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<https://doi.org/10.15017/1449029>

出版情報 : 九州大学教養部数学雑誌. 13 (1), pp.51-61, 1981-12. 九州大学教養部数学教室
バージョン :
権利関係 :

The minimal essentially complete class of symmetric exact designs with k factors on the quadratic response surfaces

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(Received August 29, 1981)

1. Notations and preliminaries

Let us consider the linear regression model

$$\mathbf{y} = X\boldsymbol{\theta} + \mathbf{e}, \quad (1.1)$$

where $\mathbf{y} = {}^t(y_1, y_2, \dots, y_n)$ is an observed vector, $\mathbf{x}_i = {}^t(x_{i1}, x_{i2}, \dots, x_{ik})$, $i = 1, 2, \dots, n$, is an observation point, $X = {}^t(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n)$ is a design matrix, $\boldsymbol{\theta} = {}^t(\theta_1, \theta_2, \dots, \theta_m)$ is a vector of unknown parameters and $\mathbf{e} = {}^t(e_1, e_2, \dots, e_n)$ is an error vector which has mean vector 0 and variance-covariance matrix $I_n\sigma^2$. σ^2 is unknown and I_n is the identity matrix of degree n .

Any observation point \mathbf{x}_i , $i = 1, 2, \dots, n$, is chosen from a compact subset of R^m . A set of observation points $D_n = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n\}$ is called an n -points design.

Let $\hat{\boldsymbol{\theta}}_{D_n}$ be the least squares estimator of $\boldsymbol{\theta}$ using a design D_n with design matrix X , we assume that $\boldsymbol{\theta}$ is estimable by D_n , then

$$\hat{\boldsymbol{\theta}}_{D_n} = ({}^tXX)^{-1} {}^tX\mathbf{y} \quad (1.2)$$

$$V(\hat{\boldsymbol{\theta}}_{D_n}) = \sigma^2 ({}^tXX)^{-1}. \quad (1.3)$$

Furthermore, the least squares estimator $\hat{\boldsymbol{\tau}}_{D_n}$ of linear combination of unknown parameters $\boldsymbol{\tau} = {}^t\mathbf{b}\boldsymbol{\theta}$ and its variance are given by

$$\hat{\boldsymbol{\tau}}_{D_n} = {}^t\mathbf{b}\hat{\boldsymbol{\theta}}_{D_n} \quad (1.4)$$

$$V(\hat{\boldsymbol{\tau}}_{D_n}) = \sigma^2 {}^t\mathbf{b}({}^tXX)^{-1}\mathbf{b}. \quad (1.5)$$

If $V(\hat{\boldsymbol{\tau}}_{D_n}) \leq V(\hat{\boldsymbol{\tau}}_{D_n'})$ holds for any linear combination $\boldsymbol{\tau}$ of parameters, we say that the n -points design D_n is better than the design D_n' , or that D_n is an improvement of D_n' and write $D_n \succ D_n'$.

A proper subset C of n -points designs is called an essentially complete

$$M_{D_n} - M_{D_n'} = \begin{pmatrix} 0 & \lambda_1 - \lambda_1' & \lambda_2 - \lambda_2' & \cdots & \lambda_m - \lambda_m' \\ & \lambda_2 - \lambda_2' & \lambda_3 - \lambda_3' & \cdots & \lambda_{m+1} - \lambda_{m+1}' \\ & & \lambda_4 - \lambda_4' & \cdots & \lambda_{m+2} - \lambda_{m+2}' \\ & & & \ddots & \vdots \\ & & & & \lambda_{2m} - \lambda_{2m}' \end{pmatrix} \quad (2.4)$$

Noting that the (1,1) element of the above matrix is zero, and from lemma 1 we can understand the following lemma.

LEMMA 2 (Kiefer and Wolfowitz [2]). A design D_n is better than D_n' if and only if the following conditions hold.

$$(i) \quad \lambda_j = \lambda_j', \quad j=1, 2, \dots, 2m-1, \quad (2.5)$$

and $(ii) \quad \lambda_{2m} \geq \lambda'_{2m}. \quad (2.6)$

A design D_n is written occasionally as $D_n = \left\{ \begin{matrix} x_1, x_2, \dots, x_p \\ n_1 \ n_2 \dots n_p \end{matrix} \right\}$ or $\left\{ \begin{matrix} x_i, i=1, 2, \dots, p \\ n_i \end{matrix} \right\}$ where $\sum n_i = n$. That means the observation point x_i is observed n_i times, $i=1, 2, \dots, p$.

