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Optimal Minimum Bias Designs for Model Discrimination

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Abstract

Designs for discriminating between two linear regression models are studied under Λ-type optimalities maximizing the measure for the lack of fit for the designs with fixed model inadequacy. The problem of selecting an appropriate Λ-type optimalities is shown to be closely related to the estimation method. Λ-type optimalities for the least squares and minimum bias estimation methods are considered. The minimum bias designs are suggested for the designs invariant with respect to the two estimation methods. First order minimum bias designs optimal under Λ-type optimalities are then derived. Finally for the case where the lack of fit test is significant, an approach to the construction of a second order design accommodating the optimal first order minimum bias design is illustrated.

1. Introduction

Many results on the optimal experimental designs are derived under the assumption that the statistical model is known at the design stage. Most often in practice, however, the experimenter will not know the correct functional form but instead will have two or more plausible models in mind. The experimenter's goal is then to implement a design that is efficient to discriminate between these rival models and select the best one.

Suppose that there are two rival models $\eta_1(\boldsymbol{x}, \boldsymbol{\theta}_1)$ and $\eta_2(\boldsymbol{x}, \boldsymbol{\theta}_2)$ expressing the expected response at a point $\boldsymbol{x}$ in some specified design space $\boldsymbol{\chi}$, where $\boldsymbol{x}$ is a vector of design variables and $\boldsymbol{\theta}_i$'s are vectors of unknown parameters. Suppose also that $\eta_2(\boldsymbol{x}, \boldsymbol{\theta}_2)$ is the true model. A design ξ is a probability measure on $\boldsymbol{\chi}$. Let Ξ denote the class of all probability measures on $\boldsymbol{\chi}$. Atkinson and Fedorov (1975a) used the non-centrality parameter

$$inf_{\boldsymbol{\theta}_1}\Delta(\xi, \boldsymbol{\theta}_1, \boldsymbol{\theta}_2) = inf_{\boldsymbol{\theta}_1}\int_{\boldsymbol{\chi}}\{\eta_2(\boldsymbol{x}, \boldsymbol{\theta}_2)-\eta_1(\boldsymbol{x}, \boldsymbol{\theta}_1)\}^2 d\xi$$

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as a measure of the capability of a design ξ for detecting the lack of fit of model $\eta_1(\boldsymbol{x}, \boldsymbol{\theta}_1)$. They suggested $\boldsymbol{T}$-optimality that maximizes $inf_{\boldsymbol{\theta}_1}\Delta(\xi, \boldsymbol{\theta}_1, \boldsymbol{\theta}_2)$ in some sense. The $\boldsymbol{T}$-optimality was extended by Atkinson and Fedorov (1975*b*) to the case of more than two rival models. Fedorov and Khabarov (1986) illuminated the connection between the $\boldsymbol{T}$-optimality and some design criteria for parameter estimation. This paper assumes that both $\eta_1(\boldsymbol{x}, \boldsymbol{\theta}_1)$ and $\eta_2(\boldsymbol{x}, \boldsymbol{\theta}_2)$ are linear regression models and $\eta_1(\boldsymbol{x}, \boldsymbol{\theta}_1)$ is a special case of $\eta_2(\boldsymbol{x}, \boldsymbol{\theta}_2)$. That is,

$$\eta_1(\boldsymbol{x}, \boldsymbol{\theta}_1) = f_1'(\boldsymbol{x})\boldsymbol{\theta}_1 \text{ and } \eta_2(\boldsymbol{x}, \boldsymbol{\theta}_2) = f_1'(\boldsymbol{x})\boldsymbol{\beta}_1 + f_2'(\boldsymbol{x})\boldsymbol{\beta}_2,$$

where $f_i(\boldsymbol{x})$ is a $p_i \times 1$ vector of known functions of $\boldsymbol{x}$ and $\boldsymbol{\theta}_2' = (\boldsymbol{\beta}_1', \boldsymbol{\beta}_2')$. In these circumstances we may assume that $\eta_2(\boldsymbol{x}, \boldsymbol{\theta}_2)$ is the true model. Then

$$\Delta(\xi, \boldsymbol{\theta}_1, \boldsymbol{\theta}_2) = (\boldsymbol{\beta}_1 - \boldsymbol{\theta}_1)'M_{11}(\xi)(\boldsymbol{\beta}_1 - \boldsymbol{\theta}_1) + 2(\boldsymbol{\beta}_1 - \boldsymbol{\theta}_1)'M_{12}(\xi)\boldsymbol{\beta}_2 + \boldsymbol{\beta}_2'M_{22}(\xi)\boldsymbol{\beta}_2$$

