 2009, Shi and Ólafsson 2000, Tang 1994). In particular, the nested partition framework has been shown to be an effective tool in globally optimizing black-box functions.

The nested partition algorithm operates by sampling from a partitioned domain and then refining the partition scheme to focus on promising regions (Shi et al. 1998, Shi and Ólafsson 2000). This method was initially shown to be effective at solving problems on finite domains and most expansions on this work have focused on discrete domains (Yu and Luo 2008). However, some work has been done applying the nested-partition framework to continuous domains or domains with an uncountable number of elements (Brantley and Chen 2005, Shi and Ólafsson 2009) by determining the most promising region from the best sampled point or averaged sample values.

In this paper we propose an algorithm in the nested partition framework that solves continuous domain problems while implementing optimal computational budget allocation (OCBA). Instead of nesting additional partitions around the best sampled point or expected value in each region, we select the most promising region as the one with the best estimated quantile. The established properties of this estimator are then used to determine sampling allocations between regions via an OCBA scheme that asymptotically maximizes the probability of selecting the region with lowest quantile.

This nested-partition-type search based on quantiles paired with an OCBA algorithm bears closest resemblance to work done by Brantley and Chen (2005) and Chen et al. (2014). However, our approach has some advantages over the previous approaches. First, branching on the quantile rather than the sampled best point allows the algorithm to gain global information about each region while avoiding the influence of sampled outliers. Secondly, the use of quantiles (and their normally distributed estimators) allows the implementation of an optimal computational budget allocation scheme without relying on parametric models for extreme values.

Developing a region of a certain size with lowest quantile might be interesting for other purposes. An application might be interested in identifying a portion of the domain with the highest concentration of good points within a given quantile. An application may also be interested in selecting a range of points for a type of sensitivity analysis.

This paper describes the implementation of the quantile-based nested partition algorithm for black-box functions. We prove that the quantile-based nested partition algorithm converges in probability to an unbranchable region (e.g., minimum volume) with the lowest specified quantile. We also prove that with a sufficiently low quantile threshold, the probability that the unbranchable region with the lowest estimated quantile contains the true global optimum approaches 1 as the number of iterations become arbitrarily large. We implement the quantile-based nested partition algorithm on a set of common test problems with and without OCBA sampling. We find that the addition of the OCBA sampling scheme results in better (closer to the global minimum) sampled points using the same allocated budget.

2 BASIC MODEL AND ALGORITHM

We consider a black-box function f on a continuous closed and bounded domain $S \subset \mathbb{R}^n$. We are interested in the minimization problem

$$min_{x \in S} \; f(x). \tag{1}$$

We also define an optimal point $x^* \in S$ such that $f(x^*) \leq f(x) \;\; \forall x \in S$.

Due to the lack of information concerning the structural properties of the function, identifying the true global minimum can be computationally expensive. Our algorithm looks for "good enough" solutions within a given specified quantile and therefore attempts to locate a region with a concentration of good points inside the domain of S by sequentially applying a series of partitions ("branching") on the domain and then sampling from and ranking regions based on estimated quantiles.

Given a partitioning scheme (typically along each dimension), we define a region as "unbranchable" when the length of each dimension i is less than or equal to some length ε_i. Other definitions for unbranchable might include a minimum volume or a contained diagonal length. Let Σ_{max} denote the set of unbranchable regions that form a partition on S (i.e., $\bigcup_{\sigma \in \Sigma_{max}} \sigma = S$ and $\sigma \bigcap \sigma' = \emptyset$ for all $\sigma, \sigma' \in \Sigma_{max}, \sigma \neq \sigma'$). The set Σ_{max} will comprise the smallest regions for which the algorithm will apply no additional partitioning.

The number of unbranchable regions may become very large, especially with large n, so it is impractical to evaluate each unbranchable region. For instance, if S is a box in n dimensions with width w along each dimension, then the number of unbranchable regions in Σ_{max} is $\left(\frac{w^n}{\prod_{i=1}^n \varepsilon_i}\right)$. Therefore, our algorithm uses quantile estimation to compare regions of various sizes, allowing the algorithm to focus on the regions with large concentrations of near optimal points.

The algorithm ranks regions based on their estimated quantiles. For a given region σ, we use the notation $y(\delta, \sigma)$ as the δ-threshold quantile such that for X sampled uniformly from the region σ then

$$y(\delta, \sigma) = argmin\{P(f(X) \leq y | X \in \sigma) \geq \delta\} \tag{2}$$

for $0 < \delta < 1$. We also define a multi-dimensional volume function $\mathbf{v}(\sigma)$ that provides the volume for a given region σ.

The algorithm proceeds by (1) sequentially partitioning a promising region of the domain S into M equal smaller regions, (2) sampling points based on a budget allocation scheme (possibly OCBA), (3) estimating the quantiles in each region, and (4) ranking the remaining regions by estimated quantiles. The complete algorithm can be formally described as follows.