THEOREM 1 (Ishii G., et al. [3]). An essentially complete class of designs on the regression curve (2.1) is constructed by designs of the following type D_n .

$$D_n = \left\{ \begin{matrix} x_i \\ n_i \end{matrix}, i=1, 2, \dots, 2m+1 \right\} \quad (2.7)$$

where $x_1 = -1 < x_2 < \dots < x_{2m} < x_{2m+1} = 1, \sum n_i = n, n_{2i}$ takes its value only 0 or 1, $i=1, 2, \dots, m$.

DEFINITION 1. A design is symmetric if an observation point x is observed n_x times, then the observation point $-x$ is observed n_x times in D_n .

Therefore, if D_n is symmetric then $\lambda_{2j+1} = 0, j=1, 2, \dots$. From the theorem 1, for $m=2$, the quadratic regression problem, any admissible design has at most three observation points in $(-1, 1)$ and if we restrict on symmetric designs, then one of them is zero.

THEREM 2. For the quadratic regression problem the class of designs

of the type

$$D_n = \begin{Bmatrix} -1, & -x, & 0, & x, & 1 \\ n_1 & 1 & n_2 & 1 & n_1 \end{Bmatrix} \quad (2.8)$$

where $x \in [0, 1)$, $2n_1 + n_2 + 2 = n$, consists the minimal essentially complete class in the class of symmetric designs.

PROOF. Let $D_n' = \{x_1', x_2', \dots, x_n'\}$ be any symmetric n point design. We attempt to improve D_n' . By lemma 2, if there exist integers n_1 , n_2 and $x \in [0, 1)$ such that

$$(i) \quad n_1 + x^2 = \sum x_i'^2 / 2 (= \lambda_2' / 2), \quad (2.9)$$

and

$$(ii) \quad n_1 + x^4 \geq \sum x_i'^4 / 2 (= \lambda_4' / 2) \quad (2.10)$$

then $D_n \succ D_n'$.

Let us consider a maximizing problem: Maximize $\sum a_i^2$, where $A = \{a =$

$(a_i) \mid \sum a_i = \alpha$ and $0 \leq a_i < 1, i = 1, 2, \dots, n\}$. Since A is a convex closed set in the positive orthant and $\sum a_i^2$ is the square of length of a , $\sum a_i^2$ takes its maximum at the boundary of A . The longest distance from the origin to the boundary of i -dimensional cube is \sqrt{i} , thus if $i \leq \alpha < i+1$ then the farthest points of A from the origin are the cross points of edges of $(i+1)$ -dimensional cube and the hyperplane $\sum a_i = \alpha$. One of those points is $a = (1, \underbrace{\dots, 1}_i, \underbrace{\sqrt{\alpha-i}, 0, \dots, 0}_1, \underbrace{0, \dots, 0}_{n-1-i})$ and others are the vectors whose components,

consist of permutations of components of a .

Now put $\alpha = \lambda_2' / 2$, then $a = (1, \underbrace{\dots, 1}_{n_1}, x, 0, \underbrace{\dots, 0}_{n-1-n_1})$, where $n_1 = [\lambda_2' / 2]$ ([]

means the Gauss notation) and $x = \sqrt{\lambda_2' / 2 - i}$, is a solution of the maximizing problem. Therefore, by using those n_1 and x we know that D_n is better than D_n' and can not be improved by any design because of its maximality.

3. The minimal essentially complete class of symmetric designs with two factors on the quadratic response surface

Let us consider the following regression model in this section.

$$y = X\theta + e \quad (3.1)$$

where $X = {}^t(x_1, x_2, \dots, x_n)$ and

$$x_i = {}^t(1, x_{1i}, x_{2i}, x_{1i}^2, x_{2i}^2, x_{1i}x_{2i}), \quad i=1, 2, \dots, n. \quad (3.2)$$

Similarly to the section 2, we write $D_n = \{(x_{1i}, x_{2i}), i=1, 2, \dots, n\}$ or

$$D_n = \left\{ \begin{matrix} (x_{1i}, x_{2i}) \\ n_i \end{matrix}, i=1, 2, \dots, p \right\} \text{ where } \sum n_i = n.$$

We give two meanings to the notion of symmetricity of designs:

(a) symmetric at the origin for any factor,

and

(b) symmetric between two factors.

DEFINITION 2. D_n is a *symmetric* design if the followings hold.

(i) If $(x_1, x_2) \in D_n$, then $(\pm x_1, \pm x_2) \in D_n$,

and

(ii) if $(x_1, x_2), x_1 \neq x_2$, is observed i times, then (x_2, x_1) is also observed i times.