and $inf_{\boldsymbol{\theta}_1}\Delta(\xi, \boldsymbol{\theta}_1, \boldsymbol{\theta}_2)$ is obtained as $\boldsymbol{\beta}_2'L(\xi)\boldsymbol{\beta}_2$ when $\boldsymbol{\theta}_1 = \boldsymbol{\beta}_1 + M_{11}^{-1}(\xi)M_{12}(\xi)\boldsymbol{\beta}_2$, where $M_{ij}(\xi) = \int_{\boldsymbol{x}} f_i(\boldsymbol{x})f_j'(\boldsymbol{x})d\xi$ and

$$L(\xi) = M_{22}(\xi) - M_{12}'(\xi)M_{11}^{-1}(\xi)M_{12}(\xi).$$

Atkinson (1972) has investigated the design criterion maximizing $det(L(\xi))$, the determinant of $L(\xi)$. The $\boldsymbol{T}$-optimality reduces to the maximization of $\boldsymbol{\beta}_2'L(\xi)\boldsymbol{\beta}_2$. Since $\boldsymbol{\beta}_2'L(\xi)\boldsymbol{\beta}_2$ depends on the unknown parameters $\boldsymbol{\beta}_2$, Atkinson and Fedorov (1975*a*) suggested a maximin approach to this problem in which the design is chosen to maximize the minimum of $\boldsymbol{\beta}_2'L(\xi)\boldsymbol{\beta}_2$ over a specified region Φ of $\boldsymbol{\beta}_2$. In order to specify a reasonable Φ, Jones and Mitchell (1978) introduced $inf_{\boldsymbol{\theta}_1}\tau(\boldsymbol{\theta}_1, \boldsymbol{\theta}_2)$ as a measure of the inadequacy of model $\eta_1(\boldsymbol{x}, \boldsymbol{\theta}_1)$, where $\tau(\boldsymbol{\theta}_1, \boldsymbol{\theta}_2)$, the integrated squared distance between $\eta_1(\boldsymbol{x}, \boldsymbol{\theta}_1)$ and $\eta_2(\boldsymbol{x}, \boldsymbol{\theta}_2)$, is defined as

$$\begin{aligned}\tau(\boldsymbol{\theta}_1, \boldsymbol{\theta}_2) &= \int_{\boldsymbol{x}}\{\eta_2(\boldsymbol{x}, \boldsymbol{\theta}_2) - \eta_1(\boldsymbol{x}, \boldsymbol{\theta}_1)\}^2 d\boldsymbol{x} \Big/ \int_{\boldsymbol{x}} d\boldsymbol{x} \\ &= (\boldsymbol{\beta}_1 - \boldsymbol{\theta}_1)'\mu_{11}(\boldsymbol{\beta}_1 - \boldsymbol{\theta}_1) + 2(\boldsymbol{\beta}_1 - \boldsymbol{\theta}_1)'\mu_{12}\boldsymbol{\beta}_2 + \boldsymbol{\beta}_2'\mu_{22}\boldsymbol{\beta}_2\end{aligned}$$

and $\mu_{ij}=\int_{\chi} f_i(\boldsymbol{x})f_j'(\boldsymbol{x})d\boldsymbol{x}\Big/\int_{\chi} d\boldsymbol{x}$. Since $\tau(\boldsymbol{\theta}_1, \boldsymbol{\theta}_2)$ achieves its minimum $\boldsymbol{\beta}_2'T\boldsymbol{\beta}_2=\boldsymbol{\beta}_2'(\mu_{22}-\mu_{12}'\mu_{11}^{-1}\mu_{12})\boldsymbol{\beta}_2$ at $\boldsymbol{\theta}_1=\boldsymbol{\beta}_1+\mu_{11}^{-1}\mu_{12}\boldsymbol{\beta}_2$, they proposed Λ-optimalities that maximize the minimum and average of $\boldsymbol{\beta}_2'L(\xi)\boldsymbol{\beta}_2$ over $\Phi=\{\boldsymbol{\beta}_2: \boldsymbol{\beta}_2'T\boldsymbol{\beta}_2=\delta\}$ for some constant $\delta>0$. The Λ-optimalities were shown to be equivalent to the maximization of $ch_{\min}(T^{-1}L(\xi))$ and $tr(T^{-1}L(\xi))$, the minimum characteristic root and trace of $T^{-1}L(\xi)$, which are respectively called Λ_1- and Λ_2-optimalities. Recently DeFeo and Myers (1992) considered Λ^*-optimalities that maximize the minimum and average of $\boldsymbol{\beta}_2'L(\xi)\boldsymbol{\beta}_2$ over $\Phi=\{\boldsymbol{\beta}_2: \boldsymbol{\beta}_2'T^*(\xi)\boldsymbol{\beta}_2=\delta\}$, where $\boldsymbol{\beta}_2'T^*(\xi)\boldsymbol{\beta}_2=\tau(\beta_1+M_{11}^{-1}(\xi)M_{12}(\xi)\boldsymbol{\beta}_2, \boldsymbol{\theta}_2)$ and

$$T^*(\xi)=\mu_{22}+M_{12}'(\xi)M_{11}^{-1}(\xi)\mu_{11}M_{11}^{-1}(\xi)M_{12}(\xi)-2\mu_{12}'M_{11}^{-1}(\xi)M_{12}(\xi).$$

