Model-Robust Process Optimization using Bayesian Model Averaging

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ABSTRACT

Traditional approaches for process optimization start by fitting a model and then optimizing the model to obtain optimal operating settings. These methods do not account for any uncertainty in the parameters of the model or in the form of the model. Bayesian approaches have been proposed recently to account for the uncertainty on the parameters of the model, assuming the model form is known. This paper presents a Bayesian predictive approach to process optimization that accounts for the uncertainty in the model form, also accounting for the uncertainty of the parameters given each potential model. It is proposed to optimize the model-averaged posterior predictive density (MAP) of the response where the weighted average is taken using the model posterior probabilities as weights. The resulting model-robust optimization is illustrated with two experiments from the literature, one involving a mixture experiment and the other a small composite design.