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Computer Experiments in the Context of Simulation-Driven Design –A Cautionary Tale

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In light of the advances of simulation technology over the last decades, engineering design increasingly turns towards simulation-driven practices. However, with the enormous possibilities for parametric optimization, it is often neglected that many other design decisions require efficient screening to gain insights about the significance of inputs. Examples include the choice of different design configurations, prioritising design variables for further investigation, or the exploitation of interaction effects for increased product robustness.

While many engineering applications for this purpose still rely on simple tools such as traditional fractional factorials, this presentation will address the challenges of applying more sophisticated designs and surrogate modelling approaches for a design rather than a detailed modelling task.

Building on Joseph's review of space-filling designs [1], sampling designs suitable for computer simulations are investigated which have advantages in their specific use cases. If the goal is to interpolate based on the samples, a meta-model can be created based on the kriging method, allowing to gain more information about the design space. The performance of a metamodel can be characterized using the Cross Validation Error (CVE) metric. Screening for significant effects and their behaviour can be done by using functional decomposition, also known as functional ANOVA.

Four designs, namely the Central Composite Design, the MiniMax, and two versions of Latin Hypercube Designs (LHD), have been used for multi-objective injection molding simulations with three varying inputs in Moldex3D. CVE values and functional decomposition of the main effects for the kriging-based metamodels are investigated for each sampling model resulting in different model accuracy and estimated variable main effects for each design.

Model dependence of the effectiveness the sampling methods apparent in the injection molding case is eliminated by carrying out a study using known true functions. Analyzing the data using functional decomposition and kriging, the LHD performed overall the best, yielding the lowest CVE and matching the true main effects the closest. The influence of interaction effects in the true model is investigated, where introducing interaction effects in the true model lead to distortion of the shape of the main effects. When there is an interaction significant but one of its components is not, it may show up as a falsely significant main effect in the functional decomposition causing misinterpretation of the results, unless the interaction effects are considered in the functional decomposition.

Overall, it can be concluded that the performance of sampling designs is heavily model dependent.
Introducing artificial interaction inputs (AII) in the metamodel for a true model lacking interaction may allow the identification of the significant interaction effects in exemplary cases. The approach of analyzing the AII may lead to more insights to the design space but requires more research to allow for an estimation of its accuracy and robustness.

References

[1] V. Roshan Joseph. "Space-filling designs for computer experiments: A review". In: Quality Engineering. Vol. 28. 1. Taylor and Francis Inc., Jan. 2016, pp. 28–35. doi: 10.1080/08982112.2015.1100447.

Primary authors: BAUCHROWITZ, Moritz Leopold (Technical University of Denmark); ATHREYA, Naganathan Krishnan (Technical University of Denmark); JUUL-NYHOLM, Herle Kjemtrup (Technical University of

Denmark); EIFLER, Tobias (Technical University of Denmark); KULAHCI, Murat (Technical University of Denmark)

Presenters: BAUCHROWITZ, Moritz Leopold (Technical University of Denmark); ATHREYA, Naganathan Krishnan (Technical University of Denmark); JUUL-NYHOLM, Herle Kjemtrup (Technical University of Denmark); EIFLER, Tobias (Technical University of Denmark); KULAHCI, Murat (Technical University of Denmark)

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