Similarly Λ^*-optimalities reduce to the maximization of $ch_{\min}(T^{*^{-1}}(\xi)L(\xi))$ and $tr(T^{*^{-1}}(\xi)L(\xi))$. They are respectively referred to as Λ_1^*- and Λ_2^*-optimalities. Λ- and Λ^*-optimalities are members of $\boldsymbol{T}$-optimality and useful for selecting the most discriminative designs from the designs that offer the same protection against the model inadequacy.

Section 2 first reviews the statistical meaning of the minimization of $\Delta(\xi, \boldsymbol{\theta}_1, \boldsymbol{\theta}_2)$ and $\tau(\boldsymbol{\theta}_1, \boldsymbol{\theta}_2)$ with respect to $\boldsymbol{\theta}_1$ and shows that $inf_{\boldsymbol{\theta}_1}\Delta(\xi, \boldsymbol{\theta}_1, \boldsymbol{\theta}_2)$ and $inf_{\boldsymbol{\theta}_1}\tau(\boldsymbol{\theta}_1, \boldsymbol{\theta}_2)$ are not always $\boldsymbol{\beta}_2'L(\xi)\boldsymbol{\beta}_2$ and $\boldsymbol{\beta}_2'T\boldsymbol{\beta}_2$, but they depend on the estimation method. We define Λ-type optimalities for given estimation method as the maximization of the minimum and average of $inf_{\boldsymbol{\theta}_1}\Delta(\xi, \boldsymbol{\theta}_1, \boldsymbol{\theta}_2)$ over $\Phi=\{\boldsymbol{\theta}_2: inf_{\boldsymbol{\theta}_1}\tau(\boldsymbol{\theta}_1, \boldsymbol{\theta}_2)=\delta\}$. Λ-type optimalities for the least squares and minimum bias estimation methods are then considered. The minimum bias designs are suggested for the designs that are invariant with respect to the estimation method. First order minimum bias designs optimal under Λ-type design criteria are obtained in Section 3. Section 4 illustrates how to construct a second order design accommodating the optimal first order minimum bias design. Efficiency of the optimal minimum bias designs is discussed in Section 5.

2. Λ-type design criteria

Usually the optimal design problem for linear regression models is solved under the assumption that the model is fitted by the least squares method. However, we do not confine ourselves to the least squares method in this paper. Suppose that $\widehat{\boldsymbol{\theta}_1}$ is a linear unbiased estimator of $\boldsymbol{\theta}_1$ and $\eta_1(\boldsymbol{x}, \boldsymbol{\theta}_1)$ is fitted by $f_1'(\boldsymbol{x})\widehat{\boldsymbol{\theta}_1}$. Let $E_{\eta_2}(\widehat{\boldsymbol{\theta}_1})$ denote the expected value of $\widehat{\boldsymbol{\theta}_1}$ under model $\eta_2(\boldsymbol{x}, \boldsymbol{\theta}_2)$. The corresponding non-centrality parameter and integrated squared bias of $f_1'(\boldsymbol{x})\widehat{\boldsymbol{\theta}_1}$ are then obtained as $\Delta(\xi, E_{\eta_2}(\widehat{\boldsymbol{\theta}_1}), \boldsymbol{\theta}_2)$ and $\tau(E_{\eta_2}(\widehat{\boldsymbol{\theta}_1}), \boldsymbol{\theta}_2)$. Once the estimator is chosen, the non-centrality parameter and integrated squared bias are also determined and Λ-type optimalities for the estimator can be derived. It is not reasonable to deal with $\Delta(\xi, \boldsymbol{\theta}_1, \boldsymbol{\theta}_2)$ and $\tau(\boldsymbol{\theta}_1, \boldsymbol{\theta}_2)$ separately and minimize them individually. The minimization of $\Delta(\xi, \boldsymbol{\theta}_1, \boldsymbol{\theta}_2)$ or $\tau(\boldsymbol{\theta}_1, \boldsymbol{\theta}_2)$ with respect to $\boldsymbol{\theta}_1$ is equivalent to finding an estimator that minimizes the non-centrality parameter or the integrated squared bias. Therefore $\boldsymbol{\beta}_2' L(\xi)\boldsymbol{\beta}_2$ is the non-centrality parameter for the estimator $\widehat{\boldsymbol{\theta}_1}$ such that $E_{\eta_2}(\widehat{\boldsymbol{\theta}_1}) = \boldsymbol{\beta}_1 + M_{11}^{-1}(\xi)M_{12}(\xi)\boldsymbol{\beta}_2$ (Condition 1), while $\boldsymbol{\beta}_2' T\boldsymbol{\beta}_2$ is the integrated squared bias for the estimator $\widehat{\boldsymbol{\theta}_1}$ such that $E_{\eta_2}(\widehat{\boldsymbol{\theta}_1}) = \boldsymbol{\beta}_1 + \mu_{11}^{-1}\mu_{12}\boldsymbol{\beta}_2$ (Condition 2). We thus focus on Λ-type optimalities for the estimators satisfying Condition 1 and/or Condition 2.

