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A CONVERGENCE THEOREM[1] IN THE THEORY OF D-OPTIMUM EXPERIMENTAL DESIGNS

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It is proved that in a sequential design of a regression problem the variance of the l.s. estimate for the response surface in the nth sequential point tends to zero with $n \to \infty$. This allows the proof of the convergence of certain procedures for computing D_s-optimum designs.

0. Introduction. In several papers (Fedorov (1971), Wynn (1970) and (1972)) sequential methods were proposed for computing D-optimum designs. The idea of such methods is that we start from an initial design (an arbitrary design with a nonsingular information matrix) and we add new points to the design following a certain rule. The main problem in the theory of such methods is proving that they allow to approximate the optimum design as closely as is necessary.

Let $\theta = (\theta_1, \cdots, \theta_k)'$ be the vector of unknown parameters and let $f(x) = (f_1(x), \cdots, f_k(x))'$ be the vector of regression functions in the considered design problem. It is supposed that $\mathscr{X}$—the domain of $f(x)$—is compact in a topology in which $f(x)$ is continuous and that the functions $f_1(x), \cdots, f_k(x)$ are linearly independent on $\mathscr{X}$. Let $\{x_n\}_1^\infty$ be the sequence of points generated by a sequential procedure (compare with Wynn (1972)). The Theorem in the present paper states that the variance of the l.s. estimate for $f'(x_{n+1})\theta$, which is computed from the n-point design $x_1, \cdots, x_n$, converges to zero with $n \to \infty$. This result allows proof of the convergence of certain sequential procedures to a D_s-optimum design (compare with the proof of Theorem 2 in Wynn (1972)).

We refer to Wynn (1970) and (1972) for the full formulation of the considered design problem. We shall also use the notation which was used in these papers.

1. Results. A design measure ξ is a probability measure on Borel subsets of $\mathscr{X}$. The design measure ξ_n associated to the discrete design $x_1, \cdots, x_n$ assigns the measure m/n to every Borel set containing m points from $x_1, \cdots, x_n$. The information matrix corresponding to ξ_n is

$$M(\xi_n) = \frac{1}{n} \sum_{i=1}^n f(x_i)f'(x_i) = \int_{\mathscr{X}} f(x)f'(x)\xi_n(dx) .$$

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[1] This convergence theorem was first presented as a part of a larger paper on the theory of D_s-optimum designs which was written simultaneously with the paper by Wynn (1972) and independently from it. The main difference between the two approaches is the presented convergence theorem.

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We suppose that starting from an integer $n(0)$ the information matrix $M(\xi_n)$ will be nonsingular.

Let

$$d(x, \xi_n) = f'(x)M^{-1}(\xi_n)f(x)$$

and

$$C(x, \bar{x}, \xi_n) = f'(x)M^{-1}(\xi_n)f(\bar{x})/n .$$

$C(x, \bar{x}, \xi_n)$ is the covariance of the estimate for $f'(x)\theta$ with the estimate for $f'(\bar{x})\theta$, when the discrete design $x_1, \cdots, x_n$ is used.

LEMMA. (Pázman (1968)).

$$C(x, \bar{x}, \xi_n) - C(x, \bar{x}, \xi_{n+1}) = \frac{C(x, x_{n+1}, \xi_n)C(\bar{x}, x_{n+1}, \xi_n)}{1 + C(x_{n+1}, x_{n+1}, \xi_n)} . \tag{1}$$

PROOF. We use the formula

$$\frac{M^{-1}(\xi_{n+1})}{n+1} = \frac{M^{-1}(\xi_n)}{n} - \frac{M^{-1}(\xi_n)f(x_{n+1})f'(x_{n+1})M^{-1}(\xi_n)}{n^2 + nf'(x_{n+1})M^{-1}(\xi_n)f(x_{n+1})} \tag{2}$$

which can be verified by a direct multiplication of the right-hand side of (2) by the matrix $(n+1)M(\xi_{n+1}) = nM(\xi_n) + f(x_{n+1})f'(x_{n+1})$. Multiplying (2) by $f'(x)$ from the left and by $f(\bar{x})$ from the right we obtain (1).

THEOREM. *For an arbitrary sequence $x_{n(0)+1}, x_{n(0)+2}, \cdots$ of points from $\mathscr{X}$*

$$\lim_{n\to\infty} \frac{d(x_{n+1}, \xi_n)}{n} = 0 . \tag{3}$$

PROOF. We shall denote

$$K = \sup_{x\in\mathscr{X}} \|f(x)\| , \qquad C = \sup_{\|a\|=1} a'M^{-1}(\xi_{n(0)})a/n(0)$$

where $\| \ \|$ is the norm in the k-dimensional space. As a consequence of (2) we have for every $n \geqq n(0)$

$$\sup_{\|a\|=1} a'M^{-1}(\xi_n)a/n \leqq C .$$

Take an arbitrary $\varepsilon > 0$ and let r be an integer greater then $2/\varepsilon$. Denote $\delta = \varepsilon/8rK^3C^2$.