The inputs to the algorithm include the δ-threshold quantile, the branching scheme M, a defined budget per iteration T, and a minimum number of iterations K. The input parameter K sets a minimum number of iterations that is typically larger than the number of iterations to achieve an unbranchable set by consecutive partitioning, to prevent the algorithm from stopping prematurely. A maximum number of iterations may also be set, however we use the discovery of an unbranchable region to determine the stopping condition.

Quantile-based Nested Partition Algorithm

STEP 0 Initialize:

Set δ, M, T, and K. Set $\Sigma_{contend}(0) = \{S\}$. Define the most promising region (best) $\sigma^B(0) = S$ and set $k = 1$.

STEP 1 Partition:

If $\sigma^B(k-1)$ is unbranchable then $\Sigma_{contend}(k) = \Sigma_{contend}(k-1)$. Otherwise, partition the most promising region, $\sigma^B(k-1)$, into M regions of equal volume $\sigma^B(k-1)_1, \ldots, \sigma^B(k-1)_M$, and update

$$\Sigma_{contend}(k) = \left(\Sigma_{contend}(k-1) \backslash \sigma^B(k-1)\right) \bigcup_{m=1}^{M} \sigma^B(k-1)_m.$$

Let $\sigma_j^k, j = 1, \ldots, \|\Sigma_{contend}(k)\|$ represent each region in $\Sigma_{contend}(k)$.

STEP 2 Sample:

Sample N_j^k points from region in $\sigma_j^k \in \Sigma_{contend}(k)$ for $j = 1, \ldots, \|\Sigma_{contend}(k)\|$ including previously sampled points such that $\sum_{j=1}^{\|\Sigma_{contend}(k)\|} N_j^k = k \cdot T$. Note there must be at least one newly sampled point in each of the regions in $\Sigma_{contend}(k)$. We specify a method for setting the budgeting allotments N_j^k using OCBA in Section 4. Denote the sampled points in σ_j^k as

$$x_1^j, \ldots, x_{N_j^k}^j.$$

Rank the sample points by their function evaluations, i.e., $x_{(1)}^j, \ldots, x_{(N_j^k)}^j$ such that $f(x_{(1)}^j) \leq f(x_{(2)}^j) \leq \cdots \leq f(x_{(N_j^k)}^j)$.

STEP 3 Estimate Quantile:

Let $\mathbf{v}_{min}(k)$ be the smallest volume of the regions in $\Sigma_{contend}(k)$. For each $\sigma_j^k \in \Sigma_{contend}(k)$ for $j = 1, \ldots, \|\Sigma_{contend}(k)\|$ determine $\hat{y}_j$ as an estimate of the quantile $y\left(\delta \cdot \frac{\mathbf{v}_{min}(k)}{\mathbf{v}(\sigma_j^k)}, \sigma_j^k\right)$, estimated as:

$$\hat{y}\left(\delta \cdot \frac{\mathbf{v}_{min}(k)}{\mathbf{v}(\sigma_j^k)}, \sigma_j^k\right) = f\left(x^j_{\left(ceil\left(N_j^k \cdot \delta \cdot \frac{\mathbf{v}_{min}(k)}{\mathbf{v}(\sigma_j^k)}\right)\right)}\right)$$

where the expression $ceil(x)$ is the lowest integer greater than x. Notice that the quantile associated with σ_j^k (using the notation as in (2)) is adjusted by the ratio of volumes $\mathbf{v}_{min}(k)/\mathbf{v}(\sigma_j^k)$.

STEP 4 Rank:

Determine a new most promising region $\sigma^B(k) \in \Sigma_{contend}(k)$ such that $\hat{y}\left(\delta \cdot \frac{\mathbf{v}_{min}(k)}{\mathbf{v}(\sigma^B(k))}, \sigma^B(k)\right) < \hat{y}\left(\delta \cdot \frac{\mathbf{v}_{min}(k)}{\mathbf{v}(\sigma_j^k)}, \sigma_j^k\right)$ $\forall \sigma_j^k \in \Sigma_{contend}(k)$. In the case of a tie, such that $\hat{y}\left(\delta \cdot \frac{\mathbf{v}_{min}(k)}{\mathbf{v}(\sigma_i^k)}, \sigma_i^k\right) = \hat{y}\left(\delta \cdot \frac{\mathbf{v}_{min}(k)}{\mathbf{v}(\sigma_j^k)}, \sigma_j^k\right)$ for sets $\sigma_i, \sigma_j \in \Sigma_{contend}(k)$ then let $\sigma^B(k)$ be the set with the greater volume, if volumes are tied break the tie arbitrarily.

STEP 5 Stopping Condition:

Record the minimum incumbent value $f_k^B = min_j f(x_{(1)}^j)$ for $j = 1, \ldots, \|\Sigma_{contend}(k)\|$. If $k \geq K$ and $\sigma^B(k)$ is unbranchable then stop the algorithm, otherwise increment k and go to Step 1.

