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Decision Support

A new Bayesian approach to multi-response surface optimization integrating loss function with posterior probability

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ABSTRACT

Multi-response surface (MRS) optimization in quality design often involves some problems such as correlation among multiple responses, robustness measurement of multivariate process, confliction among multiple goals, prediction performance of the process model and the reliability assessment for optimization results. In this paper, a new Bayesian approach is proposed to address the aforementioned multi-response optimization problems. The proposed approach not only measures the reliability of an acceptable optimization result, but also incorporates expected loss (i.e., bias and robustness) into a uniform framework of Bayesian modeling and optimization. The advantages of this approach are illustrated by one example. The results show that the proposed approach can give more reasonable solutions than the existing approaches when both quality loss and the reliability of optimization results are important issues.

1. Introduction

Robust design (RD), introduced by Taguchi (1986), has been proven very useful for improving the quality of products or processes at low cost. RD is a useful tool for controlling the variance of products or processes performance while keeping the difference between the output characteristics and the desired targets as small as possible (Nha, Shin, & Jeong, 2013). Although the experimental design and data analysis methodology proposed by Taguchi have been argued frequently, there is great consensus that the philosophy of robust design has been considered as a milestone in the field of quality engineering (Nair et al., 1992). Response surface methodology (RSM) is viewed as a collection of statistical design, empirical modeling methodologies and numerical optimization techniques used to optimize product designs (He, Zhu, & Park, 2012; Myers, Montgomery, Vining, Borror, & Kowalski, 2004). A common problem in robust design is the selection of optimum parameter levels for optimizing multiple responses simultaneously, which is called a multi-response surface (MRS) optimization problem (Myers, Montgomery, & Anderson-Cook, 2009).

If there are multiple responses involved, a series of research issues need to be addressed to optimize products or processes performance because they are often in conflict (Lee, Kim, & Köksalan, 2011; Murphy, Tsui, & Allen, 2005; Tansel İç & Yıldırım, 2013). In general, the MRS problem usually consists of three stages (Kim & Lin, 2006): (1) index construction (i.e., constructing an effective index to measure the robustness and correlation among multiple responses), (2) model building (i.e., building a suitable process model to consider the conflict among multiple objectives and the prediction performance of process model), (3) parameter optimization (i.e., selecting an appropriate optimization algorithm to obtain robust optimal solution and assess the reliability of optimization results).

In the last three decades, various creative approaches for MRS optimization have been proposed to solve the aforementioned problems in literature. One common approach to MRS optimization has been the use of dimensionality reduction strategy (Ko, Kim, & Jun, 2005). This strategy usually constructs a simplified performance index which can convert a MRS problem into a single objective optimization problem. The simplified performance index has often been defined as a desirability function, a loss function or a reliability function. The desirability function approach, firstly put forth by Harrington (1965), gives a numerical value between zero (i.e., unacceptable quality) and one (i.e., perfect quality) for a quality characteristic of a product or process. This approach is modified to consider the process economics by adjusting the desirability function shapes (Jeong & Kim, 2009) or the relative weights of multiple responses (Derringer, & Suich, 1980). However, these improved desirability approaches do not take into consideration the correlations among multiple responses, the variance–covariance structure of the responses and the variability of the predictions. In fact, ignoring such information may

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lead to an unrealistic solution if the responses are highly correlated (Chiao & Hamada, 2001; Gomes, Paiva, Costa, Balestrassi, & Paiva, 2013) or have significantly different variance levels (Ko et al., 2005). As stressed by Myers (1999), understanding the variability of predicted responses is a critical issue for practitioners. Recently, several approaches have been proposed to consider the correlation or robustness using the desirability function. Wu (2005) presented an approach to optimize the correlated multiple quality characteristics based on the modified double-exponential desirability function. He, Wang, Oh, and Park (2010) proposed an overall desirability function which makes the balance between robustness and optimization for MRS problem. Goethals and Cho (2012) extended the desirability function by fitting higher-order variance models and covariance models, which are available with model estimation techniques such as ordinary least squares, to account for the variability measures (i.e., robustness and correlation). Although higher-order models can achieve an ideal fitting accuracy, it also easily results in over-fitting problems (Zhou, Ma, Tu, & Feng, 2013). Besides, Vining and Bohn (1998) also pointed out that the process variance typically is rather "noise" system which results in poor fit or prediction results.

Another popular approach to assessing the performance of MRS optimization is based on loss function. Taguchi, Elsayed, and Hsiang (1989) introduced a univariate loss function to obtain a parameter setting where the response value is close to the target with a low variance. Pignatiello (1993) proposed a general multi-response loss function by extending Taguchi's univariate loss function, to resolve the correlation problem among multiple responses. Ames, Mattucci, MacDonald, Szonyi, and Hawkins (1997) presented a quadratic quality loss function, which is applied to MRS optimization with experimentally derived polynomials, to find the optimal parameter setting by minimizing the loss function with respect to process inputs. Vining (1998) improved Pignatiello's method to consider the correlation among multiple responses, the process economics and the quality of prediction. Ko et al. (2005) combined the advantages of Pignatiello's and Vining's methods to propose a new loss function, which allows the analyst to consider both robustness and quality of predictions as well as bias in a single loss function framework. The major advantages of the loss function approach are that it incorporates the variance–covariance structure of the responses and the quality of predictions (Ouyang, Ma, & Byun, 2015). As noted by Ko et al. (2005), a major drawback of their proposed loss function approach is that they ignore the robustness to process parameter fluctuations, which is a very common phenomenon in practice.