The linear unbiased estimator satisfying Condition 1 is the least squares estimator. If $\eta_1(\boldsymbol{x}, \boldsymbol{\theta}_1)$ is fitted by the least squares method, the values of $\Delta(\xi, \boldsymbol{\theta}_1, \boldsymbol{\theta}_2)$ and $\tau(\boldsymbol{\theta}_1, \boldsymbol{\theta}_2)$ are obtained as $\boldsymbol{\beta}_2' L(\xi)\boldsymbol{\beta}_2$ and $\boldsymbol{\beta}_2' T^*(\xi)\boldsymbol{\beta}_2$ by replacing $\boldsymbol{\theta}_1$ in $\Delta(\xi, \boldsymbol{\theta}_1, \boldsymbol{\theta}_2)$ and $\tau(\boldsymbol{\theta}_1, \boldsymbol{\theta}_2)$ with $\boldsymbol{\beta}_1 + M_{11}^{-1}(\xi)M_{12}(\xi)\boldsymbol{\beta}_2$. Since $\boldsymbol{\beta}_2' L(\xi)\boldsymbol{\beta}_2$ and $\boldsymbol{\beta}_2' T^*(\xi)\boldsymbol{\beta}_2$ do not contain $\boldsymbol{\theta}_1$, it is not necessary to minimize them with respect to $\boldsymbol{\theta}_1$. Λ-type optimalities become the Λ_1^*- and Λ_2^*-optimalities proposed by DeFeo and Myers (1992). If the least squares estimator is used, $\tau(\boldsymbol{\theta}_1, \boldsymbol{\theta}_2)$ does not attain its minimum $\boldsymbol{\beta}_2' T\boldsymbol{\beta}_2$ in general. It is not practical to minimize or average $\boldsymbol{\beta}_2' L(\xi)\boldsymbol{\beta}_2$ over a region expressed with the unattainable term $\boldsymbol{\beta}_2' T\boldsymbol{\beta}_2$. Therefore Λ_1- and Λ_2-optimalities may produce somewhat impractical designs. For example, according to Example 2 of Jones and Mitchell (1978), Λ_1-optimal designs that are available only for $k \leq 4$ require too many support points and Λ_2-optimal designs for $k \geq 4$ are powerless.

We next consider the linear unbiased estimator satisfying Condition 2. Karson, Manson and Hader (1969) advocated the linear estimator minimizing the integrated squared bias of the estimated response. The estimator satisfies Condition 2 and is unbiased under model $\eta_1(\boldsymbol{x}, \boldsymbol{\theta}_1)$. Among the estimators satisfying Condition 2 the estimator having the minimum integrated variance is called the minimum bias estimator. If $\eta_1(\boldsymbol{x}, \boldsymbol{\theta}_1)$ is fitted by the minimum bias estimation, the corresponding values of $\Delta(\xi, \boldsymbol{\theta}_1, \boldsymbol{\theta}_2)$ and $\tau(\boldsymbol{\theta}_1, \boldsymbol{\theta}_2)$ are given by $\boldsymbol{\beta}_2' L^*(\xi)\boldsymbol{\beta}_2$ and $\boldsymbol{\beta}_2' T\boldsymbol{\beta}_2$, where

$$L^*(\xi) = M_{22}(\xi) + \mu_{12}'\mu_{11}^{-1}M_{11}(\xi)\mu_{11}^{-1}\mu_{12} - 2\mu_{12}'\mu_{11}^{-1}M_{12}(\xi).$$

Λ-type optimalities for the minimum bias estimation then reduce to the maximization of $ch_{\min}(T^{-1}L^{*(\xi)})$ and $tr(T^{-1}L^*(\xi))$, which will be respectively referred to as $\tilde{\Lambda}_1$- and $\tilde{\Lambda}_2$-optimalities.

