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A QUANTILE ADAPTIVE SEARCH FOR BLACK-BOX SIMULATION OPTIMIZATION ON CONTINUOUS DOMAINS WITH PRACTICAL IMPLEMENTATIONS

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ABSTRACT

Due to the use of complex models in simulation, black-box optimization methods have been useful in the field of simulation optimization. Since black-box functions lack exogenous information about the structure of the function, optimization methods often employ random search to focus sampling inside a domain. This poster describes an optimization framework, Quantile Adaptive Search (QAS), for focusing sampling inside a nested set of quantile level sets on a continuous domain. The poster describes theoretical results regarding the complexity of QAS. In addition, methods for implementing the framework using Probabilistic Branch and Bound and Hit-and-Run are discussed.

EXTENDED ABSTRACT

Due to the complex nature of systems, advanced simulation and optimization algorithms are required to develop good or near optimal solutions (e.g., for parameter selection or model tuning). The optimization of complex simulation systems often involve functions with no additional structural information (e.g., convexity), or "black box" functions, which involve key challenges for optimization algorithms. First, algorithms can only practically generate solutions within a certain distance from a true optimum (such as an indifference region). Second, global optimization algorithms must balance the need to explore the domain versus focusing sampling on areas that have already generated promising solutions. To address these problems, both theory and practical algorithms have been developed to sample within improving level sets with a consistent probability to ensure that a given algorithm neither converges too quickly to a local optimum nor spends too much time sampling inside of non-promising regions in the domain (Zabinsky and Smith 1992, Zabinsky 2003).

This poster explores the issue of global optimization algorithms that attempt to sample from a nested sequence of level sets based on increasing quantiles. The work begins with the description of a framework called Quantile Adaptive Search (*QAS*), which allows the use of a variety of different methods to obtain samples within targeted quantiles. The analysis makes basic assumptions about the function, the continuous domain, and the sampling distributions, and characterizes computational performance. In *QAS*, the use of quantiles allows an optimization search to focus its search efforts on a more refined subset of the domain, using information about a function from previous samples. Under the framework, we provide an analysis of complexity to be used as a basis for controlling the sampling distributions of random search for a variety of optimization approaches.

The complexity analysis provided builds on previously developed theoretical global optimization frameworks such as Pure Adaptive Search (*PAS*) and Hesitant Adaptive Search (*HAS*) which describe algorithms that iteratively sample inside improving level sets (Bulger and Wood 1998, Wood et al. 2001, Zabinsky 2003, Zabinsky 2015). The analysis of *PAS* and *HAS* show that, under some conditions, the algorithm's expected number of iterations before obtaining a desired minimum value increases only linearly in dimension. Additional research has shown that relating other algorithms to *HAS* and *PAS*, such as Annealing Adaptive Search (*AAS*), can be used to develop theoretically sound sampling strategies for finding near global optimum solutions. In (Shen et al. 2007), the analysis is used to derive a cooling schedule in the context of simulated annealing.

We demonstrate conditions under which *QAS* can achieve theoretical properties similar to the ideal performance of *PAS* and more relaxed properties of *HAS* and *AAS*. The analysis focuses on selecting a sequence of increasing quantiles to guide a sampling distribution, balancing between selecting low quantiles (easy to sample from) and high quantiles (better objective values, but difficult to sample from), analogous to developing a cooling schedule for *AAS*. By targeting an adaptive sequence of nested quantile level sets, the algorithm balances the probability of sampling within a quantile with the computational expense of sampling (Romeijn and Smith 1994, Shen et al. 2007).

We provide some initial results concerning the estimation of a target level set for a general sampling distribution. On each iteration, the sampling distribution and quantile can be controlled to achieve a targeted computational budget with probabilistic quality of solution. This analysis also has practical uses for algorithm stopping time (Zabinsky et al. 2010).

The poster will discuss various implementations of optimization algorithms with several different ways of adapting the sampling distributions based on the provided theoretical results. We expand existing algorithms such as Probabilistic Branch and Bound, and a Hit-and-Run Monte Carlo Markov Chain method in order to statistically sample within a sequence of nested level sets defined by increasing quantiles (Huang and Zabinsky 2014, Zabinsky and Smith 2013, Linz et al. 2016). Some initial numerical results will be presented. We comment briefly on expanding the methodology to mixed continuous and integer domains and functions with noise.

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