Ph.D. Defense
by
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"A Sequential Adaptive Sampling Technique Based on Local Linear Model for Computer Experiment Applications"

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Abstract:
The objective of this dissertation research is to develop a model independent sequential adaptive sampling technique for surrogate model (SM) applications based on a local linear model. This technique, called Nearest Neighbors Adaptive Sampling (NNAS), is conceived to be conceptually simple, computationally robust, and easy to apply, all characteristics that are crucial for effective surrogate modeling application during early phases of the engineering design process. SMs are now regarded as powerful engineering tools for the approximation of expensive responses – obtained either from computer simulations or real experiments – via less computationally expensive mathematical models. The use of SMs is especially valuable during the preliminary design phase when engineers need fast and accurate tools to assess the performance of different configurations and to define the top-level specifications that will guide the entire design process. Due to the increasing importance of SMs, new strategies are continuously being devised to build more flexible SM formulations, to rigorously select an SM technique from a set of candidates, and to efficiently sample the design space to collect the data required to train an SM.

The considerable influence of the sample distribution on SM accuracy motivates efforts to develop advanced strategies to improve the sampling process. In particular, the adoption of sequential adaptive sampling techniques has been empirically shown to reduce the number of samples required to obtain an SM of specified accuracy. However, these techniques are typically challenging to implement, limited by assumptions about the response, and dependent on the SM formulation selected to supervise the sampling process (e.g. cross validation and Kriging based strategies), making them impracticable for most engineering design applications. In particular, model dependence – a common characteristic of most state-of-the-art adaptive sequential sampling techniques – may decrease the sampling efficiency if the guiding SM is inappropriately chosen.

The proposed NNAS technique avoids the limitations of model dependence by introducing a new refinement metric – the Non Linearity Index (NLI) – which estimates the local nonlinear characteristics as the difference between the actual response value \( f(x_{T,i}) \) and the local function approximation represented by the hyperplane obtained via Weighted Least Squares Regression of the closest \( D+k \) points in the neighborhood of \( x_{T,i} \), where \( D \) is the domain dimensionality. The use of local linear models to assess the nonlinear characteristics of the response without the need for a global SM is the key characteristic of NNAS that makes this strategy model independent. Additionally, NNAS introduces a new stochastic Pareto-ranking-based selection criterion to simultaneously maximize the refinement and exploration of the design space search, thereby ensuring a balance between the two behaviors. The initial NNAS and NLI formulations have also been expanded to include a form of directional sampling in which the algorithm identifies both region and direction of sampling.
NNAS embodies the capabilities of sampling multi-response design spaces, working in batch-mode (i.e. adding more than one sample at a time), and continuing the sampling process even in the event of a critical error in the f evaluation, e.g. the lack of convergence of a computational model at points in the design space. These characteristics together with its ease of implementation make NNAS a valuable, efficient and robust sampling strategy to use during the early phases of engineering design.

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