DeFeo and Myers (1992) developed the designs that are efficient under Λ^*-optimalities. Many authors ([5], [8], [9], [13], [14], [15]) have studied the designs for the minimum bias estimation. Unfortunately it is difficult to characterize Λ_i^*- and $\tilde{\Lambda}_i$-optimum designs. This is because the classical optimal design theory based on the convex optimization can not be applied to Λ^*- and $\tilde{\Lambda}$-optimalities, since $T^{*^{-1}}(\xi)L(\xi)$ is not convex with respect to ξ and the set of designs permitting the minimum bias estimation is not convex. In order to derive the designs optimal under Λ-type design criteria, we reduce the design problem to a manageable problem by the following invariance requirement. Data are usually collected by performing the experiment designed to optimize the chosen design criterion. However, the data analyst may use an estimation method different from the one used in the design stage. It is therefore desirable to use an experimental design that is efficient and invariant with respect to the estimation method. One approach is to design the experiment so that both Conditions 1 and 2 are simultaneously satisfied irrespective to which of the least squares and minimum bias estimation methods is used. This can be accomplished by confining our attention to $\Xi_0 = \{\xi: M_{12}(\xi) = M_{11}(\xi)\mu_{11}^{-1}\mu_{12}\}$, the class of minimum bias designs for estimating the expected response advocated by Box and Draper (1963) and considered by several authors ([7], [8]). Then Λ^*- and $\tilde{\Lambda}$-optimalities become identical and any of the two types can be used for selecting designs from Ξ_0. The minimum bias designs for other design objectives have been studied by Myers and Lahoda (1975) and Park (1990). It is interesting that the minimum bias designs for the estimation of the expected response are also useful for the model discrimination.

3. Optimal minimum bias designs for model discrimination

In this section we suppose that $\eta_1(\boldsymbol{x}, \boldsymbol{\theta}_1)$ is fitted by the least squares or minimum bias esitmation method. Then the non-centrality parameter and integrated squared bias for the minimum bias designs can be written as $\beta_2' L(\xi) \beta_2$ and $\beta_2' T \beta_2$. Both Λ^*- and $\bar{\Lambda}$-optimalities reduce to the maximization of $ch_{\min}(T^{-1}L(\xi))$ and $tr(T^{-1}L(\xi))$. They will be simply called Λ'-optimalities. The Λ'-optimalities may appear similar to the Λ-optimalities. But the Λ'-optimalities are different from the Λ-optimalities at the point that ξ is restricted within Ξ_0, instead of Ξ. The Λ_i'-optimal designs are obtained as follows: It is well-known that $ch_{\min}(T^{-1}L(\xi))$ and $tr(T^{-1}L(\xi))$ are concave and increasing functions of $T^{-1}L(\xi)$ when ξ ranges over Ξ, i.e., if $T^{-1}L(\xi_1) \geq T^{-1}L(\xi_2)$ in the sense of positive definiteness, then $ch_{\min}(T^{-1}L(\xi_1)) \geq ch_{\min}(T^{-1}L(\xi_2))$ and $tr(T^{-1}L(\xi_1)) \geq tr(T^{-1}L(\xi_2))$. The concavity and monotonicity hold when ξ ranges over Ξ_0, since Ξ_0 is a convex subset of Ξ. Let G be a group of orthogonal transformations g on χ and let ξ^g be the rotation of ξ under g. Assume that for each $g \in G$ and $i = 1, 2$, there exist orthogonal matrices Q_{ig} such that $f_i(g(\boldsymbol{x})) = Q_{ig} f_i(\boldsymbol{x})$ for all $\boldsymbol{x} \in \chi$. Then it can be shown that $T^{-1}L(\xi^g) = T^{-1}Q_{2g}L(\xi)Q_{2g}'$, $Q_{2g}TQ_{2g}' = T$ and the minimum characteristic root and trace of $T^{-1}L(\xi^g)$ are equal to those of $T^{-1}L(\xi)$. If the design space χ is invariant with respect to G, the concavity ensures that it suffices to consider the minimum bias designs that are invariant with respect to G, i.e., the minimum bias designs such that $Q_{2g}L(\xi)Q_{2g}' = L(\xi)$ for all $g \in G$. The invariance condition implies that $Q_{ig}M_{ij}(\xi)Q_{jg}' = M_{ij}(\xi)$ for all i, j and $g \in G$. Such designs are called the invariant minimum bias designs. The Λ_i'-optimal designs can be found within the invariant minimum bias designs.