Since $\mathscr{X}$ is compact and $f(x)$ is continuous, there are open sets $U_i^\delta \subset \mathscr{X}$; $i = 1, \cdots, N$, such that $\bigcup_{i=1}^N U_i^\delta = \mathscr{X}$ and that $\|f(x^{(1)}) - f(x^{(2)})\| < \delta$ for arbitrary points $x^{(1)}, x^{(2)} \in U_i^\delta$. This implies that for such points and for $n \geqq n(0)$ also the following inequalities are valid:

$$|C(x^{(1)}, x^{(1)}, \xi_n) - C(x^{(2)}, x^{(2)}, \xi_n)| < 2KC\delta \tag{4}$$

and

$$|C^2(x^{(1)}, x^{(2)}, \xi_n) - C^2(x^{(2)}, x^{(2)}, \xi_n)| < 2K^3C^2\delta . \tag{5}$$

Denote $\mathscr{X}^\delta$ the union of all sets U_i^δ each of which contains an infinite subsequence from $\{x_i\}_{i=n(0)+1}^\infty$. Evidently there is an integer $n(1)$ such that for every $n \geqq n(1)$ there is an $x_n \in \mathscr{X}^\delta$ and there is an integer $n(2)$ such that the finite sequence $x_{n(0)+1}, \cdots, x_{n(2)}$ has at least r terms in each set $U_i^\delta \subset \mathscr{X}^\delta$.

We take a fixed integer $n \geqq \max[n(1), n(2)]$. Since $x_{n+1} \in \mathscr{X}^{\delta}$, one of the sets $U_i^{\delta} \subset \mathscr{X}^{\delta}$ contains the point x_{n+1} and also r points from the sequence $x_{n(0)+1}, \cdots, x_n$, say the last r points. Denote by $\xi_n^{(s)}$ the design measure associated to the n-point discrete design $x_1, \cdots, x_{n-s}, x_{n+1}, \cdots, x_{n+1}$. Obviously

$$C(x_{n+1}, x_{n+1}, \xi_n^{(r)}) < \frac{1}{r} < \frac{\varepsilon}{2}. \tag{6}$$

Denote by Δ the difference

$$\Delta = C(x_{n+1}, x_{n+1}, \xi_{n-1}) - C(x_{n+1}, x_{n+1}, \xi_n).$$

Using (1) and the inequalities (4) and (5) we obtain

$$\Delta < C(x_{n+1}, x_{n+1}, \xi_{n-1}) < K^2C$$

$$\Delta = \frac{C^2(x_{n+1}, x_n, \xi_{n-1})}{1 + C(x_n, x_n, \xi_{n-1})} > \frac{C^2(x_{n+1}, x_{n+1}, \xi_{n-1}) - 2K^3C^2\delta}{1 + C(x_{n+1}, x_{n+1}, \xi_{n-1}) + 2KC\delta}. \tag{7}$$

From (7) it follows that

$$\begin{aligned}[1 + C(x_{n+1}, x_{n+1}, \xi_{n-1})]\Delta + 2K^3C^2\delta &> [1 + C(x_{n+1}, x_{n+1}, \xi_{n-1}) + 2KC\delta]\Delta \\ &> C^2(x_{n+1}, x_{n+1}, \xi_{n-1}) - 2K^3C^2\delta.\end{aligned}$$

Hence

$$\Delta > \frac{C^2(x_{n+1}, x_{n+1}, \xi_{n-1})}{1 + C(x_{n+1}, x_{n+1}, \xi_{n-1})} - 4K^3C^2\delta. \tag{8}$$

Comparing the right-hand side of (8) with (1) we obtain from (8)

$$C(x_{n+1}, x_{n+1}, \xi_n) < C(x_{n+1}, x_{n+1}, \xi_n^{(1)}) + 4K^3C^2\delta. \tag{9}$$

Applying r times the inequality (9) we obtain

$$C(x_{n+1}, x_{n+1}, \xi_n) - C(x_{n+1}, x_{n+1}, \xi_n^{(r)}) < 4rK^3C^2\delta = \varepsilon/2. \tag{10}$$

Comparing (6) with (10) we obtain

$$C(x_{n+1}, x_{n+1}, \xi_n) < \varepsilon$$

for every $n \geqq \max[n^{(1)}, n^{(2)}]$. The theorem is proved.

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