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Exact D_s-efficient Designs for Quadratic Response Surface Model†

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ABSTRACT

Exact D_s-efficient designs for the precise estimation of all the coefficients of the quadratic terms are studied in a quadratic response surface model. Efficient exact designs are constructed for $2 \leqslant q \leqslant 5$ w.r.t. D_s-optimaity criterion based on Pesotchinsky's(1975) and approximate D_s-optimal design given in Lim & Studden(1988). Moreover, they seem to have reasonably good D-efficiencies. Similar idea could apply to $q \geq 6$ cases.

1. Introduction

Consider a quadratic response surface model of the form :

$$Y(x) = \beta_0 + \sum_{i=1}^{q} \beta_i x_i + \sum_{i=1}^{q} \beta_{ii} x_i^2 + \sum_{1 \leq i < j}^{q} \beta_{ij} x_i x_j + \epsilon \quad . \tag{1}$$

In this model, $Y(x)$ is the response or dependent variable, x_i's are the independent experimental variables, the β's are parameters to be estimated using the data from the experiment and ϵ is an experimental error term with the common variance σ^2. Suppose each independent experimental variable is properly scaled, so that the experimental region becomes the q-cube

$$X = \{x : |x_i| \leq 1, \ i = 1, \cdots, q\}.$$

Often the purpose of the response surface analysis is to find the optimum operating conditions. Also it is very important to determine the nature of the response contour system. Thus, we put more emphasis on the precise estimation of all the coefficients of the quadratic terms.

For the quadratic polynomial regression on the hypercube Kiefer(1961a), Kono(1962) and Farrell, et al(1967) give a rather complete description of the approximate D-optimal design and further considerations of minimum number of points of support of the D-optimal design are inclu-

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ded in Pesotchinsky(1975). The approximate D_s-optimal design for estimating all the coefficients of the quadratic terms is described by Lim & Studden(1988). The main result of the paper is the construction of efficient exact designs for $2 \le q \le 5$ w.r.t. D_s-optimaity criterion based on Pesotchinsky's minimal second-order symmetric sets and approximate D_s-optimal design given in Lim & Studden(1988). Moreover, they seem to have reasonably good D-efficiencies. Similar idea could apply to $q \ge 6$ cases.

2. Preliminaries

Let $f(x)$ be a $(q+1)(q+2)/2 \times 1$ vector of all the monomials of degree upto two and β be a vector of regression coefficients. Then it is assumed that for each $x=(x_1, \cdots, x_q)$ in the q-cube

$$EY(x)=f(x)'\beta.$$

A design ξ is a probability measure on X. The information matrix is given by

$$M(\xi)=\int f(x)f(x)'\xi(dx). \quad (2)$$

If the design is implementable and N uncorrelated observations are taken, then the covariance matrix of the least square estimates(l.s.e.) $\hat{\beta}$ of β is given by

$$Var(\hat{\beta})=\frac{\sigma^2}{N}M^{-1}(\xi). \quad (3)$$

A design ξ^* is an approximate D-optimal design iff $|M(\xi^*)|=Max_\xi |M(\xi)|$.

In the case where interest is in only all the coefficients of quadratic terms in β, it is customary to decompose $f(x)$ into $f(x)'=(f_1(x)', f_2(x)')$, where $f_1(x)'=(1, x_1, \cdots, x_q)$ and $f_2(x)'=(x_1^2, \cdots, x_q^2, x_1x_2, \cdots, x_{q-1}x_q)$. The vector $f_2(x)$ contains all the quadratic terms. Similarly the information matrix is decomposed into

$$M(\xi)=\begin{pmatrix} M_{11}(\xi) & M_{12}(\xi) \\ M_{21}(\xi) & M_{22}(\xi) \end{pmatrix}$$

The covariance matrix of l.s.e. of all the coefficients of quadratic terms in β is proportional to the inverse of

$$\Sigma_s(\xi)=M_{22}(\xi)-M_{21}(\xi)M_{11}^{-1}(\xi)M_{12}(\xi).$$

A design ξ_s^* is an approximate D_s-optimal design iff $|\Sigma_s(\xi_s^*)|=Max_\xi |\Sigma_s(\xi)|$. To find the maximum of $|\Sigma_s(\xi)|$, we use the result that

$$|\Sigma_s(\xi)|=\frac{|M(\xi)|}{|M_{11}(\xi)|} \quad (4)$$

Using the invariance theorem(Kiefer(1961b)) and equivalence theorem(Karlin & Studden

