The Summer Undergraduate Research Fellowship (SURF) Symposium
4 August 2016
Purdue University, West Lafayette, Indiana, USA

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

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ABSTRACT

Multi-objective optimization (MOO) problems arise frequently in science and engineering situations. In an optimization problem, we want to find the set of input parameters that generate the set of optimal outputs, mathematically known as the Pareto frontier (PF). Solving the MOO problem is a challenge since expensive experiments can be performed only a constrained number of times and there is a limited set of data to work with, e.g. a roll-to-roll microwave plasma chemical vapor deposition (MPCVD) reactor for manufacturing high quality graphene. State-of-the-art techniques, e.g. evolutionary algorithms; particle swarm optimization, require a large amount of observations and do not completely reveal the true PF. Recent extensions of Bayesian global optimization (BGO) are able to address the problems where the objective functions are expensive to evaluate, by replacing the expensive objective functions with cheap-to-evaluate surrogates trained with few input-output pairs. These surrogates provide prediction error bars that correspond to the epistemic uncertainty induced by limited data. BGO uses an information acquisition function (IAF) to quantify the improvement that a hypothetical experiment could make to the state of knowledge of the Pareto front in the MOO problem. This allows us to sequentially select the designs that maximize this enhancement. In this work we developed a NanoHUB tool that enables experimentalists to use BGO using an extension of the expected improvement over hypervolume (EHVI) IAF to provide solutions to MOO problems under uncertainty. We verified the tool through synthetic examples and we used it in the challenging task of optimizing the manufacturing of high-quality graphene using an MPCVD reactor.

KEYWORDS

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