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EFFICIENT D_s-OPTIMAL DESIGNS FOR MULTIVARIATE POLYNOMIAL REGRESSION ON THE q-CUBE[1]

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Polynomial regression in q variables of degree n on the q-cube is considered. Approximate D-optimal and approximate D_s-optimal designs for estimating higher degree terms are investigated. Numerical results are given for $n = 2$ with arbitrary q and for $n = 3, 4, 5$ and $q = 2, 3$. Exact solutions are given within the class of product designs together with some efficiency calculations.

1. Introduction. Consider the polynomial regression model in q variables of degree n on the q-cube. Thus it is assumed that for each $x = (x_1, \dots, x_q)$ in the q-cube,

$$\mathscr{X} = \{x: |x_i| \le 1, i = 1, \dots, q\}, \tag{1.1}$$

a random variable $Y(x)$ with mean $\sum_{i=1}^{K} \theta_i f_i(x) = f(x)'\theta$ and variance σ^2 independent of x can be observed. Here the regression functions $f_i(x)$ are known functions of the form $\prod_{j=1}^{q} x_j^{m_j}$, where m_j are nonnegative integers with sum less than or equal to n. It is well known [e.g., Scheffé (1958)] that the number of such functions is $\binom{n+q}{q}$.

A design ξ is a probability measure on $\mathscr{X}$. The information matrix is given by

$$M(\xi) = \int f(x) f(x)' \xi(dx). \tag{1.2}$$

If the design is implementable and N uncorrelated observations are taken, then the covariance matrix of the least squares estimates $\hat{\theta}$ of θ is given by

$$\operatorname{Var}(\hat{\theta}) = \frac{\sigma^2}{N} M^{-1}(\xi). \tag{1.3}$$

Much of the Kiefer type optimal design theory is concerned in minimizing some functional of $M^{-1}(\xi)$ over ξ.

The basic criterion of design optimality we shall use here is that of D-optimality (or D_s-optimality) developed largely by Kiefer (1959, 1961a, b) and Kiefer and Wolfowitz (1959, 1960). The D-optimality criterion is known by the celebrated Kiefer–Wolfowitz theorem to be equivalent to the G-optimality criterion. So the design ξ^* is D-optimal iff the variance function $d(x, \xi^*) \le K$ for all $x \in \mathscr{X}$, where $d(x, \xi^*) = f(x)' M^{-1}(\xi^*) f(x)$.

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In the case where interest is in only s of the K parameters in θ, it is customary to decompose f into $f' = (f_1', f_2')$ where f_2 corresponds to the s parameters of interest. Similarly the information matrix is decomposed into

$$M = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}.$$

The covariance matrix of the s parameters is proportional to the inverse of

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

[Here we must interpret M_{11}^{-1} as a generalized inverse if rank $(M_{11}) < K - s$.] Corresponding to the D_s-optimality criterion, we have the following theorem [Kiefer (1961a), Karlin and Studden (1966b) and Atwood (1969)].

THEOREM 1.1. *If $M(\xi^*)$ is nonsingular, then the following assertions,*

(i) *the design ξ^* maximizes $|\Sigma_s(\xi)|$,*
(ii) *the design ξ^* minimizes $\max_x d_s(x, \xi)$ where $d_s(x, \xi) = d(x, \xi) - f_1(x)'M_{11}^{-1}(\xi)f_1(x)$ and*
(iii) $\max_x d_s(x, \xi^*) = s$,

are equivalent.

To find the maximum of $|\Sigma_s(\xi)|$, we use the result that

$$|\Sigma_s(\xi)| = \frac{|M(\xi)|}{|M_{11}(\xi)|}. \tag{1.4}$$

The model under consideration is invariant or symmetric with respect to the group consisting of permutations and sign changes of the coordinates. The invariance theorem [Kiefer (1959, 1961b) and Giovagnoli, Pukelsheim and Wynn (1987)] which concludes that there exists a symmetric D- and D_s-optimal design is a very important tool for obtaining D- and D_s-optimal designs either theoretically or numerically. All of the designs we consider will be symmetric with respect to the preceding group.