(1966) and Atwood(1969)), Lim & Studden(1988) have shown that there exist D_s-optimal designs which are symmetric w.r.t. permutations and sign changes of x_i's, $i=, \cdots, q$ and they must be supported on E, where $E=\{x : |x_i|=0 \text{ or } 1\}$. For symmetric designs supported on E, we let

$$u=\int x_1^2\xi(dx)=\int x_1^4\xi(dx) \text{ and } v=\int x_1^2x_2^2\xi(dx). \qquad (5)$$

It is then easy to show (see Kiefer(1961a)) that

$$|\Sigma_s(\xi)| = \frac{|M(\xi)|}{|M_{11}(\xi)|}=v^{q(q-1)/2}(u-v)^{q-1}(u+(q-1)v-qu^2). \qquad (6)$$

Simple algebra shows tht $|\Sigma_s(\xi)|$ is maximized at

$$u^*=\frac{(2q^2+q+5)(q-1)\sqrt{4q^2+4q+9}}{4(q^2+q+2)} \qquad (7)$$

and $$v^*=\frac{(2q^2-q+3)u^*-(q+1)}{2q^2-2} \qquad (8)$$

For $i=1, 2, \cdots, q$, let E_i be the subset of E consisting of those$\binom{q}{i}\cdot 2^i$ elements with $q-i$ components of x being equal to zeros. The following theorem characterizes those sets of the form $\cup_{i=1}^3 E_{r_i}$, which can support a symmetric approximate D_s-optimal design.

Theorem 1(**Lim & Studden(1988)**) *The set* $\cup_{i=1}^3 E_{r_i}$, *supports a symmetric approximate D_s-optimal design if and only if*

$$0\leqslant r_1\leqslant(q-1)\cdot\frac{u^*-v^*}{1-u^*}\leq r_2\leq q-1,\ r_3=q. \qquad (9)$$

The weights for a symmetric approximate D_s-optimal design with $r_1=0$ and $r_2=q-1$ are listed in Table 1 for $2\leq q\leq 5$. For more details, refer to Lim & Studden(1988).

Table 1. Weights for a symmetric approximate D_s-optimal design on E

		D_s-optimal design
q=2	$\xi^*(E_2)$	.472
	$\xi^*(E_1)$	.352
	$\xi^*(E_0)$	.176
q=3	$\xi^*(E_3)$	.417
	$\xi^*(E_2)$	.475
	$\xi^*(E_0)$	.108
q=4	$\xi^*(E_4)$	.366
	$\xi^*(E_3)$	.562
	$\xi^*(E_0)$	.072
q=5	$\xi^*(E_5)$	.324
	$\xi^*(E_4)$	.625
	$\xi^*(E_0)$	.051

3. Exact D_s-efficient Designs

When the design is implementable, i.e. the weight of each design point is proportional to 1/N, we call such a design an exact design. An exact design ξ_N is called second order symmetric if any moments upto quartic involving odd powers are zeros, for example, $E^{\xi N} x_1^3 x_2$, $E^{\xi N} x_1 x_2$, $E^{\xi N} x_1^2 x_2$, etc. We will construct efficient symmetric exact designs based on approximate D_s-optimal design and Pesotchinsky's minimal second order symmertic sets for the practical purpose.

The value of $|\Sigma_s(\xi)|$ gives an indication of the information per point for a design w.r.t. D_s-optimality criterion, so designs with different total numbers of design points can be compared. The designs are compared by calculating D_s-efficiencies defined by

$$D_s(\xi)=\left[\frac{|\Sigma_s(\xi)|}{|\Sigma_s(\xi_s^*)|}\right]^{q(q+1)/2} \tag{10}$$

Composite designs (Box & Wilson(1951)) are often used for estimating quadratic response surfaces. They are difficult to beat in practice. Pesotchinsky(1975) considered designs whose supports were subsets of the supports for D-optimal designs and obtained DP, designs with support on the minimal second-order symmetric sets and on the center point, which has better D-efficiencies than best composite designs. Here we take the similar approach to Pesotchinsky (1975). But we allow to replicate observations on some of the minimal second-order symmetric sets to get better D_s-efficiencies.