The algorithm proceeds at each iteration to partition the most-promising region if it is unbranchable. It then samples a positive number of points (determined by a budgeting scheme) and estimates quantiles for each of the remaining regions. For purposes of selecting the most promising region, larger regions have proportionally smaller quantiles estimated (relative to the volume of the smallest contending region) and therefore the algorithm has a probability of selecting larger volumes as the "most promising" and "backtracking" to other areas of the domain for consideration. The algorithm terminates once an unbranchable region has been developed and a minimum number of iterations have elapsed. Therefore the algorithm ends with an unbranchable region with the lowest estimated quantile.

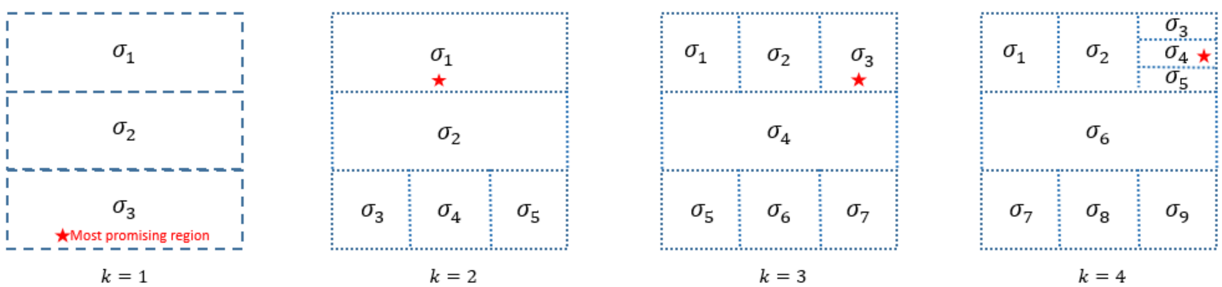

Figure 1: An example illustrating four iterations on a two dimensional domain, with $M = 3$.

An example is shown in Figure 1 for a two dimensional domain. On the first iteration the algorithm creates $M = 3$ different regions, and selects the most promising region indicated by a $\star$. On the second iteration the most promising region is partitioned (replacing σ_3 with σ_3, σ_4 and σ_5). In this example, the most promising region on iteration 2 is σ_1, illustrating backtracking. The algorithm finally lands on the most promising region σ_4 at $k = 4$ with σ_4 being an unbranchable region.

3 ASYMPTOTIC ANALYSIS

The quantile-based nested partition, has a number of useful convergence properties that mirror the original nested partition algorithm. First, we can observe that, as the number of iterations approaches infinity, the most promising region will be the subregion in Σ_{max} with the lowest true quantile. Let σ^* be the best unbranchable region, $\sigma^* \in \Sigma_{max}$ such that $y(\delta, \sigma^*) < y(\delta, \sigma)$ for all $\sigma \in \Sigma_{max}$ with $\sigma \neq \sigma^*$. For purposes of analysis we assume σ^* is unique.

Theorem 1 As $k \to \infty$ then $P\left(\sigma^B(k) = \sigma^*\right) \to 1$.

Proof. On every iteration, the algorithm either branches the most promising region $\sigma^B(k)$, or the most promising region is unbranchable in which case $\sigma^B(k) \in \Sigma_{max}$ and $\hat{y}\left(\delta, \sigma^B(k)\right) < \hat{y}\left(\delta \cdot \frac{\mathbf{v}_{min}(k)}{\mathbf{v}(\sigma_j)}, \sigma_j^k,\right)$ for all $\sigma_j^k \in \Sigma_{contend}(k)$ and $\sigma_j^k \notin \Sigma_{max}$.

As $k \to \infty$ then $v_{min}(k) \to v(\sigma^*)$ and the number of samples $N_j^k \to \infty$ in every σ_j^k in $\Sigma_{contend}(k)$, therefore

$$\hat{y}\left(\delta \cdot \frac{\mathbf{v}_{min}(k)}{\mathbf{v}(\sigma_j^k)}, \sigma_j^k\right) \to y\left(\delta \cdot \frac{\mathbf{v}(\sigma^*)}{\mathbf{v}(\sigma_j^k)}, \sigma_j^k\right)$$

with probability arbitrarily close to 1 by the consistency of the quantile estimator (Serfling 1980, Conover 1980).

Due to the consistency of the estimator and since the number of possible regions in $\Sigma_{contend}(k)$ is finite, as $k \to \infty$, it is true with probability approaching 1 that for any region $\sigma_j^k \in \Sigma_{contend}(k)$ either $\sigma_j^k \in \Sigma_{max}$ (unbranchable) or $\exists\ \bar{\sigma}_j^k \in \Sigma_{max} \bigcap \Sigma_{contend}(k)$ such that $y\left(\delta, \bar{\sigma}_j^k(k)\right) < y\left(\delta \cdot \frac{\mathbf{v}(\sigma^*)}{\mathbf{v}(\sigma_j^k)}, \sigma_j^k\right)$ and $\sigma^* \in \Sigma_{contend}(k)$.

