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Acceleration of Optimal Bayesian Experimental Design via Decision Trees Methods with Orthgonality Constraint

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Optimal Bayesian Experimental Design is one of the methods for data acquisition system optimization that is frequently utilized in subsurface flow problems. In this method utility function that measures expected quality of the experiment is derived from the first principles of probability and statistics as a function of design parameters (aka sensor location). Therefore, the optimal experimental scheme can be found as a maximum of that utility function.

The most significant advantage of this method is solid Mathematical foundations.
Unfortunately, direct calculation of the Utility Function is computationally expensive, because it requires nested MCMC integration [1].

In the author's previous work [2] it was shown that Polynomial Chaos Expansion (PCE) can be utilized to accelerate Bayesian Experimental Design significantly. Basically, a novel approach for the utilization of PCE to avoid nested MCMC integration was proposed. The key idea for developing of that novel technique was the orthogonality of basis polynomial functions in PCE.

Despite the advantages of PCE, Decsiion Trees and Gradient Boosting methods seems to be an attractive alternative to PCE due to high popularity and simplicity in tuning. Therefore, the present work shows how orthogonality ideas can be extended to Decision Trees or Gradient Boosting like methods to provide acceleration of Bayesian Experimental Design. In other words, the novel algorithm for construction of the Gradient Boosted trees with specific orthogonality constraint was developed and examined on several test cases that include flow in porous media. Additionally, validation against classical methods is provided.

Participation

In-Person

References

[1]Xun Huan, Youssef M. Marzouk, Simulation-based optimal Bayesian experimental design for nonlinear systems, Journal of Computational Physics, Volume 232, Issue 1, 2013, Pages 288-317, ISSN 0021-9991, https://doi.org/10.1016/j.jcp.2012.08.013

[2] Alexadner Tarakanov, Ahmed H. Elsheikh, Optimal Bayesian experimental design for subsurface flow problems, Computer Methods in Applied Mechanics and Engineering, Volume 370, 2020, 113208, ISSN 0045-7825, https://doi.org/10.1016/j.cma.2020.113208.

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