Define $n(E_i)$ by the number of design points assigned on E_i. When $2\leq q\leq 3$, *minimal second order symmetric sets are* E_q and E_{q-1}, themselves. By fixing the number of replications on E_q and E_{q-1}, and then, varying the number of trials at the center point, the best symmetric exact designs take single replication at all the points on E_q & E_{q-1}, i.e.,

when $q=2$; $n(E_2)=4$, $n(E_1)=4$, $n(E_0)=1$
when $q=3$; $n(E_3)=8$, $n(E_2)=12$, $n(E_0)=2$.

When $q=4$, weights for a symmetric approximate D_s-optimal design are $\xi^*_s(E_4)=.366$ and $\xi^*_s(E_3)=.562$ from Table 1. From Pesotchinsky(1975), minimal second order symmertic sets are as follows :

on E_4 : 8 points with the defining relation $x_1x_2x_3=1$
on E_3 : $x_4=0$; 2×4 points with $x_1x_2x_3=-1$
all 8 points for $x_1=0$, $x_2=0$, $x_3=0$.

By adding all sixteen design points in E_4, the relative weight of E_4 to E_3 increases to 24/32, which is close to the optimal relative weight .366/.562. By allocating $n(E_4)=24$, $n(E_3)=32$ and then, varying the number of trials at the center point, the best D_s-efficiency is attained at $n(E_0)=4$.

When $q=5$, weights for a symmetric approximate D_s-optimal designs are $\xi^*_s(E_5)=.324$ and $\xi^*_s(E_4)=.625$ from Table 1. From Pesotchinsky(1975), minimal second order symmetric sets are as follows :

on E_5 : **8 points with** $x_1x_2x_4=x_2x_3x_5=x_1x_3x_4x_5=1$

on E_4 : $x_1=0$; 8points with $x_2x_4x_5=1$
$x_2=0$; 8points with $x_1x_3x_4x_5=-1$
$x_3=0$; 8points with $x_2x_4x_5=-1$
$x_4=0$; 8points with $x_2x_3x_5=-1$
$x_5=0$; 8points with $x_1x_2x_4=-1$.

By adding sixteen design points with the defining relation $x_1x_2x_4x_5=1$ on E_5, the relative weight of E_5 to E_4 increases to 24/40, which is close to the optimal relative weight .324/.625. By allocating $n(E_5)=24$, $n(E_4)=40$ and then, varying the number of trials at the center point, the best D_s-efficiency is attained at $n(E_0)=3$.

Table 2. Design Comparison

No. of Factors	Designs	No. of Trials	$\lvert \Sigma_s(\xi) \rvert$	D_s-eff.	D-eff.
q=1	Best Composite	10	.233e-1	.987	.974
q=3	Lim DL	22	.129e-2	.994	.987
	Best Composite	14	.382e-3	.882	.976
q=4	Lim DL	60	.504e-4	.999	.993
	Pesotchinsky DP	42	.371e-4	.970	.967
	Best Composite	24	.760e-5	.828	.936
q=5	Lim DL	67	.153e-5	.999	.996
	Pesotchinsky DP	50	.121e-5	.984	.978
	Best Composite	42	.537e-7	.813	.899

The design efficiencies are listed in Table 2. When $q=2$, the design is the best composite design. The best composite designs are included for the comparison purpose.

4. Concluding Remarks

Composite designs are often used in practice for estimating quadratic response surfaces. The main advantage over other type of symmertic designs is that they need fewer design points. The best composite designs for $q \geq 3$ do not have design points at the center, i.e., adding a center point to a composite design decreases the information per experimental point. But the center point is quite important in the sense that it is usually expected to be near the best operating condition. Moreover D_s-efficiencies of best composite designs seem to be poor. Thus we suggest to use exact D_s-efficient symmetric designs if we can afford to take enough number of design points. They seem to have reasonably good D-efficiency as well as a few replications at the center point.

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