To see this, consider two regions, $\sigma_j, \sigma_{j'}$ such that $\sigma_j \subset \sigma_{j'}$. Then $y(\delta \cdot \frac{\mathbf{v}(\sigma_j)}{\mathbf{v}(\sigma_{j'})}, \sigma_{j'}) \leq y(\delta, \sigma_j)$ since the set of points $\{x : f(x) < y(\delta, \sigma_j)\}$ is also contained in σ_j and therefore constitutes at least $\delta \cdot \frac{\mathbf{v}(\sigma_j)}{\mathbf{v}(\sigma_{j'})}$ of the total volume of σ_j'. Now, if for all regions $\sigma_j^k \in \Sigma_{contend}(k)$ either $\sigma_j^k \in \Sigma_{max}$ (unbranchable) or $\exists \bar{\sigma}_j^k \in \Sigma_{max} \bigcap \Sigma_{contend}(k)$ such that $y\left(\delta, \bar{\sigma}_j^k(k)\right) < y\left(\delta \cdot \frac{\mathbf{v}(\sigma^*)}{\mathbf{v}(\sigma_j^k)}, \sigma_j^k,\right)$ then for any branchable region that contains σ^*, i.e., $\sigma^* \subset \tilde{\sigma}_j^k$, we have $y(\delta \cdot \frac{\mathbf{v}(\sigma^*)}{\mathbf{v}(\tilde{\sigma}_j^k)}, \tilde{\sigma}_j^k) \leq y(\delta, \sigma^*) < y(\delta, \bar{\sigma}_j^k)$ for all $\bar{\sigma}_j{}^k \in \Sigma_{max} \bigcap \Sigma_{contend}(k)$ and therefore $\tilde{\sigma}_j^k \notin \Sigma_{contend}(k)$. Since at least one region in $\Sigma_{contend}(k)$ contains σ^* then $\sigma^* \in \Sigma_{contend}(k)$.

Therefore as $k \to \infty$ the probability that $\sigma^* \in \Sigma_{contend}(k)$ and $y(\delta, \sigma^*) < y\left(\delta \cdot \frac{\mathbf{v}(\sigma^*)}{\mathbf{v}(\sigma_j^k)}, \sigma_j^k\right)\ \ \forall \sigma_j^k \in \Sigma_{contend}(k)$ goes to 1, and as $k \to \infty$ then $P(\hat{y}(\delta, \sigma^*) < \hat{y}(\delta, \sigma^m(k))) \to 1$ and the probability $P\left(\sigma^B(k) = \sigma^*\right) \to 1$. □

In addition to proving the convergence properties of the algorithm to an unbranchable region with lowest specified quantile, we also prove that the final unbranchable region contains the true global optimum with probability approaching 1 as the number of iterations approaches infinity. For purposes of the analysis, we assume that global optimum x^* is unique.

Theorem 2 If f is a function that satisfies the Lipschitz condition with Lipschitz constant L, there exists a value δ^* such that for all $\delta < \delta^*$ then P($x^* \in \sigma^B(k)) \to 1$ as $k \to \infty$.

Proof. Consider $\sigma_i \in \Sigma_{max}$ for $i = 1, \ldots, \|\Sigma_{max}\|$. Let $x_i^* = argmin_{x \in \sigma_i} f(x)$. Order the unbranchable regions in Σ_{max} by their minimum values, i.e., $\sigma_{(1)}, \cdots, \sigma_{(\|\Sigma_{max}\|)}$ such that $f(x_{(1)}^*) \leq \cdots \leq f(x_{(\|\Sigma_{max}\|)}^*)$.

Consider $\sigma_{(1)}$ and $\sigma_{(2)}$ with $f(x_{(1)}^*) < f(x_{(2)}^*)$. From the Lipschitz condition there must be a hypersphere $\mathbf{h}$ centered at $x_{(1)}^*$ and $\mathbf{v}\left(\mathbf{h} \bigcap \sigma_{(1)}\right) > 0$, such that $\forall x \in \mathbf{h} : f(x) < f(x_{(2)}^*)$. Therefore for $\delta < \delta^* = \frac{\mathbf{v}(\mathbf{h} \bigcap \sigma_{(1)})}{\mathbf{v}(\sigma_{(1)})}$, we are assured that $y(\delta,\sigma_{(1)}) < y(\delta,\sigma_{(i)})\ \ \forall i \neq 1$. The best σ^* relative to a $\delta < \delta^*$ satisfies $y(\delta,\sigma^*) \leq y(\delta,\sigma_{(i)})$ for all i, and therefore $\sigma^* = \sigma_{(1)}$ and $x^* \in \sigma^*$.

By Theorem 1, $P\left(\sigma^B(k) = \sigma^*\right) \to 1$ as $k \to \infty$. Therefore $P\left(x^* \in \sigma^B(k)\right) \to 1$ as $k \to \infty$. □

Therefore with a sufficiently small quantile threshold δ, the algorithm asymptotically develops an optimal region that contains the global minimum.

4 OPTIMAL BUDGETING

Although the quantile-based nested partition algorithm is guaranteed to eventually find the unbranchable region with lowest specified quantile, the efficiency of the algorithm will largely depend on the allocated budget N_j^k in each contending region $\sigma_j^k \in \Sigma_{contending}(k)$. At each iteration k the algorithm will sample points and branch the most promising region in order to focus more sampling in the newly branched regions on the next iteration. It is therefore important for efficiency to choose the most promising region with the lowest quantile to minimize backtracking and focus sampling in the regions likely to contain optimal points.

