ON D- AND A-OPTIMAL DESIGNS OF EXPERIMENTS

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Abstract

It is shown that for linear multiple model of heteroscedastic observations for which variances changing linearly D-optimal designs take place when all points of spectrum of these designs lay in vertices of unite cube and not only. The structure such D- and A-optimal designs for heteroscedastic observations is investigated.

1 Introduction

Consider the linear multiple model of heteroscedastic observations:

$$y_i = \theta_1 x_{1i} + ... + \theta_m x_m + \varepsilon(x^{(i)}), i = 1, 2, ..., n, n \geq m, \tag{1}$$

where y_i are observed variables; $\theta_1, ..., \theta_m$ are unknown parameters; $x^{(i)}= (x_{1i}, ..., x_{mi})$ are m-vectors of controllable variables and components of these vectors taken from the interval $[-1, 1]$; $\varepsilon(x^{(i)})$ are uncorrelated random errors of observations with mean zero and limited variance

$$D(\varepsilon(x^{(i)}) = a_0 + a_1 x_{1i} + ... + a_m x_{mi} > 0, \tag{2}$$

for each realization $x^{(i)}$ from m-dimensional unit cube and $a_0 > 0, | a_1 | +...+ | a_m |< a_0$. In the article [1] it is proved that for homoscedastic observations (1) the D-optimal design is obtained by setting $x_{ij} = \pm 1$. In this paper we obtain the same result for heteroscedastic observations (1), (2). In the paper [2] it is investigated the structure of saturated D-optimal designs ε_n^0 for homoscedastic model of observations (1) when $n = 3, 4, 5, 6$. In our article it is shown that the set of designs ε_3^0 for homoscedastic observations (1) is much wider than the set which is described in [2]. The set of such designs ε_3^0 infinitely and has power of a continuum. The structure of A-optimal designs for a line of regress with square-law change of a variance of observations is investigated.These results generalize results received in [3] for linear change of variance of observations.

2 The model of heteroscedastic observations

We have the following theorem for heteroscedastic observations (1), (2).

Theorem 1. *Exist exact D-optimal design ε_n^0 of experiments (1), (2) all spectrum points of it lay in the vertices of m-dimensional unit cube.*

Consider that ε_n^0 is D-optimal design of experiments (1), (2) and that $\mid x_{ij} \mid < 1$. Make this point "floating", i.e. $x_{11} = x \in [-1.1]$. Denote the design of experiment being obtain from ε_n^0 by changing x_{11} as ε_x. Information matrix of design ε_x can be written as $M(\varepsilon_x) = A(x) + B$, where

$$A(x) = \frac{1}{d_1(x)} \begin{pmatrix} x \\ t \end{pmatrix} (x, t'), B = \sum_{i=2}^{n} \frac{x^{(i)}(x^{(i)})'}{d_i},$$

$d_1(x) = a_1x+c_1, c_1 = a_0+a_{21}+...+a_mx_{m1}, d_i = a_0+a_1x_{1i}+...+a_mx_{mi}, t' = (x_{21}, ..., x_{m1})'$. Matrix B does not depend on x and $rank A(x) = 1$. Matrixes B and $A(x)$ can be written as

$$B = (b_1, ..., b_m), A(x) = (a_1(x), ..., a_m(x)),$$

where b_i and $a_i(x)$ are m-dimensional columns, $i = 1, 2, ..., m$. Determinant $\mid A(x)+B \mid$ may be presented as a sum of determinants of matrixes containing different combinations of columns matrixes $A(x)$ and B. Determinants of these combinations containing more than one column of $A(x)$ is equal to zero. Hence

$$\mid A(x) + B \mid = \mid a_1(x), b_2, b_3, ..., b_m \mid + \mid b_1, a_2(x), b_3, ..., b_m \mid + ... + \mid b_1, b_2, b_3, ..., a_m(x) \mid$$
$$+ \mid b_1, b_2, ..., b_m \mid . \tag{3}$$

Calculating determinants in the rigt part of (3) with respect elements of columns $a_1(x), a_2(x), , ..., .a_m(x)$ we obtain

$$f(x) = \mid A(x) + b \mid = \frac{\alpha x^2 + \beta x + \gamma}{a_1x + c_1} + m, \tag{4}$$

where

$$m = \mid B \mid, \alpha = \mid \sum_{i=2}^{n} \frac{x^{(i)}(x^{(i)})'}{d_i} \mid \geq 0, z^{(i)} = (x_{2i}, ..., x_{mi})'$$

and β, γ are constants which do not depend on x. If the function $f(x)$ do not depend on x then we can set $x = \pm 1$ in the D-optimal design ε_n^0. Hence we obtain the result of theorem. If the function $f(x)$ depend on x then $f(-1)$ or $f(1)$ take value more than $f(x_{11})$. It is impossible. We have contradiction. Indeed, the derivative of function $f(x)$ is

$$\frac{df(x)}{dx} = \frac{\alpha a_1 x^2 + 2\alpha c_1 x + c_1\beta - a_1\gamma}{(a_1x + c_1)^2}. \tag{5}$$

Let is designate though $D = 4\alpha(\alpha c_1^2 - a_1(c_1\beta - a_1\gamma))$ numerator discriminant in (5). If $D \leq 0$, the derivative (5) does not change his signum in the interval $[-1, 1]$, i.e. the function $f(x)$ is increasing or decreasing in $[-1, 1]$. If $D > 0$, than the function $f(x)$ is convex downwards. Indeed,

$$\frac{d^2 f(x)}{dx^2} = \frac{D}{2\alpha(a_1x + c_1)^2} > 0.$$

Hence, the function $f(x)$ takes maximum value at $x = \pm 1$ and it value more than $f(x_{11})$.Theorem 1 is proved.