Suppose that $\eta_1(\boldsymbol{x}, \boldsymbol{\theta}_1)$ and $\eta_2(\boldsymbol{x}, \boldsymbol{\theta}_2)$ are respectively first and second order polynomials of k dimensional vector $\boldsymbol{x}$ $(k \geq 2)$ and $\chi = \{\boldsymbol{x} : |x_i| \leq 1, i = 1, \cdots, k\}$. Then $f_1'(\boldsymbol{x}) = (1, x_1, x_2, \cdots, x_k)$ and $f_2'(\boldsymbol{x}) = (x_1^2, x_2^2, \cdots, x_k^2, x_1x_2, x_1x_3, \cdots, x_{k-1}x_k)$. Let $\boldsymbol{G_0}$ denote the invariant group of all permutations and sign changes of the coordinates of $\boldsymbol{x}$. Q_{ig}'s are then orthogonal matrices of which columns are unit vectors multiplied by 1 or -1. The design space χ is invariant with respect to $\boldsymbol{G_0}$. It is therefore sufficient to consider only the first order invariant minimum bias designs. The invariance condition mentioned in the previous paragraph is equivalent to the following design moment conditions:

(i) $\int_\chi x_i d\xi = 0$ for all i;

(ii) $\int_{\mathcal{X}} x_i^2 d\xi$ are equal for all i;

(iii) $\int_{\mathcal{X}} x_i^2 x_j^2 d\xi$ are equal for all $i \neq j$;

(iv) $\int_{\mathcal{X}} x_i^4 d\xi$ are equal for all i;

(v) Other design moments up to degree 4 are zero.

The design moment matrices $M_{ij}(\xi)$ of first order invariant designs and μ_{ij} are then obtained as

$$M_{11}(\xi)=\begin{pmatrix}1 & 0' \\ 0 & m_2 I_k\end{pmatrix},\quad M_{12}(\xi)=\begin{pmatrix}m_2 1_k' & 0' \\ o & 0\end{pmatrix},$$

$$M_{22}(\xi)=\begin{pmatrix}(m_4-m_{22})I_k+m_{22}J_k & 0' \\ 0 & m_{22}I_{k(k-1)/2}\end{pmatrix},\quad \mu_{11}=\begin{pmatrix}1 & 0' \\ 0 & \frac{1}{3}I_k\end{pmatrix},$$

$$\mu_{12}=\begin{pmatrix}\frac{1}{3}1_k' & 0' \\ 0 & 0\end{pmatrix} \text{ and } \mu_{22}=\begin{pmatrix}\frac{4}{45}I_k+\frac{1}{9}J_k & 0' \\ 0 & \frac{1}{9}I_{k(k-1)/2}\end{pmatrix},$$

where $m_2=\int_{\mathcal{X}} x_i^2 d\xi$, $m_{22}=\int_{\mathcal{X}} x_i^2 x_j^2 d\xi$, $m_4=\int_{\mathcal{X}} x_i^4 d\xi$, I_k is the identity matrix of order k, 1_k is the vector of ones and $J_k=1_k 1_k'$. The design moment matrices $M_{ij}(\xi)$ of the invariant minimum bias designs are obtained by replacing m_2 with $1/3$, the solution of the equations $M_{12}(\xi)=M_{11}(\xi)\mu_{11}^{-1}\mu_{12}$. $ch_{\min}(T^{-1}L(\xi))$ and $tr(T^{-1}L(\xi))$ of the invariant minimum bias designs are simplified to

$$ch_{\min}(T^{-1}L(\xi))=\min\left\{\frac{45}{4}(m_4-m_{22}),\frac{45}{4}m_4+\frac{45}{4}(k-1)m_{22}-\frac{5}{4}k, 9m_{22}\right\} \tag{1}$$

and

$$tr(T^{-1}L(\xi))=\frac{9}{4}k\{5m_4+2(k-1)m_{22}\}-\frac{5}{4}k.$$

We first consider the Λ_2'-optimal designs. Since $m_{22}\leq m_4\leq m_2=1/3$, $tr(T^{-1}L(\xi))$ is maximized when $m_{22}=m_4=m_2=1/3$. The corresponding maximum is $3k^2/2+k$. Equality of the three non-zero design moments suggests that the support of the Λ_2'-optimal designs consist of the vertices and center point of χ. It is further required that the weight for the vertices is 1/3 and that for the center point is 2/3. Consequently the Λ_2'-optimal designs are 2^{k-f} (fractional) factorial designs plus the center point with $1/(2^{k-f}3)$ and 2/3 weights allocated to each vertex and the center point. One noteworthy point is that Λ_2'-optimal designs put 2/3 weight on the center point and consequently require too many experiments at the center point. Therefore it is highly recommended that fractional factorial designs be utilized for constructing Λ_2'-optimal designs.

Next we derive the Λ_1'-optimal designs. We first need to evaluate the minimum of the three values listed in the brace of the right hand side of equation (1). Then the values of design moments maximizing the minimum should be determined. The minimum, i.e. $ch_{\min}(T^{-1}L(\xi))$, is $45(m_4 - m_{22})/4$ for the following two disjoint cases:

(i) $\frac{5}{9} m_4 \le m_{22}$ and $\frac{1}{5} \le m_4 \le \frac{1}{3}$;

(ii) $\frac{1}{9} \le m_{22}$ and $m_4 \le \frac{1}{5}$.

