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Computationally Efficient Solution of Inverse Problem Using Bayesian Global Optimization Approach

Zixuan Liu
Department of Computer Science, Purdue University
Ilias Billionis, Piyush Pandita
Department of Mechanical Engineering, Purdue University

ABSTRACT

Models have parameters that need to be determined from experimental observations. The problem of determining these parameters is known as the *inverse problem* or the *model calibration* problem. Solving inverse problems can be ubiquitously difficult because when the models involved are computationally expensive, one can only make a limited number of simulations. This work addresses the issue of solving an inverse problem with a limited data budget. Towards this end, we pose the inverse problem as the problem of minimizing a loss function that measures the discrepancy between model predictions and experimental measurements. Then, we employ Bayesian global optimization (BGO) to actively select the most informative simulations until either the expected improvement falls below a user defined threshold or our computational budget has been exhausted. We apply our results to the problem of estimating the kinetic rate coefficients modeling the catalytic conversion of nitrate to nitrogen using real experimental data.

KEYWORDS

Inverse problems, Bayesian Global optimization, Gaussian process, square loss function, nanoHUB, rappture