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A BAYESIAN OPTIMIZATION ALGORITHM FOR CONSTRAINED PROBLEMS WITH HETEROSCEDASTIC NOISE

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ABSTRACT

In this research, we develop a Bayesian optimization algorithm to solve expensive constrained problems. We consider the presence of heteroscedastic noise in the evaluations, and propose an identification procedure that considers this uncertainty in recommending the final optimal solution(s). The primary experimental results show that the proposed algorithm is capable of finding a set of optimal (or near-optimal) solutions in the presence of noisy observations.

1 INTRODUCTION

Simulation optimization is an often-used approach for optimizing black-box problems. Different approaches exist and have been used successfully in, e.g., engineering design (Qing et al. 2021) and hyperparameter tuning of machine learning algorithms (Wu et al. 2019). Most of these approaches (e.g., evolutionary algorithms) require many function evaluations before converging to the optimal solution(s). Yet, this causes a problem when the simulation model is expensive to run (because of long running times, high monetary cost, or hazardous experiments), implying that data-efficient optimization algorithms are needed. Moreover, in many simulation optimization problems, the true objective and constraint functions are not observable with perfect accuracy; only noisy observations are available (Amaran et al. 2016). This noise makes it harder to study/predict the effect of the input vector on the output values. While replication is a common strategy to reduce this noise, this again poses a problem in settings with an expensive simulator (Zhan and Xing 2020).

This research proposes a Bayesian optimization (BO) algorithm to solve expensive and noisy constrained problems in a data-efficient way. Work on using Bayesian optimization for solving noisy constrained problems is scarce . All these articles pose a questionable assumption on the distribution of the noise; they assume that the noise is homoscedastic. Furthermore, when the stopping criterion is met and they switch to the identification phase, they return a single feasible solution with the best observed (or predicted) mean and disregard uncertainty on the values of the functions because of noise. Contrary to the current algorithms, the goal is not to return a single solution; given the noisy outcomes for objective and constraint functions, obtaining such result may require a large budget to be used in the ranking and selection phase. Instead, the proposed algorithm identifies the solution with the best expected performance, and then returns the subset of all solutions in the search space that are estimated to be statistically equivalent to this solution in terms of the goal function, while ensuring that they reach a user-defined probability of feasibility.

2 PROPOSED ALGORITHM

The proposed algorithm follows the general framework of the BO algorithms, using a Latin hypercube sample to obtain a space-filling set of initial design points, and approximating the objective function and the m constraints using m+1 independent stochastic kriging surrogates (Ankenman et al. 2008). The search space is discretized into a (very large) set of candidate points. In the first phase, the search tries to move to an estimated optimal solution using a modification of the barrier acquisition function proposed in (Pourmohamad and Lee 2022). When the variation of the objective function at the optimal solution is below a user-defined threshold, the algorithm moves to the accuracy phase. In this phase, using two novel acquisition functions the algorithm improves (1) the accuracy of the approximated functions among solutions that fall in the vicinity of the optimal solution so far , and (2) the probability of feasibility among the same solutions. In the identification phase, the most recent metamodel information is used to screen out candidate solutions that do not meet a prespecified probability of feasibility, or that are statistically inferior (to that end, we modify the screen-to-the-best procedure proposed in (Boesel et al. 2003)). The algorithm then returns the remaining solutions.

To assess the performance of the algorithms, we solve three problems: the synthetic problem proposed originally in (Gramacy et al. 2016), a modified version of this synthetic problem, and a popular mechanical engineering test problem focusing on the design of a spring (used also, for instance, in (Tao et al. 2020)). We modify the objective and constraint functions with different noise patterns. The primary experimental results show that the proposed algorithm is capable of finding a set of optimal (or near-optimal) solutions in the presence of noisy observations.

3 CONCLUSION

This research proposes a Bayesian optimization algorithm for constrained problems with heteroscedastic noise, including a novel identification procedure that considers the uncertainty in recommending the final optimal solution(s). The algorithm’s performance are examined and its efficiency are demonstrated.

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