For case (i) it is not difficult to verify that $45(m_4 - m_{22})/4$ attains its maximum 5/3 when $m_4 = 1/3$ and $m_{22} = 5/27$. For case (ii) $45(m_4 - m_{22})/4$ is maximized when $m_{22} = 1/9$ and $m_4 = 1/5$. The corresponding maximum is 1. Next we consider the case where the right hand side of equation (1) becomes $45m_4/4 + 45(k-1)m_{22}/4 - 5k/4$. This occurs when either (iii) or (iv), mentioned below, holds.

(iii) $m_{22} \le \frac{5(k-9m_4)}{9(5k-9)}$ and $\frac{1}{5} \le m_4 \le \min\left(\frac{1}{3}, \frac{k}{9}\right)$;

(iv) $m_{22} \le \frac{1}{9}$ and $\frac{1}{5} \le m_4 \le \frac{1}{3}$.

It can be shown that the values of design moments maximizing $ch_{\min}(T^{-1}L(\xi))$ and corresponding $ch_{\min}(T^{-1}L(\xi))$ for cases (iii) and (iv) are identical with those for case (ii). Finally $ch_{\min}(T^{-1}L(\xi))$ becomes $9m_{22}$ when

(v) $\frac{5(k-9m_4)}{9(5k-9)} \le m_{22} \le \frac{5}{9} m_4$ and $\frac{1}{5} \le m_4 \le \frac{1}{3}$.

$9m_{22}$ attains its maximum $5/3$ when $m_4=1/3$ and $m_{22}=5/27$. Therefore $ch_{\min}(T^{-1}L(\xi))$ is maximized when $m_{22}=5/27$ and $m_4=1/3$ and corresponding maximum is $5/3$.

These design moment conditions imply that the Λ_1'-optimal designs put all weight on the points having coordinates 0 and ± 1 only, i.e., on $\boldsymbol{A}_j$'s where $\boldsymbol{A}_j$ denotes the set of points with j coordinates equal to 0 and the remaining coordinates equal to ± 1. Appealing to Galil and Kiefer (1986), we can construct the Λ_1'-optimal designs consisting of $\boldsymbol{A}_j$'s. A simple and well-known method is to use $\boldsymbol{A}_0$, $\boldsymbol{A}_{k-1}$ and $\boldsymbol{A}_k$, which are respectively the vertices, $2k$ axial points and center point of $\boldsymbol{\chi}$. The weights for each vertex, each axial point and the center point are respectively $5/(2^{k-f}27)$, $2/27k$ and $2/3$.

4. Second order design accommodating first order design

First order Λ_1'-optimal designs allow us to fit a second order model. Therefore, even if significant lack of fit is found, we can fit a second order model without further experiments. However, if a first order Λ_2'-optimal design is employed and the lack of fit test is significant, an additional experiment should be performed to fit a second order model. The problem of designing the additional experiment is considered in this section. Let us suppose that the experiment was performed according to a first order Λ_2'-optimal design and the lack of fit test is significant. Then an additional experiment should be designed so that the augmented design ξ^* enables us to fit the second order model $\eta_2(\boldsymbol{x}, \boldsymbol{\theta}_2)$ optimally in some sense. In this case we may consider the optimality criteria associated with the information matrix $M(\xi^*)$ for the second order model, where

$$M(\xi^*)=\begin{pmatrix} M_{11}(\xi^*) & M_{12}(\xi^*) \\ M_{12}'(\xi^*) & M_{22}(\xi^*) \end{pmatrix}.$$

The well-known optimality criteria are $\boldsymbol{A}$-, $\boldsymbol{D}$-, $\boldsymbol{E}$- and G-optimalities which have the convexity and monotonicity properties. For the purpose of illustration this section considers $\boldsymbol{D}$-optimality, the maximization of $det(M(\xi^*))$. Since $det(M(\xi^*))$ is invariant with respect to $\boldsymbol{G}_0$, it is enough to consider only the invariant second order designs. One method to derive invariant second order designs from the (fractional) factorial first order designs is to perform the supplementary experiments at the $2k$ axial points $(\pm a, 0, \cdots, 0)$, $\cdots$, $(0, \cdots, \pm a)$. Let w be the weight for the first order design portion in the augmented design. Then the weight for each axial point is $(1-w)/2k$. The corresponding information matrix is given by

$$M(\xi^*)=\begin{pmatrix} 1 & \mathbf{0}' & m_2^*\mathbf{1}_k' & \mathbf{0}' \\ \mathbf{0} & m_2^* I_k & \mathbf{0} & \mathbf{0} \\ m_2^*\mathbf{1}_k & \mathbf{0} & (m_4^*-m_{22}^*)I_k+m_{22}^*J_k & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & \mathbf{0} & m_{22}^* I_{k(k-1)/2} \end{pmatrix}.$$

