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Design Optimization of a Stochastic Multi-Objective Problem: Gaussian Process Regressions for Objective Surrogates

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# ABSTRACT

# Global optimization of expensive, multi-modal and noisy multi-objective functions is a common problem that comes up frequently in various areas of computational and experimental research. Along with being expensive to evaluate and noisy, we are also particularly interested in cases where the objective function under consideration is a black box and does not provide gradient information of the quantity of interest (QoI) with reference to the inputs. Because of the high cost of every single evaluation of such objective functions, we can only obtain a limited number of evaluations. This necessarily induces epistemic uncertainty (lack of knowledge due to limited data) on our problem. The Bayesian approach provides a natural framework to tackle this problem, building Gaussian process surrogates that model the objective functions and allow a sequential optimization process. The method applies the expected improvement (EI) information acquisition function in each iteration to perform an efficient global optimization (EGO) and discover the Pareto front of the problem, which contains the set of optimal solutions of the objectives. We implemented this method in a NanoHUB tool and tested it with synthetic examples and real observations of an expensive experiment, where it proved to be efficient in finding the corresponding set of optimal solutions for each problem. This methodology demonstrates how the efficiency of the Bayesian approach for handling epistemic uncertainty in multi-objective optimization problems, dealing with limited observations and avoiding a high amount of evaluations of time-consuming codes or expensive experiments.

# KEYWORDS

Gaussian process, Multi-Objective, Optimization, Regression, Surrogate, Uncertainty