To ensure efficiency of the algorithm, values for N_j^k are chosen to maximize the probability of correctly selecting the most promising region. At a given iteration, we define an index b such that $y\left(\delta \cdot \frac{\mathbf{v}_{min}(k)}{\mathbf{v}(\sigma_j^k)}, \sigma_j^k\right) \geq y\left(\delta \cdot \frac{\mathbf{v}_{min}(k)}{\mathbf{v}(\sigma_b^k)}, \sigma_b^k\right)\ \ \forall \sigma_j^k \in \Sigma_{contend}^k$ for $j \neq b$. As in Chen et al. (2000), we formulate a program that maximizes the probability of correct selection as the following.

$$max_{N_1^k,\cdots,N_j^k}\quad P\left(Correct\ Selection\right) = P\left(\bigcap_{\forall j \neq b} \bar{y}\left(\delta \cdot \frac{\mathbf{v}_{min}(k)}{\mathbf{v}(\sigma_j^k)}, \sigma_j^k\right) \geq \bar{y}\left(\delta \cdot \frac{\mathbf{v}_{min}(k)}{\mathbf{v}(\sigma_b^k)}, \sigma_b^k\right)\right)$$

$$\text{subject to} \quad \sum_{j=1}^{\|\Sigma_{contend}(k)\|} N_j^k = k \cdot T$$

where $\bar{y}\left(\delta \cdot \frac{\mathbf{v}_{min}(k)}{\mathbf{v}(\sigma_j^k)}, \sigma_j^k\right)$ is a random variable representing an estimated quantile in the region σ_j^k after sampling. This creates an optimal computational budgeting program that can be further specified by describing the distribution of the quantile estimator. Based on non-parametric order statistics, we can establish that the estimator $\bar{y}\left(\delta \cdot \frac{\mathbf{v}_{min}(k)}{\mathbf{v}(\sigma_j^k)}, \sigma_j^k\right)$ for the quantile is normally distributed with specified mean and variance, such that:

$$\bar{y}\left(\delta \cdot \frac{\mathbf{v}_{min}(k)}{\mathbf{v}(\sigma_j^k)}, \sigma_j^k\right) \sim Nor\left(\hat{y}\left(\delta \cdot \frac{\mathbf{v}_{min}(k)}{\mathbf{v}(\sigma_j^k)}, \sigma_j^k\right), \frac{\left(1 - \delta \cdot \frac{\mathbf{v}_{min}(k)}{\mathbf{v}(\sigma_j^k)}\right) \cdot \left(\delta \cdot \frac{\mathbf{v}_{min}(k)}{\mathbf{v}(\sigma_j^k)}\right)}{\mathbf{f}\left(y(\delta \cdot \frac{\mathbf{v}_{min}(k)}{\mathbf{v}(\sigma_j^k)}, \sigma_j^k)\right)^2 \cdot N_j^k}\right)$$

where N is the number of points sampled, $\mathbf{f}$ is the probability density function of the sample distribution from the region σ_j^k, and $\hat{y}\left(\delta \cdot \frac{\mathbf{v}_{min}(k)}{\mathbf{v}(\sigma_j^k)}, \sigma_j^k\right)$ is the value of the quantile estimate in region σ_j^k (Serfling 1980).

Because of the normality of the estimator, we can extend the methodology for OCBA across a partitioned domain in order to asymptotically maximize the probability of correctly selecting the most promising region. The formula derived by Chen et al. (2000) specifies equations that asymptotically optimize the probability of correct selection when choosing sampling points to divide between a discrete number of normally distributed estimators,

$$\frac{N_{j'}}{N_j} = \left(\frac{\frac{s_j}{\delta_{b,j}}}{\frac{s_{j'}}{\delta_{b,j'}}} \right)^2 \qquad \forall j, j' \neq b$$

$$N_b = s_b \sqrt{\sum_{j=1, j\neq b}^{\|\Sigma_{contend}(k)\|} \frac{N_j^2}{s_j^2}}$$

where $\delta_{b,j} = \hat{y}\left(\delta \cdot \frac{\mathbf{v}_{min}(k)}{\mathbf{v}(\sigma_j^k)}, \sigma_j^k\right) - \hat{y}\left(\delta \cdot \frac{\mathbf{v}_{min}(k)}{\mathbf{v}(\sigma_b^k)}, \sigma_b^k\right)$ and $s_j^2 = \frac{(1-\delta\cdot\frac{\mathbf{v}_{min}(k)}{\mathbf{v}(\sigma_j^k)})\cdot\delta\cdot\frac{\mathbf{v}_{min}(k)}{\mathbf{v}(\sigma_j^k)}}{\mathbf{f}(y(\delta\cdot\frac{\mathbf{v}_{min}(k)}{\mathbf{v}(\sigma_j^k)}, \sigma_j^k))^2}$. These equations therefore fully specify a division of the budget between partitions and with a total budget per iteration of $k \cdot T$.