An outline of this paper is as follows. In Section 2 we discuss the case $n = 2$. Kiefer (1961a), Kono (1962) and Farrell, Kiefer and Walbran (1967) give a complete description of a symmetric D-optimal design. We give a similar analysis for estimating only the quadratic terms and simplify the corresponding geometrical considerations. In Section 3 we give some numerical results for $q = 2, 3$ and $n = 3, 4, 5$. These results support the general idea that the D- and D_s-optimal design are "close to" product designs. Thus for the cubic regression in one dimension we use four support points in our design while for $q = 2$, the D-optimal design is on a nearly rectangular grid of 16 points. This motivated the use of product designs in Section 5. Through the use of certain canonical moments we are able to describe more or less explicitly the D- and D_s-optimal product design. These turn out to be fairly efficient. Section 4 has some preliminary discussion and lemmas regarding the canonical moments.

2. Quadratic D_s-optimal design. Kiefer (1961a), Kono (1962) and Farrell, Kiefer and Walbran (1967) give a rather complete description of the D-optimal design when $n = 2$ and q is arbitrary. Further considerations of a similar nature are included in Lim, Studden and Wynn (1988) where an example involving a factorial model of type $3^q 2^r$ is analyzed. Here we describe the details for estimating all of the quadratic terms. The analysis used here originates with Kiefer (1961a). Our analysis of the resulting geometrical considerations is somewhat simpler.

The regression vector is $f'(x) = (f_1'(x), f_2'(x))$, where $f_1'(x) = (1, x_1, \dots, x_q)$ and $f_2'(x) = (x_1^2, \dots, x_q^2, x_1x_2, \dots, x_{q-1}x_q)$. The vector $f_2(x)$ contains all the quadratic terms.

By the invariance theorem, there exist D- and D_s-optimal designs which are symmetric with respect to permutations and sign changes of x_i's, $i = 1, \dots, q$. Both $d(x, \xi)$ and $d_s(x, \xi)$ are quartic functions when considered as functions of each variable separately. Moreover they are symmetric with positive coefficient for x_i^4, so that their maximum can occur only at $x_i = \pm 1$ or 0. Thus the symmetric optimal design must be supported on E, where $E = \{x\colon |x_i| = 0 \text{ or } 1\}$.

For symmetric designs supported on E, we let

$$u = \int x_1^2 \xi(dx) = \int x_1^4 \xi(dx) \quad \text{and} \quad v = \int x_1^2 x_2^2 \xi(ds). \tag{2.1}$$

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

$$|\Sigma_s(\xi)| = \frac{|M(\xi)|}{|M_{11}(\xi)|} = v^{q(q-1)/2}(u - v)^{q-1}(u + (q-1)v - qu^2). \tag{2.2}$$

Some algebra shows that $|\Sigma_s(\xi)|$ is maximized at

$$u^* = \frac{(2q^2 + q + 5) + (q-1)\sqrt{4q^2 + 4q + 9}}{4(q^2 + q + 2)} \tag{2.3}$$

and

$$v^* = \frac{(2q^2 - q + 3)u^* - (q+1)}{2q^2 - 2}. \tag{2.4}$$

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

THEOREM 2.1. *The set $\bigcup_{i=1}^3 E_{r_i}$ supports a quadratic D_s-optimal design for quadratic regression on the q-cube if and only if*

$$0 \le r_1 \le (q-1)\frac{u^* - v^*}{1 - u^*} \le r_2 \le q - 1, \qquad r_3 = q. \tag{2.5}$$

PROOF. For ξ supported on E the space of possible (u, v) is the convex hull of $\{(i/q, i(i-1)/(q(q-1))),\ i = 1, \dots, q\}$ since $u = \sum_{i=0}^{q}(i/q)\xi(E_i)$ and $v = \sum_{i=0}^{q} i(i-1)/(q(q-1))\xi(E_i)$. It is not clear at this point that u^* and v^* in (2.3) and (2.4) are of this form.

Let $z_1 = i/q$ and $z_2 = i(i-1)/(q(q-1))$. Then

$$z_2 = \frac{q}{q-1} z_1^2 - \frac{1}{q-1} z_1. \tag{2.6}$$

Consider z_1 as a random variable on $[0, 1]$ and let c_1 and c_2 be the "first" and "second" moments of z_1. The set of all possible values or moment

