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Process Optimization Using Bayesian Models for Bounded Data

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Design space construction is a key step in the Quality by Design paradigm in manufacturing process development. Construction typically follows the development of a response surface model (RSM) that relates different process parameters with various product quality attributes and serves the purpose of finding the set of process conditions where acceptance criteria of the objectives are met with required level of assurance. If a potentially large number of process parameters is being looked at, this RSM can be developed from a screening plus augmentation study.

Although normal RSM is typically fitted for this investigation, this is often no longer applicable for bounded response. Using the incorrect model can lead to identification of the wrong parameters in the screening study, thereby leading to a non-optimal design space.

In this work, we show the use of Beta-regression and Fractional-response generalized linear models as alternatives to the normal RSM. All models are fitted in the Bayesian framework since the expected posterior distribution is typically used in characterizing the design space. We compare the performance of the two models across different location and spread scenarios. We demonstrate this technique using simulated data that was derived based on a real optimization study in chemical synthesis.

Keywords

Bayesian RSM, Beta-regression, Fractional-response

Classification

Both methodology and application

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