Estimating the difference $\delta_{b,j}$ can be computed through estimating $\hat{y}\left(\delta \cdot \frac{\mathbf{v}_{min}(k)}{\mathbf{v}(\sigma_j^k)}, \sigma_j^k\right)$ based on previously sampled points. The approximation of s_j can be estimated through a jack-knife approximation, a sectioning approximation, or by estimating the pdf $\mathbf{f}$ through kernel density estimation. As such, given a constant budget per each iteration, we can determine the number of samples N_j^k from each of the contending regions that is asymptotically optimal for maximizing the probability of selecting the contending region with the lowest true quantile.

5 NUMERICAL RESULTS

In this section we apply the algorithm described in Section 2 to three test functions in order to demonstrate the effectiveness of the algorithm with the *OCBA* scheme. The test problem is formulated as

$$min_{x\in S} f(x) \tag{3}$$

where S is a square domain and the three different test functions $f(x)$ taken from Ali et al. (2005) are specified as:

1. **General Sinusoidal Function:** $f(x) = -[A \cdot \prod_{i=1}^{n} sin(x_i - z) + \prod_{i=1}^{n} sin(B \cdot (x_i - z))]$ with $A = 2.5$, $B = 5$, $z = 30$ in two dimensions on the domain $S = \{[0,180],[0,180]\}$ with a true minimum at $(90,90)$ with value -3.5.

2. **Rosenbrock Function:** $f(x) = \sum_{i=1}^{n-1} [100 \cdot (x_{i+1} - x_i^2)^2 + (x_i - 1)^2]$ in two dimensions on the domain $S = \{[-2,2],[-2,2]\}$ with a true minimum at $(1,1)$ with value 0.

3. **Ackley's Function (Problem):** $f(x) = -20 \cdot exp\left(-0.02\sqrt{n^{-1}\sum_{i=1}^{n} x_i^2}\right) - exp\left(n^{-1}\sum_{i=1}^{n} cos(2\pi x_i)\right) + 20 + e$ in two dimensions on the domain $S = \{[-32.768, 32.768],[-32.768, 32.768]\}$ with a true minimum at $(0,0)$ with value 0.

The first numerical experiment compares the performance of the quantile-based nested partition algorithm under two different sampling schemes that determine the values of N_j^k. The first sampling scheme uniformly allocates an equal division of the budget to each region, i.e., σ_j^k gets $ceil\left(\frac{T}{\|\Sigma_{contend}(k)\|}\right)$ new samples. The second sampling scheme is the OCBA scheme, where N_j^k is determined by the equations developed in Section 4. For OCBA, we use a sectioning approach with size of 20 samples to approximate the variance of the quantile estimator.

In order to evaluate the performance of the algorithms, we allocate a budget $T = 1200$ for each iteration, $M = 6$ as the number of divisions via branching, and δ threshold 0.05, and $K = 6$. We allow the algorithm

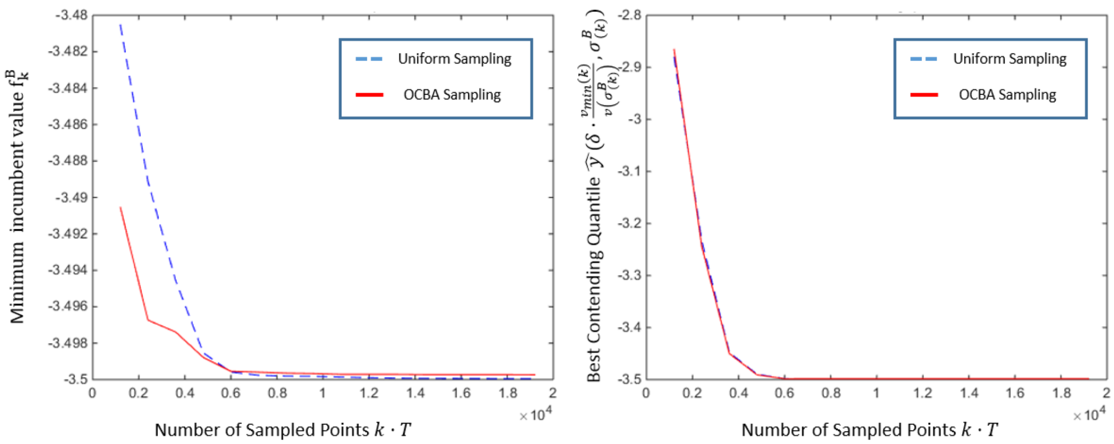

Figure 2: The minimum sampled point (left) and minimum quantile (right) plotted against the total number samples for the sinusoidal function. The plots for the uniform (broken line) and OCBA sampling (solid line) are both shown.

to make 5 branching operations before hitting an unbranchable region which means the lengths that define the unbranchable set are $(\varepsilon_1, \varepsilon_2) = (5, 0.8333)$ for the sinusoidal function, $(\varepsilon_1, \varepsilon_2) = (0.1111, 0.0185)$ for the Rosenbrock function, and $(\varepsilon_1, \varepsilon_2) = (1.8204, 0.3034)$ for the Ackley function. To measure consistent performance we report the average incumbent minimum value (f_k^B) and the average best contending quantile estimate $\left(\hat{y}\left(\delta \cdot \frac{v_{min}(k)}{v(\sigma^B(k))}\right), \sigma^B(k)\right)$ across 20 replications and plot the values relative to the number of samples taken at every iteration. The results for the algorithm run with equal allocation of budget (uniform sampling) and run with the OCBA sampling for the three test functions are shown in Figures 2, 3, and 4.