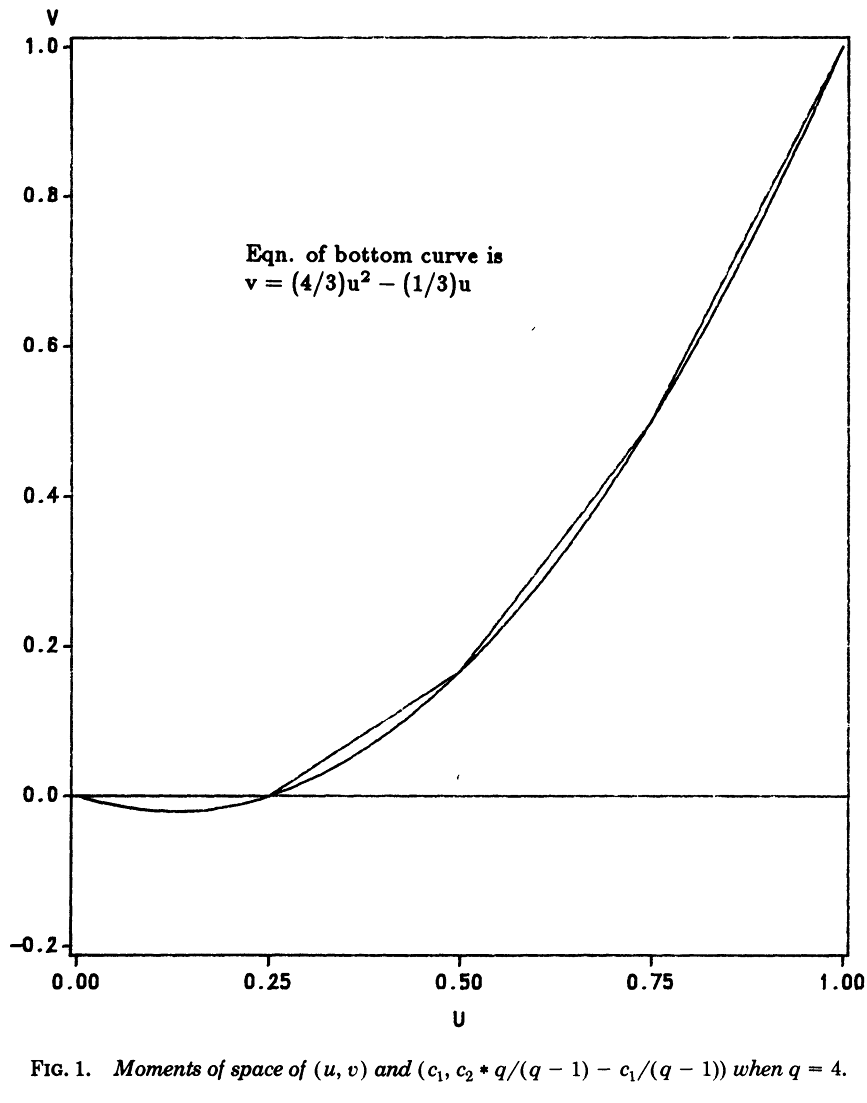

FIG. 1. *Moments of space of* (u, v) *and* $(c_1, c_2 * q/(q-1) - c_1/(q-1))$ *when* $q = 4$.

space of $(c_1, q/(q-1)c_2 - 1/(q-1)c_1)$ is the convex hull of (z_1, z_2) where $z_2 = q/(q-1)z_1^2 - 1/(q-1)z_1$. Note that $z_2 = 1$ for $z_1 = 1$ and $z_2 = 0$ for $z_1 = 0$ or $1/q$. The possible values for (u, v) are a subset of these corresponding to z_1 having mass only on $z_1 = i/q$, $i = 0, 1, \ldots, q$. Figure 1 provides a sketch of both sets when $q = 4$.

Since $u^* > (q-1)/q$, we have to choose r_3 to be q which corresponds to $(1,1)$ in the moment space. Let L be the line which passes through $(1,1)$ and (u^*, v^*) and u_0 be the abscissa of the intersection point of L and the lower boundary of the moment space $(c_1, q/(q-1)c_2 - 1/(q-1)c_1)$. Then

$$\frac{r_1}{q} \le u_0 \le \frac{r_2}{q} \tag{2.7}$$

iff (u^*, v^*) is in the convex hull of $\{(r_1/q, r_1(r_1-1)/(q(q-1))), (r_2/q, r_2(r_2-1)/(q(q-1))), (1,1)\}$. Thus there exists a symmetric D_s-optimal design on $E_{r_1} \cup E_{r_2} \cup E_q$. It can be easily checked that

$$u_0 = \frac{q-1}{q}\,\frac{u^* - v^*}{1 - u^*}. \tag{2.8}$$

By substitution of (2.8) into (2.7), we get

$$0 \le r_1 \le (q-1)\frac{u^* - v^*}{1 - u^*} \le r_2, \qquad r_3 \equiv q.$$

Substitute (2.3) and (2.4) into $(u^* - v^*)/(1 - u^*)$ and use $\sqrt{4q^2 + 4q + q} < 2q + 1 + 4/(2q+1)$. Then it follows that

$$\frac{u^* - v^*}{1 - u^*} < 1.$$

Thus $r_2 \le q - 1$, which assures the existence of a symmetric D_s-optimal design on $E_0 \cup E_{q-1} \cup E_q$. □