Theorem 1 says that it is possible that among D-optimal designs exist design in which not all points lay in the vertices of unite cube. It will be shown in following section that such possibility is realized for saturated design ε_3^0.

3 Saturated D-optimal designs

Information matrix for saturated design ε_n (when $n = m$) for model heteroscedastic observations (1), (2) is

$$M = X_1' X_1, X_1 = \begin{pmatrix} \frac{x_{11}}{\sqrt{d_1}} & \frac{x_{21}}{\sqrt{d_1}} & \dots & \frac{x_{n1}}{\sqrt{d_1}} \\ \dots & \dots & \dots\dots & \\ \frac{x_{1n}}{\sqrt{d_n}} & \frac{x_{2n}}{\sqrt{d_n}} & \dots & \frac{x_{nn}}{\sqrt{d_n}} \end{pmatrix}$$

Determinant of matrix M is equal to $\mid M \mid= (\mid X_1 \mid)^2$. So, D-optimal saturated design ε_n^0 is such design which takes maximum of $\mid X_1 \mid$ in absolute value. Using theorem 1 we can prove the following theorem.

Theorem 2. *Saturated D-optimal designs ε_3^0 for homoscedastic observations (1) form infinite set of designs having following structure. Three spectrum points of this design should lay on one of six sides of unite cube, $-1 \leq x_i \leq 1, i = 1, 2, 3$. Two points are the ends of same edge and the third point is any point laying on opposite edge of the same side.*

It has been shown in article [2], that the absolute value of a determinant matrix X_1 corresponding to design ε_3^0 at which all points of spectrum lays in vertices of unite cube is equal 4. It is easy to check up, that such situation takes place for the matrixes X_1 which structure is described in theorem 2. Hence, such matrixes correspond to optimal designs and such designs there are an infinite set. Theorem 2 is proved.
Following theorem is correct for heteroscedastic observations.

Theorem 3. *Saturated D-optimal design ε_3^0 for heteroscedastic observations coincides with design ε_3^0 for homoscedastic observations at which spectrum points lay in vertices of unite cube $\mid x_i \mid\leq 1, i = 1, 2, 3$ and at which product of variances of observations in these points is minimal.*

Construction of ε_3^0 is reduced to maximization of absolute value of

$$\mid X_1 \mid= \frac{\mid X \mid}{\sqrt{d_i d_j d_k}}, \tag{6}$$

where X is the matrix of design ε_3,

$$X = \begin{pmatrix} x_{1i} & x_{2i} & x_{3i} \\ x_{1j} & x_{2j} & x_{3j} \\ x_{1k} & x_{2k} & x_{3k} \end{pmatrix}. \tag{7}$$

In matrix (7) i, j, k are various numbers of vertices of unite cube. Determinants of matrixes X with such structure are equal on absolute value to zero or 4. The matrixes (7) which determinants are equal ± 4 and product of observations minimum define the optimum designs ε_3^0. Theorem 3 is proved.
For example, for variance $d(x) = 10 - 2x_1 + x_2 - x_3$ design with spectrum points $x^{(1)} = (1, 1, 1)$, $x^{(2)} = (1, -1, 1)$, $x^{(3)} = (1, -1, -1)$ is saturated D-optimal and it is unique.

4 Structure of A-optimal designs for regress line with heteroscedastic observations

Consider regress line

$$y_i = \theta_0 + \theta_1 x_i + \varepsilon(x_i), \mid x_i \mid \leq 1, i = 1, 2, \ldots, n, \tag{8}$$

with variance of observations

$$D(\varepsilon(x_i)) = a_2 x_i^2 + a_1 x_i + a_0 = a_0(k_2 x_i^2 + k_1 x_i + 1) > 0, a_0 > 0, \tag{9}$$

where $k_2 = \frac{a_2}{a_0}, k_1 = \frac{a_1}{a_0}$ and constants are such that for which one of following conditions is carried out
$i) \mid k_1 \mid < 2\sqrt{k_2}, k_2 > 0,$
$ii) \mid k_1 \mid < 1 + k_2, -1 < k_2 \leq 0,$
$iii) 2\sqrt{k_2} < \mid k_1 \mid < 1 + k_2, 0 < k_2 < 1.$
These conditions guarantee that inequality (9) will be carried out. In [3] it is investigated structure of A-optimal designs for model (8), (9) when $a_2 = 0$. It is possible to generalize the result obtained in [3] and receive the following theorem.

Theorem 4. *Let one of conditions i), ii), iii) is carried out. Then for* $p_{s-1} \leq k_1 \leq p_s$ *A-optimal designs for model of observations (8), (9) are following:*

$$\varepsilon_n^0 = \begin{pmatrix} -1; & 1 \\ n_1 - s; & n - n_1 + s \end{pmatrix}, s = 0, \pm 1, \pm 2, \ldots,$$

where $n_1 = [\frac{n}{2}]$ *is the whole part from* $\frac{n}{2}$, $n_1 - s = 1, 2, \ldots,$ *and*

$$p_s = \frac{n(1 + k_2)(n - 2n_1 + 2s + 1)}{2n_1(n_1 - 2s - n - 1) + n(2s + n + 1) + 2s(s + 1)}.$$

References

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