Generally, the numerical results demonstrate that the algorithm converges to a near-optimal value (relative to the target quantile), and the OCBA sampling scheme performs better than the algorithm paired with an equal allocation sampling scheme. For all three test functions, the best contending quantile estimate at each iteration for both sampling schemes are almost identical. However, generally the algorithm paired with OCBA shows a lower minimum incumbent value f_k^B. For the sinusoidal function in Figure 2, the OCBA algorithm develops lower values at early iterations and then tapers off after it locates the region with lowest quantile. For the Rosenbrock function in Figure 3, the opposite behavior is observed with the OCBA making mis-allocations early on and then developing better solutions at later iterations. The OCBA version of the algorithm consistently develops better incumbent points across all iterations on the Ackley function in Figure 4. Further testing will be done for different test functions.

To further explore the performance, we compared the quantile-based nested partition method (with uniform and OCBA sampling) to two other variations of nested-partition method: one that branches based on the sample mean in a region (i.e., estimated expected value over a region); and the other that uses the minimum-sampled value in a region.

We examined the performance of each of the four variations on the three test functions in 4 dimensions. To account for the additional resources needed for a 4-dimensional problem, we set new parameters $\delta = 0.0005$, $T = 10000$, $K = 20$ and maximum branching equal to 10. Running 20 replications we plot the average minimum values for the four variations and the three test functions in Figure 5. For the sinusoidal and Ackley's test functions, the quantile-based algorithm with the OCBA sampling scheme converges to a near minimum value with lower (better) points at the same iteration than the other variations. For the Rosenbrock function, the OCBA scheme does not consistently produce better performance results. The performance of the quantile-based nested partition algorithm with uniform sampling is shown to be generally

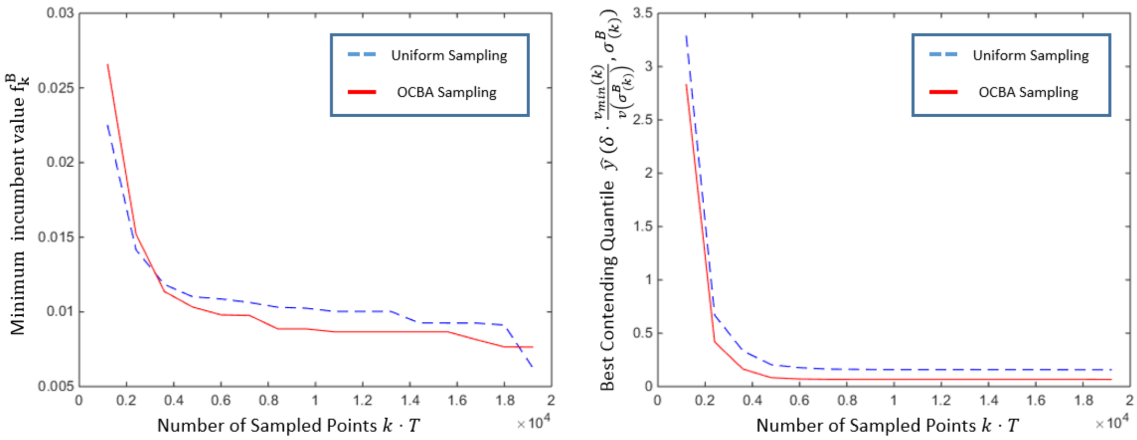

Figure 3: The minimum sampled point (left) and minimum quantile (right) plotted against the total number samples for the Rosenbrock function. The plots for the uniform (broken line) and OCBA sampling (solid line) are both shown.

