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Algorithmic construction of R-optimal designs for second-order response surface models[☆]

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ABSTRACT

The R-optimality criterion introduced by Dette (1997) minimizes the volume of Bonferroni t-intervals. The present paper is devoted to the construction of R-optimal designs for second-order response surface models with $k \geq 1$ predictors. An equivalence theorem are given as an important tool for determining the R-optimal designs. The algorithms are given for constructing the R-optimal designs for second-order response surface models on the k-dimensional unit cube and ball, respectively. Numerical results of the R-optimal designs for $2 \leq k \leq 25$ are obtained by using the proposed algorithms.

1. Introduction

To develop an adequate functional relationship between a response of interest, say y, and a number of associated input (or control) variables denoted as, say $x_1, x_2, \ldots, x_k$, response surface methodology (RSM) can be used which consists of a group of mathematical and statistical techniques. Such a relationship is, in general, unknown but can be approximated by a low-degree polynomial model, e.g., the first-order model and the second-order model. In this respect, mention may be made of the monograph by Myers and Montgomery (2002).

Optimal designs are those that are constructed on the basis of a certain optimality criterion that pertains to the closeness of the predicted response to the mean response over a certain region of interest. Literature review reveals that numerous authors have worked on the construction of optimal (or nearly optimal) experimental designs for response surface models. Literature review also reveals that for the first-order models, 2^k factorial and 2^{k-p} fractional factorial designs of resolution III are optimal with respect to the D-, G- and I-optimality criteria. In this respect mention may be made of the article by Anderson-Cook et al. (2009). Several authors investigated approximate designs for these models in the sense of Kiefer (1974). Kiefer (1959, 1961), Kiefer and Wolfowitz (1959), Kôno (1962) and Farrel et al. (1967) explicitly determined D-optimal approximate designs for the second-order polynomial regression model on the ball and cube. Moreover, it is also established that D-optimal designs on a ball are rotatable designs. A numerical study on A- and Q-optimal designs was initiated by Laptev (1974), Denisov and Popov (1976) and Golikova and Pantchenko (1977). Galil and Kiefer (1977b) obtained numerically

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optimal rotatable designs for the second-order response surface model. Moreover, mention may be made to Draper et al. (2000) and Draper and Pukelsheim (2003) who investigated optimal design problems in second-order mixture models. Dette and Grigoriev (2014) proved the conjecture posed by Galil and Kiefer (1977a) on the determination of optimal designs when the design space is the k-dimensional unit cube. Moreover, they initiated the challenging work on the determination of E-optimal designs for second-order response surface models on the k-dimensional unit ball and provided a complete solution to this optimal design problem.

In the present paper, we are concerned with the second-order response surface model only and their optimality aspect with respect to the R-optimality criterion. The R-optimality criterion proposed by Dette (1997) minimizes the volume of the rectangular confidence region for the parameters θ based on Bonferroni t-intervals. This is proportional to the square root of product of the diagonal entries of information matrix. Besides a nice statistical interpretation, the R-criterion satisfies an extremely useful invariance property which allows an easy calculation of optimal designs on many linearly transformed design spaces. Moreover, it was indicated by Dette (1997) that the loss of efficiency might be substantial, if a rectangular confidence region is constructed on the basis of a D-optimal design or a confidence ellipsoid is constructed on the basis of a R-optimal design, for polynomial regression on intervals. The R-criterion has been applied to the cases of multiresponse experiments, multi-factor experiments and random coefficients regression models by Liu and Yue (2013) and Liu et al. (2014a,b).

The present paper is organized as follows. In Section 2, a brief discussion on the R-optimality criterion for response surface models is presented. This section also provides an equivalence theorem as an important tool for the determination of R-optimal designs. Sections 3 and 4 consider R-optimal designs on the k-dimensional unit cube and ball, and algorithms for constructing the R-optimal designs are given, respectively. Numerical results of the R-optimal designs for $2 \le k \le 25$ are also presented there by using the proposed algorithms.

2. R-optimality criterion for response surface models

The second-order response surface model considered in this paper is as follows:

$$E(y|\boldsymbol{x}) = \boldsymbol{f}^T(\boldsymbol{x})\boldsymbol{\theta}, \quad \boldsymbol{x} \in \mathcal{X}, \tag{1}$$

where y denotes the response, $\boldsymbol{x}$ is the input variable varying in a compact design space $\mathcal{X} \subset \mathbb{R}^k$, and $\boldsymbol{f}$ is the vector of regression functions of the form

$$\boldsymbol{f}(\boldsymbol{x}) = (1, x_1^2, \ldots, x_k^2, x_1, \ldots, x_k, x_1x_2, \ldots, x_{k-1}x_k)^T,$$

and $\boldsymbol{\theta}$ is the vector of m unknown parameters, where $m = (k+1)(k+2)/2$.

Throughout this paper we consider approximate designs in the sense of Kiefer (1974) which is of the form

$$\xi = \begin{Bmatrix} \boldsymbol{x}_{(1)} & \cdots & \boldsymbol{x}_{(q)} \\ w_1 & \cdots & w_q \end{Bmatrix}, \quad \boldsymbol{x}_{(i)} \in \mathcal{X}, \qquad 0 < w_i < 1, \quad \sum_{i=1}^{q} w_i = 1.$$

It is to be noted that here $\boldsymbol{x}_{(1)}, \boldsymbol{x}_{(2)}, \ldots, \boldsymbol{x}_{(q)}$ refer to different design points. Denote the set of all approximate designs with non-singular information matrix on $\mathcal{X}$ by Ξ. For the model (1), the information matrix of a design $\xi \in \Xi$ is defined by

$$M(\xi) = \int_{\mathcal{X}} \boldsymbol{f}(\boldsymbol{x})\boldsymbol{f}^T(\boldsymbol{x})d\xi(\boldsymbol{x}). \tag{2}$$

The following definition, due to Dette (1997), provides the R-optimality criterion for a design belonging to Ξ.

Definition 1. A design $\xi^* \in \Xi$ is called R-optimal for θ in the model (1) if it minimizes

$$\psi(\xi) = \prod_{i=1}^{m} \left(M^{-1}(\xi)\right)_{ii} = \prod_{i=1}^{m} \boldsymbol{e}_i^T M^{-1}(\xi)\boldsymbol{e}_i \tag{3}$$

over Ξ, where $\boldsymbol{e}_i$ denotes the ith unit vector in $\mathbb{R}^m$.

The following equivalence theorem provides an important tool for the determination of R-optimal designs which has been proved by Dette (1997).

Theorem 2.1. *For the model (1) let*

$$\phi(\boldsymbol{x}, \xi) = \boldsymbol{f}^T(\boldsymbol{x})M^{-1}(\xi)\left(\sum_{i=1}^{m} \frac{\boldsymbol{e}_i\boldsymbol{e}_i^T}{\boldsymbol{e}_i^T M^{-1}(\xi)\boldsymbol{e}_i}\right)M^{-1}(\xi)\boldsymbol{f}(\boldsymbol{x}). \tag{4}$$

Then a design $\xi^* \in \Xi$ is R-optimal if and only if

$$\sup_{\boldsymbol{x} \in \mathcal{X}} \phi(\boldsymbol{x}, \xi^*) = m. \tag{5}$$

Moreover, the supremum is achieved at the support points of ξ^*.