Coupling Constraints in Bayesian Optimization with Uncertainties

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ABSTRACT

In this work, the problem of chance constrained optimization is considered. The objective is to optimize a function while satisfying constraints, both of which are affected by uncertainties. The high computational cost of realistic simulations strongly limits the number of evaluations and makes this type of problems particularly challenging. In this context, Bayesian optimization algorithms are a popular approach. In this work, it is assumed that the uncertainty comes from random input variables, which makes it possible to define a joint space of deterministic design variables and uncertain input parameters. A Gaussian process is then built in this joined space of design and uncertain variables.

Our first contribution is a two-step acquisition function allowing to optimize the expected objective function value while ensuring that the constraints satisfaction probability is above a given threshold. The first step consists in identifying the most promising location in the (deterministic) design space by optimizing the expected feasible improvement. During the second step, the uncertain variables which minimize the one-step-ahead variance of the feasible improvement are computed. To improve the computational efficiency, a semi-analytical proxy to this one-step-ahead variance is devised. The calculated deterministic and uncertain variables are then used to update the Gaussian process indexed over the joint space.

The second contribution is based on the additional assumption that the constraints are correlated. This is the case in practice because many constraints depend on the same underlying physical phenomena (e.g., displacements and mechanical stresses). Here, the constraints are modeled as a single multi-output Gaussian Process relying on an "output as input" encoding. This can improve the model accuracy by better exploiting the information provided by the available data set, thus resulting in a faster and more robust optimization convergence. This idea is further developed by enabling that each constraint is evaluated at a different uncertain variable, thus improving the refinement of the model of the constraints. Finally, the output-as-input coding makes it possible for the acquisition criterion to optimally select a subset of the constraints to be evaluated at each iteration, thus avoiding unnecessary computations.

The proposed optimization algorithm and associated variants are tested on a number of analytical and engineering related test-cases. The results show promising results both in terms of convergence speed and robustness with respect to the initial training data set.

The authors would like to thank the OQUAIDO consortium for partly funding this work.