Sequential Designs Based on Bayesian Uncertainty Quantification in Sparse Representation Surrogate Modeling

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Abstract

A numerical method, called OBSM, was recently proposed which employs overcomplete basis functions to achieve sparse representations. While the method can handle non-stationary response without the need of inverting large covariance matrices, it lacks the capability to quantify uncertainty in predictions. We address this issue by proposing a Bayesian approach which first imposes a normal prior on the large space of linear coefficients, then applies the MCMC algorithm to generate posterior samples for predictions. From these samples, Bayesian credible intervals can then be obtained to assess prediction uncertainty. A key application for the proposed method is the efficient construction of sequential designs. Several sequential design procedures with different infill criteria are proposed based on the generated posterior samples. Numerical studies show that the proposed schemes are capable of solving problems of positive point identification, optimization, and surrogate fitting.