where $m_2^*=\int_{\mathcal{X}} x_i^2\xi^* = w/3+a^2(1-w)/k$, $m_{22}^*=\int_{\mathcal{X}} x_i^2x_j^2 d\xi^* = w/3$ and $m_4^*=\int_{\mathcal{X}} x_i^4 d\xi^* = w/3+a^4(1-w)/k$. We will determine a and w so that $det(M(\xi^*))$ is maximized. It can be shown that

$$det(M(\xi^*)) = 3^{-(k^2+k+4)/2}k^{-2k}a^{4(k-1)}w^{(k^2-k+2)/2}(1-w)^{k-1}\{kw+3(1-w)a^2\}^k \cdot \{k^2(3-w)-6k(1-w)a^2+9(1-w)a^4\}$$

is an increasing function of a for $0\leq a\leq 1$. Therefore the D-optimal value of a is 1 and the corresponding $det(M(\xi^*))$ is obtained as

$$det(M(\xi^*)) = 3^{-(k^2+k+4)/2}k^{-2k}w^{(k^2-k+2)/2}(1-w)^{k-1}\{(k-3)w+3\}^k \{2k^2(k-3)^2(1-w)\}.$$

The optimal value of w is then obtained by equating the derivative of $det(M(\xi^*))$ with respect to w to zero. Similarly A-, E- and G-optimal second order designs can be derived.

5. Discussion

This paper considered the optimal designs under Λ-type design criteria for discriminating between two linear regression models. Specific Λ-type design criteria are determined by the estimation method. Λ^*-optimalities are to be used for the least squares method, while $\tilde{\Lambda}$-optimalities are for the minimum bias estimation. However, Λ-type optimalities for other estimation methods may also be considered. Since characterization of Λ_i^*- and $\tilde{\Lambda}_i$-optimal designs are not yet available and the designs invariant with respect to the estimation method are often useful, the minimum bias designs for estimating the expected response were suggested. The Λ-type optimalities for the minimum bias designs were named Λ'-optimalities. It was shown that Λ'-optimal designs could be found within the invariant minimum bias designs. First order Λ_i'-optimal designs were then derived. A Λ_1'-optimal design can be constructed as the well-known central composite design. The Λ_2'-optimal designs are 2^{k-f} (fractional) factorial designs plus the center point. For the case where data obtained from a first order Λ_2'-optimal design shows significant lack of fit, we illustrated how to construct a second order design accommodating the first order Λ_2'-optimal design.

Finally we make some comments on the efficiency of Λ_i'-optimal designs. Such efficiency study is not easy, since Λ_i^*- and $\widetilde{\Lambda}_i$-optimal designs are not available. Alternatively we may compare Λ_i'-optimal designs with Λ_i-optimal designs, even though the Λ-optimalities are somewhat irrelevant. Λ_1-optimal designs for $k \leq 4$ and Λ_2-optimal designs were derived in Example 2 of Jones and Mitchell (1978). The Λ_1-optimal designs for $k \leq 4$ consist of $\boldsymbol{A}_0$, $\boldsymbol{A}_1$, $\boldsymbol{A}_{k-1}$ and $\boldsymbol{A}_k$ and the corresponding values of m_2, m_4 and m_{22} are respectively 5/9, 5/9 and 25/81. The Λ_2-optimal designs for $k \leq 3$ are composed of $\boldsymbol{A}_0$ and $\boldsymbol{A}_k$, but only $\boldsymbol{A}_0$ is concerned with the Λ_2-optimal designs for $k \geq 4$. Therefore the Λ_2-optimal designs for $k \geq 4$ are powerless to detect model inadequacy. Thus a comparison between Λ_1'- and Λ_1-optimal designs is made for $k \leq 4$. It can be shown that $ch_{\min}(T^{*\ 1}(\xi)L(\xi))$ and $ch_{\min}(T^{-1}L^*(\xi))$ of Λ_1-optimal designs are 25/9 and $25/(9+5k)$, between which 5/3, $ch_{\min}(T^{-1}L(\xi))$ of Λ_1'-optimal designs, is. If the least squares method is employed, Λ_1-optimal designs are more efficient than Λ_1'-optimal designs. If the minimum bias estimation is used, Λ_1'-optimal designs are more efficient. This is partly because the Λ-optimalities are developed under the assumption that the least squares method is used and partly because the invariance with respect to the estimation method causes some loss in efficiency. In addition it should be noted that Λ_1-optimal designs are not available for all practical values of k and Λ_1-optimal designs for $k \leq 4$ require too many support points. These suggest that Λ'-optimal designs are useful in practice. However, Λ^*- and $\widetilde{\Lambda}$-optimal designs need to be derived at least numerically. Further researches are also necessary for the situations where more than two and/or higher order regression models are involved.

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