An Adaptive Design of Experiments Methodology with Noise Resistance for Unreplicated Experiments

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Abstract

A new heuristic adaptive sampling method is proposed for Design of Experiments applications. It balances space-filling, local refinement, and error minimization objectives, while minimizing reliance on delicate tuning parameters. Metamodeling is performed using a variation of HOLMES approximants which take advantage of boundary-corrected kernel density estimation to increase accuracy and robustness on highly clumped datasets. HOLMES approximants confer the resulting metamodel with some robustness against data noise to provide a practical approach for the common case of unreplicated experiments. The method compares favourably against Full Factorial and Latin Hypercube Sampling designs on numerous two-dimensional, noiseless test cases. Comparisons against a comparable adaptive sampling method are also performed for the case of unreplicated designs with measurement error, and the results demonstrate the superiority of the proposed approach. A final example explores an interesting and novel application of Design of Experiments technology to particle-based numerical solutions to PDEs - and specifically the burgeoning field of Adaptive Spatial Resolution - by using Design of Experiments techniques in the particle refinement process. Results from a simple crack propagation example suggest potential for this approach in the future.