Recently, a posterior predictive approach which measures the reliability of an acceptable optimization result for any set of operating conditions, has received a great deal of attention for its attempt to tackle MRS optimization problems. The Bayesian reliability approach takes into account the correlation structure of the data, the variability of the process distribution, and the uncertainty of the model parameters (Peterson, 2004). As noted by Peterson (2004), ignoring parameter uncertainty in the optimization criterion (desirability function or loss function) can lead to reliability estimates that are too large. Miro-Quesada, Del Castillo, and Peterson (2004) extended the work of Peterson (2000) for MRS optimization to the robust parameter design case, which considers the noise variables in the integration of the predictive density. Furthermore, Peterson, Miro-Quesada, and Del Castillo (2009) refined the work of Peterson (2004) to consider the case having different covariance structure across response types with seemingly unrelated regression models. In addition, Del Castillo, Colosimo, and Alshraideh (2012) extended this earlier approach of Peterson (2004) to the functional response case based on a hierarchical two-stage mixed-effects model. Robinson, Pintar, Anderson-Cook, and Hamada (2012) also extended the work of Miro-Quesada et al. (2004) to develop a new Bayesian robust parameter design approach involving both normal and non-normal responses within a split-plot experiment. The major advantage of the existing posterior predictive approaches is that they provide a more feasible solution by assessing the reliability of a good future response which falls within the specific region. However, existing posterior predictive approaches may pay more attention to the reliability of optimization results rather than the bias and robustness. As pointed out by Kazemzadeh, Bashiri, Atkinson, and Noorossana (2008), the posterior predictive approach can help practitioners to control the responses in their specification regions; however it does not consider the deviation from the targets. As observed in this paper, the optimization results obtained by the posterior predictive approaches having high posterior probability can also yield undesirable solution with respect to the expected loss (i.e., bias and robustness). In such a case, optimization results based on the existing posterior predictive approaches may be misleading.

The purpose of this paper is to develop a new Bayesian approach for multi-response optimization, building on quality loss function (Ko et al., 2005) and a posterior predictive approach (Peterson, 2004). The proposed approach allows the analyst to consider both quality loss and reliability of optimization results in a single framework of Bayesian modeling and optimization. Section 2 reviews several existing loss functions which are the basic ingredient of the proposed approach. A detail description of the proposed approach is provided in Section 3. Section 4 illustrates the proposed approach through one example. Some discussion issues are presented in Section 5. Finally, conclusions are made in Section 6.

2. An overview of the existing loss function approach

Loss functions provide an aggregate performance measure through incorporating different optimization criteria (i.e., robustness, bias and quality of prediction) into a single objective function. Several loss functions have been proposed in the literature. Pignatiello (1993) extended Taguchi's univariate loss function to a general multi-response loss function:

$$L(\mathbf{Y}(\mathbf{x}),\theta) = (\mathbf{Y}(\mathbf{x}) - \theta)^T \mathbf{C}(\mathbf{Y}(\mathbf{x}) - \theta) \tag{1}$$

where $\mathbf{Y}(\mathbf{x})$ is a $p \times 1$ vector of responses at a parameter setting $\mathbf{x}, \theta$ is the $p \times 1$ vector of the specified target values, and $\mathbf{C}$ is a $p \times p$ positive definite cost matrix which represents the losses incurred when $\mathbf{Y}(\mathbf{x})$ deviates from the target θ. It can be shown that the expected loss function can be expressed as

$$E[L(\mathbf{Y}(\mathbf{x}),\theta)] = (E[\mathbf{Y}(\mathbf{x})] - \theta)^T \mathbf{C}(E[\mathbf{Y}(\mathbf{x})] - \theta) + \text{trace}[\mathbf{C}\textstyle\sum_{\mathbf{Y}}(\mathbf{x})] \tag{2}$$

where $\sum_{\mathbf{Y}}(\mathbf{x})$ is a $p \times p$ variance–covariance matrix for responses $\mathbf{Y}$ at a parameter setting $\mathbf{x}$. The term $(E[\mathbf{Y}(\mathbf{x})] - \theta)^T \mathbf{C}(E[\mathbf{Y}(\mathbf{x})] - \theta)$ in Eq. (2) denotes a squared bias component, which refers to the expected deviation of responses from their targets. Another term $\text{trace}[\mathbf{C}\sum_{\mathbf{Y}}(\mathbf{x})]$ in Eq. (2) is a variance component which represents the robustness measured by the variance–covariance matrix $\sum_{\mathbf{Y}}(\mathbf{x})$ among multiple responses $\mathbf{Y}$ at $\mathbf{x}$. As the variance component decreases, the robustness improves. Therefore, Pignatiello's approach is useful when robustness and bias are both significant issues.

In addition to robustness and bias, quality of predictions is also an important issue in multi-response optimization. Vining (1998) proposed another loss function by substituting the model predicted value $\hat{\mathbf{Y}}(\mathbf{x})$ for $\mathbf{Y}(\mathbf{x})$ in Eq. (1). The new loss function is given as

$$L(\hat{\mathbf{Y}}(\mathbf{x}),\theta) = (\hat{\mathbf{Y}}(\mathbf{x}) - \theta)^T \mathbf{C}(\hat{\mathbf{Y}}(\mathbf{x}) - \theta) \tag{3}$$

where $\hat{\mathbf{Y}}(\mathbf{x})$ is a $p \times 1$ vector for the predicted responses $\hat{\mathbf{Y}}$ at $\mathbf{x}$. With the definition of loss function given above, the expected loss function is given as

$$E[L(\hat{\mathbf{Y}}(\mathbf{x}),\theta)] = (E[\hat{\mathbf{Y}}(\mathbf{x})] - \theta)^T \mathbf{C}(E[\hat{\mathbf{Y}}(\mathbf{x})] - \theta) + \text{trace}[\mathbf{C}\mathbf{\Sigma}_{\hat{\mathbf{Y}}}(\mathbf{x})] \tag{4}$$