Bayesian Optimal Experimental Design for Surrogate Model Training

Xun Huan
University of Michigan
xhuan@umich.edu

Coauthor(s): Aniket Jivani

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Surrogate models can bring substantial computational accelerations to multi-query tasks such as uncertainty propagation, Bayesian inference, and design optimization. The training of parametric surrogate models is typically conducted in a deterministic manner, without quantified uncertainty, from a set of randomly selected high-fidelity computer simulations. We present a Bayesian approach for training surrogate models that captures the uncertainty from surrogate approximation, and employ optimal experimental design (OED) to guide the selection of next input values to run the high-fidelity simulations. We achieve this through a myopic OED procedure by iterating between inference and OED: update the prior to posterior through methods of Markov chain Monte Carlo or variational inference, and from the updated prior identify inputs for running new simulations that would yield the greatest expected information gain. Such a procedure can bring benefits of quantifying uncertainty in surrogate models, and enabling greater sampling efficiency in the simulation training points.