Targeted Variance Reduction: Robust Optimization of Expensive Black-Box Simulators with Noise Parameters

Simon Mak
Department of Statistical Science, Duke University, USA

Abstract

The problem of optimizing an expensive black-box function arises in many complex scientific and engineering problems, from rocket engine design to pandemic intervention analysis. In many such situations, this black-box function has not only a set of controllable inputs that the user can optimize, but also a set of random inputs that are uncontrollable in practice. Here, random inputs may arise from uncontrollable noise factors or from unknown simulation model parameters that need to be probabilistically inferred from data. We thus propose a new robust Bayesian optimization method that factors in the presence of random input factors for black-box optimization. Leveraging a carefully constructed Gaussian process surrogate, we derive a closed-form acquisition function that jointly balances exploration, exploitation and solution precision over the random inputs for adaptive sampling of the black-box objective function. We then demonstrate the effectiveness of our approach for optimizing a suite of numerical test functions and the design of braking materials for automobile brake design.