The information matrix of a symmetric design $D_n = \{(x_{1i}, x_{2i}), i=1, 2, \dots, n\}$ is

$$M_{D_n} = \begin{pmatrix} n & 0 & 0 & \lambda_2 & \lambda_2 & 0 \\ & \lambda_2 & 0 & 0 & 0 & 0 \\ & & \lambda_2 & 0 & 0 & 0 \\ & & & \lambda_4 & \lambda_{2,2} & 0 \\ & & & & \lambda_4 & 0 \\ & & & & & \lambda_{2,2} \end{pmatrix} \quad (3.3)$$

where $\lambda_{2,2} = \sum x_{1i}^2 x_{2i}^2$.

THEOREM 3. *The class of designs of the type*

$$D_n = \left\{ (\pm 1, \pm 1), (\pm x, \pm x), (\pm 1, 0), (0, \pm 1), (0, 0) \right\} \quad (3.4)$$

$$\begin{matrix} n_1 & 1 & n_2 & n_2 & n_3 \end{matrix}$$

where $0 \leq x, y < 1$ and $4(n_1 + n_2) + 8 + n_3 = n$, consists the minimal essentially complete class in the class of symmetric designs.

The proof is from the next four lemmas.

LEMMA 3. A design $D_n = \{(x_{1i}, x_{2i})\}$ is better than $D_n' = \{(x'_{1i}, x'_{2i})\}$ if and only if

$$(i) \quad \lambda_2 = \lambda_2', \quad (3.5)$$

$$(ii) \quad \lambda_{2,2} \geq \lambda'_{2,2}, \quad (3.6)$$

and

$$(iii) \quad \lambda_4 - \lambda_{2,2} \geq \lambda_4' - \lambda'_{2,2} \quad (3.7)$$

hold, where $\lambda_2^{(j)} = \sum x_j^{(j)2}$, $\lambda_4^{(j)} = \sum x_j^{(j)4}$, $j=1, 2$, and $\lambda_{2,2}^{(j)} = \sum x_1^{(j)2} x_2^{(j)2}$.

PROOF. The difference of the information matrices of D_n and D_n' is

$$M_{D_n} - M_{D_n'} = \begin{pmatrix} 0 & 0 & 0 & \lambda_2 - \lambda_2' & \lambda_2 - \lambda_2' & 0 \\ \lambda_2 - \lambda_2' & 0 & 0 & 0 & 0 & 0 \\ & \lambda_2 - \lambda_2' & 0 & 0 & 0 & 0 \\ & & \lambda_4 - \lambda_4' & \lambda_{2,2} - \lambda'_{2,2} & 0 & 0 \\ & & & \lambda_4 - \lambda_4' & 0 & 0 \\ & & & & \lambda_{2,2} - \lambda'_{2,2} & 0 \end{pmatrix} \quad (3.8)$$

That $M_{D_n} - M_{D_n'}$ is nonnegative definite implies conditions (3.5), (3.6) and (3.7).

LEMMA 4. Any design of the type

$$D' = D_0 \cup \{(\pm x_1, \pm x_2), (\pm x_2, \pm x_1)\}, \quad 0 < x_1 \neq x_2 < 1, \quad (3.9)$$

can be improved by a design

$$D = D_0 \cup \{(\pm u, \pm u), (\pm v, 0), (0, \pm v)\} \quad (3.10)$$

for some u and v , $0 \leq u, v < 1$, where D_0 is any design.

PROOF. We shall show the existence of u and v , $0 \leq u, v < 1$, that satisfy (3.5), (3.6) and (3.7). Since the design D_0 is included in both D and D' , we can omit the contributions of D_0 to those conditions. Conditions are reduced to

$$(i) \quad 4u^2 + 2v^2 = (x_1^2 + x_2^2) = 8A \text{ (say)} \quad (3.11)$$

$$(ii) \quad 4u^4 \geq 16x_1^2 x_2^2 = 8B^2 \text{ (say)} \quad (3.12)$$

and

$$(iii) \quad 2v^4 \geq 8(A^2 - 4B^2). \quad (3.13)$$

Substituting $u^2 \geq 2B$ (from (3.10)) to (3.9), we get

$$v^2 \leq 4A - 2\sqrt{2}B. \quad (3.14)$$

By straightforward calculation, we get that $4A - 2\sqrt{2}B \geq 2\sqrt{A^2 - 4B^2}$. Thus, from (3.11) and (3.12) the existence of u and v is assured.

Note that the existence of u and v is not unique.

LEMMA 5. Any design of the type

$$D' = D_0 \cup \{(\pm x_i, \pm x_i), i=1, 2, \dots, m\} \quad (3.15)$$

can be improved by

$$D = D_0 \cup \left\{ \begin{array}{ccc} (\pm 1, \pm 1), (\pm u, \pm u), & (0, 0) \\ m' & 1 & 4(m-m'-1) \end{array} \right\} \quad (3.16)$$

for some integer m' and $u \in [0, 1)$.