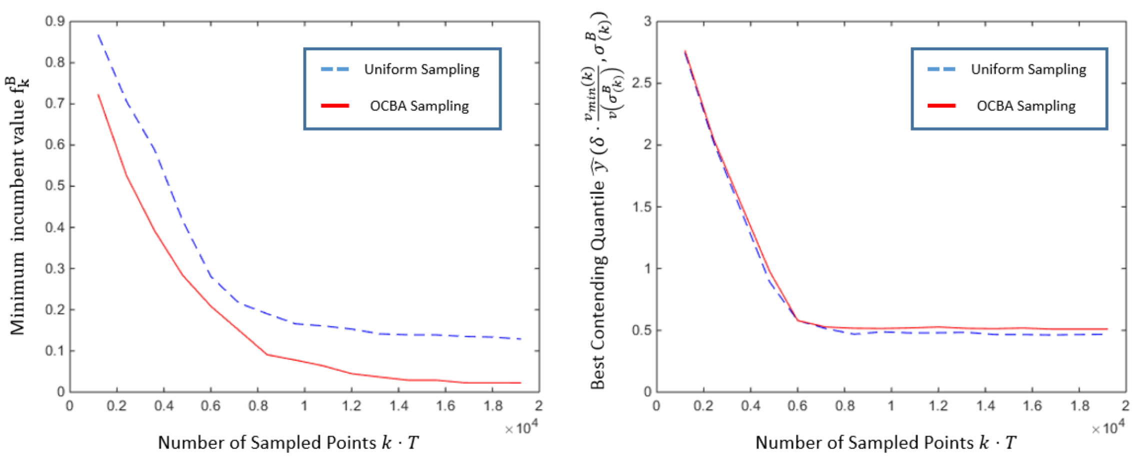

Figure 4: The minimum sampled point (left) and minimum quantile (right) plotted against the total number samples for the Ackley function. The plots for the uniform (broken line) and OCBA sampling (solid line) are both shown.

comparable to the nested partition based on minimum values. However, the addition of the OCBA scheme allows better performance in the case of the sinusoidal and Ackley's function.

6 DISCUSSION

This paper has developed an algorithm for finding optimal points for a black-box function on a continuous domain. The algorithm works within the framework of the nested partition method and uses a calculation of an adjusted sampled quantile to determine the most promising region. The algorithm then subsequently branches the most promising region in order to concentrate sampling in regions likely to contain global optimal solutions. We are able to directly prove that the developed algorithm will find a region with the lowest quantile with probability approaching 1 as the number of iterations goes to infinity. With a low

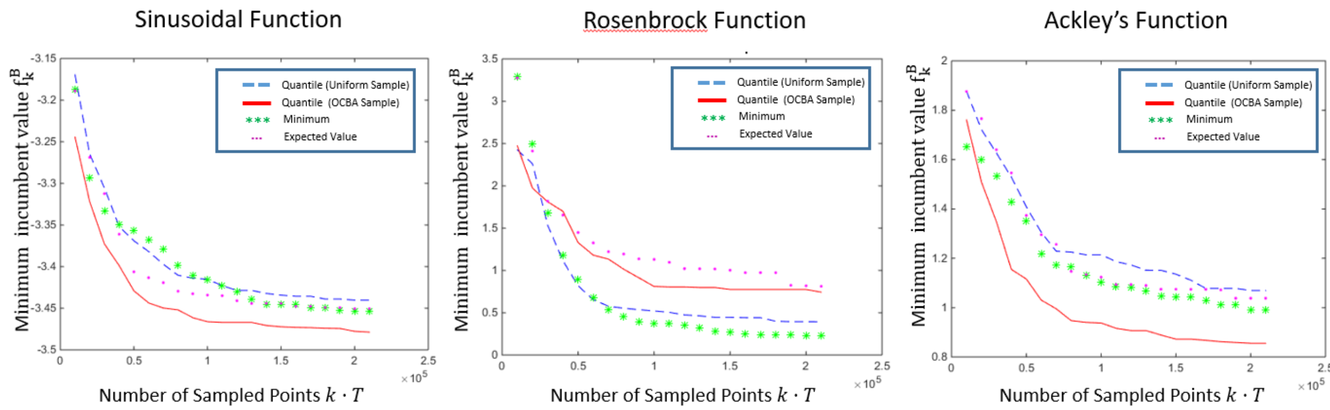

Figure 5: The minimum sampled point for the three test functions in four dimensions with four variations: the quantile-based nested partition with uniform and OCBA sampling schemes, and the nested partition method using minimum and estimated expected value for determining the most promising subregion.

enough quantile threshold, we prove that the region found will contain the true global minimum with probability approaching 1 as the number of iterations approach infinity.

The paper then determines an optimal sampling scheme at each iteration in order to maximize the probability of selecting the region with lowest adjusted quantile. Based on asymptotically normal properties of the quantile estimator, we derive sampling levels in each region that will maximize the probability of selecting the most promising region as the number of samples approaches infinity.

With the developed OCBA scheme, we apply our algorithm to several common test functions to demonstrate the effectiveness of employing the quantile-based nested partition algorithm. In all three cases we show that the algorithm quickly converges to a near optimal solution and also that the application of the OCBA budgeting scheme allows the algorithm to more efficiently reach near-minimum points. Comparison with other nested-partition methods shows that the quantile-based algorithm can achieve better values for selected problems.

Several extensions of the current algorithm might be developed in order to improve the quantile-based nested partition algorithm. First, the algorithm could be modified in order to regroup previously branched regions in order to avoid sampling in less promising areas. The proof developed in Theorem 1 might be extended to this algorithm to show convergence. A second possible extension is to iteratively adjust the quantile thresholds at each iteration of the algorithm. This modification would satisfy the condition described in Theorem 2 in the limit while avoiding the problems of using extreme values to determine the most promising regions early in the algorithm when the number of sampled points are low.

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