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ON AN ALTERNATIVE DERIVATION OF THE MOMENTS OF A-OPTIMAL SECOND ORDER DESIGNS FOR REGRESSION ON CUBES

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SUMMARY

The moments of A-optimal second-order designs for regression on cubes are derived using a method that requires solving an univariate equation rather than a pair of equations involving two variables as required by the 'standard' method.

Keywords : A-optimal, Cubic region, Second-order design.

Introduction

Galil and Kiefer (1977) considered designs for quadratic regression on cubes and studied the performance of various optimal designs under variation of criteria. Among the new results presented by them was the derivation of A-optimal designs. Their method for deriving these designs required numerical solution of a pair of 6th degree equations in two variables. In the present paper an alternative derivation of these designs is provided. In this method the problem is reduced to solving a single univariate equation.

2. The Method

Under A-optimality criterion the objective is to minimize tr $M^{-1}(\xi)$ where $M(\xi)$ is the information matrix of the design ξ. As stated by Galil and Kiefer (1977), for our problem we only need to consider symmetric ξ's. For a second-order symmetric ξ, among the moments of order four or less only three are nonzero and

$$\text{tr } M^{-1}(\xi) = V(\alpha_2, \alpha_4, \alpha_{22})$$
$$= 1 + k/\alpha_2 + k(k-1)/(2\alpha_{22}) + (k-1)/(\alpha_4 - \alpha_{22})$$
$$+ (1 - k\alpha_2^2)/\{\alpha_4 + (k-1)\alpha_{22} - k\alpha_2^2\},$$

where

$$\alpha_2 = \int_{\mathscr{X}} x_i^2 \xi(dx), \alpha_4 = \int_{\mathscr{X}} x_i^2 \xi(x,) \quad \alpha_{22} = \int_{\mathscr{X}} \xi x_j^2 x_i^2 \xi(dx) \ (i \neq j).$$

Here $\mathscr{X} = \{x = (x_1, \ldots, x_k) : |x_i| \leqslant R\}$ is the experimental region and $x_1, \ldots, x_k$ are the explanatory variables. Without loss of generality, we take $R = 1$. Then under A-optimality criterion the objective is to minimize $V(\alpha_2, \alpha_4, \alpha_{22})$ with respect to α_2, α_4 and α_{22} subject to the constraint $1 > \alpha_2 > \alpha_{22} \geqslant 0$, $\alpha_4 + (k-1)\alpha_{22} > k\alpha_2^2$.

Since V is strictly decreasing in α_4, for the A-optimal design we must have $\alpha_4 = \alpha_2$ and then the problem is to minimize

$$V(\alpha_4, \alpha_{22}) = 1 + k/\alpha_2 + k(k-1)/(2\alpha_{22}) + (k-1)/(\alpha_2 - \alpha_{22})$$
$$+ (1 + k\alpha_2^2)/\{\alpha_2 + (k-1)\alpha_{22} - k\alpha_2^2\},$$

subject to $1 > \alpha_2 \geqslant \alpha_{22} > 0$, $\alpha_{22} > \alpha_2(k\alpha_2 - 1)/(k-1)$.

substituting $t = \alpha_{22}/\alpha_2$ we may write

$$V(\alpha_4, \alpha_{22}) = V^*(t, \alpha_2) = A(t)/\beta + B(t)/(1-\beta)$$

where $\beta = k\alpha_2/\{1 + (k-1)t\}$,

$$A(t) = k[k + k(k-1)/(2t) + (k-1)/(1-t)$$
$$+ 1/\{1 + (k-1)t\}]/\{1 + (k-1)t\},$$

$$B(t) = [1 + k/\{1 + (k-1)t\}^2],$$

and consider the equivalent problem of minimizing $V^*(t, \alpha_2)$ with respect to t and α_2. The constraints now are $1 > t > 0$, $1 > \beta > 0$.

For a given t, partial differentiation of V^* with respect to α_2 immediately shows that V^* is minimized when $\beta = \beta(t) = \{A(t)\}^{1/2}/[\{A(t)\}^{1/2} + \{B(t)\}^{1/2}]$. Substituting the corresponding value $\alpha_2(t)$ of α_2 in V^* we obtain

$$V^*(t), \alpha_2(t)) = V^{**}(t) = [\{A(t)\}^{1/2} + \{B(t)\}^{1/2}]^2,$$

which we have to minimize with respect to t or equivalently minimize

$\{V^{**'}(t)\}^{1/2}$ with respect to t. Thus the problem is reduced to an univariate minimization problem which can be easily tackled numerically. If $t = t_0$ is the solution then the minimizing value of β is $\beta = \beta_0 = \beta(t_0)$. The solutions to the original problem are $\alpha_2 = \alpha_2^{(0)} = \{1 + (k-1) t_0\} \beta_0/k$ and $\alpha_{22} = \alpha_{22}^{(0)} = t_0 \alpha_2^{(0)}$.

3. Discussion

The method illustrated above was applied to derive the moments of *A*-optimal designs for regression on *k*-dimensional cubes. The results obtained for $k = 2$ to $k = 10$ are displayed in Table 1.

TAALE 1—OPTIMAL VALUES OF t, α_2, α_{22}

k	t	α_2	α_{22}
2	0.6579	0.5714	0.3759
3	0.6915	0.6148	0.4251
4	0.7153	0.6457	0.6419
5	0.7335	0.6695	0.4911
6	0.7481	0.6886	0.5152
7	0.7600	0.7044	0.5353
8	0.7702	0.7179	0.5529
9	0.7790	0.7296	0.5683
10	0.7868	0.7399	0.5821

The results clearly match those obtainable from Galil and Kiefer (1977), the discrepancies in third and fourth decimal places being explained by rounding off errors.

The method may be useful in other contexts as well

REFERENCE

Galil, Z. and Kiefer, J. (1977) : Comparison of design for quadratic regression on cubes. *J. Statist. Plann. Inf.*, 1 : 121-132.