PROOF. The conditions (3.5), (3.6) and (3.7) become

$$(i) \quad m' + u^2 = \sum x_i^2, \quad (3.17)$$

$$(ii) \quad m' + u^4 \geq \sum x_i^4 \quad (3.18)$$

and

$$(iii) \quad 0 \geq 0. \quad (3.19)$$

(3.19) is trivial. Conditions (3.17) and (3.18) are satisfied by choosing $m' = [\sum x_i^2]$, $u = \sqrt{\sum x_i^2 - m'}$. That appeared in the proof of theorem 2.

LEMMA 6. Any design of the type

$$D' = D_0 \cup \{(\pm x_i, 0), (0, \pm x_i), i=1, 2, \dots, m\}, 0 \leq x_i < 1, \quad (3.20)$$

can be improved by

$$D = D_0 \cup \left\{ \begin{array}{cccc} (\pm 1, 0), (0, \pm 1), (\pm u, 0), (0, \pm u), & (0, 0) \\ m' & m' & 1 & 1 & 4(m-m'-1) \end{array} \right\} \quad (3.21)$$

for some integer m' and $u \in [0, 1)$.

PROOF. The conditions (3.5), (3.6) and (3.7) are reduced to

$$(i) \quad m' + u^2 = \sum x_i^2 \quad (3.22)$$

$$(ii) \quad 0 \geq 0 \quad (3.23)$$

and

$$(iii) \quad m' + u^4 \geq \sum x_i^4. \quad (3.24)$$

Those are the same conditions of above lemma.

Any design which is not of the type of (3.4) can be improved and there is not other design which is better than a design of the type (3.4) because of their construction of improvement. Thus theorem 3 is proved.

The definition 3 of the symmetricity of designs seems too strong. Though any admissible design has not these observation points, if (x_1, x_2, \dots, x_k) , all x_i 's are distinct each other, is in a design D_n then n must be greater than $2^k k!$. For $k=3, 4$ and 5 those numbers are 48, 192 and 1920, respectively.

Let $H=(h_{ij})$ be a $2^m \times k$ matrix such that each element h_{ij} is 1 or -1 , ${}^t H H = 2^m I_k$ and none of its column vectors equals to ${}^t(1, 1, \dots, 1)$, and m is the smallest integer which satisfies $2^m > k$. As H , we can use a submatrix of Hadamard matrix.

DEFINITION 4. A design is *pseudo-symmetric* if the followings hold.

(i) If $(x_1, x_2, \dots, x_k) \in D$, then $(h_{i1}x_1, h_{i2}x_2, \dots, h_{ik}x_k) \in D$ for $i=1, 2, \dots, 2^m$,

and

(ii) if a pair (x, y) is contained in some two column vectors of the design matrix X of D , then the pair is also contained in any two column vectors of X .

Any pseudo-symmetric design has no longer (a) the origin symmetricity and (b) the factor symmetricity with respect to observation points. But, it remains the form (4.3) of its information matrix unchanged. Symmetric or pseudo-symmetric design defined in this paper are ones of the second order symmetric designs. (See [5] the definition of second order symmetry).

Numbers of observation points of pseudo-symmetric designs are relatively smaller than that of symmetric designs. When k is a prime number or a power of some prime number, the complete orthogonal system of Latin squares, having letters $1, 2, \dots$, and k , exists. Let $(\sigma_1, \sigma_2, \dots, \sigma_k)$ be any row of latin square in that system. If $(x_{\sigma_1}, x_{\sigma_2}, \dots, x_{\sigma_k}) \in D$ for any $(x_1, x_2, \dots, x_k) \in D$, then the condition (ii) of definition 4 is satisfied. In this case, the numbers of observation points are at least $2^m k(k-1)$, those are 24, 96 and 180 when $k=3, 4$ and 5 , respectively.

The next theorem is proved by the same manner of previous theorems.

THEOREM 5. *The class of designs of the type*

$$D = \left\{ \begin{array}{l} (h_{i1}, h_{i2}, \dots, h_{kk}), (h_{i1}x, h_{i2}x, \dots, h_{ik}x), (\pm 1, 0, \dots, 0), \dots, \\ \quad n_1 \qquad \qquad \qquad 1 \qquad \qquad \qquad n_2 \qquad \dots \\ (0, \dots, 0, \pm 1), (\pm y, 0, \dots, 0), \dots, (0, \dots, 0, \pm y), (0, 0, \dots, 0) \\ \quad n_2 \qquad \qquad \qquad 1 \qquad \dots \qquad 1 \qquad \qquad \text{others} \end{array} \right\} \quad (4.11)$$

consists the minimal essentially complete class in the class of pseudo-symmetric designs, where $H=(h_{ij})$ is defined above and $0 \leq x, y < 1$.

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