TABLE 1
Weights for a symmetric D- and D_s-optimal design on E with a minimal support for quadratic polynomial regression on the q-cube

		D-Optimal Design	**D_s-Optimal Design**
$q = 2$	$\xi^*(E_2)$	0.583	0.472
	$\xi^*(E_1)$	0.321	0.352
	$\xi^*(E_0)$	0.096	0.176
$q = 3$	$\xi^*(E_3)$	0.510	0.417
	$\xi^*(E_2)$	0.424	0.475
	$\xi^*(E_0)$	0.066	0.108
$q = 4$	$\xi^*(E_4)$	0.451	0.366
	$\xi^*(E_3)$	0.502	0.562
	$\xi^*(E_0)$	0.047	0.072
$q = 5$	$\xi^*(E_5)$	0.402	0.324
	$\xi^*(E_4)$	0.562	0.625
	$\xi^*(E_0)$	0.036	0.051

The weights for a symmetric D_s-optimal design with $r_1 = 0$ and $r_2 = q - 1$ are listed in Table 1 for $2 \le q \le 6$. These would be beneficial if fewer points in the design are desired. For comparison purposes, included are the weights for a symmetric D-optimal design from Kono (1962) and Kiefer (1961a). For estimating all of the quadratic terms only, more weight is on the center and E_{q-1} and less weight on the corners of the q cube.

3. Numerical D_s-optimal designs. In this section we consider some numerical results for $q = 2, 3$ and $n = 3, 4, 5$. For convenience we shall call ξ^* a numerical D_s-optimal design if $\sup_x d_s(x, \xi^*)$ is found to be less than or equal to s to five significant digits. The five digits is somewhat arbitrary. The results were obtained on a CDC 6500 using single precision.

For $q = 2$ and $n = 3$, Farrell, Kiefer and Walbran (1967) considered a symmetric design ξ which puts mass $w_1/4$ at $(\pm 1, \pm 1)$, $w_2/8$ at $(\pm 1, \pm a)$ and $(\pm a, \pm 1)$ and the remaining $(1 - w_1 - w_2)/4$ at $(\pm b, \pm b)$ and showed numerically that $|M(\xi)|$ was maximized at

$$a = 0.3588, \qquad b = 0.4800, \qquad w_1 = 0.3677 \quad \text{and} \quad w_2 = 0.4610.$$

For this design ξ^*, they also computed $\sup_x d(x, \xi^*)$ numerically and found $\sup_x d(x, \xi^*)$ to be less than or equal to 10 to five decimal places.

We have done a similar analysis for the fourth and fifth degree regression on the 2-cube. Resulting numerical symmetric D-optimal designs are listed in Table 2. We include the cubic case for completeness and comparison with Table 3. In Table 2 a typical point is indicated. The full design is obtained by taking permutations and sign changes of typical points. The divisors in the weight column are the number of symmetric points.

TABLE 2
Numerical symmetric D-optimal designs on the 2-cube

	Design Point	Weight
$n = 3$	(1, 1)	0.3677/4
	(1, 0.3588)	0.4610/8
	(0.4800, 0.4800)	0.1713/4
$n = 4$	(1, 1)	0.2473/4
	(1, 5811)	0.3508/8
	(1, 0)	0.1582/4
	(0.6442, 0.6442)	0.1203/4
	(0.6854, 0)	0.0722/4
	(0, 0)	0.0512/1
$n = 5$	(1, 1)	0.1785/4
	(1, 0.7039)	0.2590/8
	(1, 0.2549)	0.2453/8
	(0.7574, 0.7574)	0.0939/4
	(0.3208, 0.3208)	0.1079/4
	(0.7446, 0.1963)	0.1154/8

TABLE 3
Numerical symmetric D_s-optimal designs for the highest order coefficients on the 2-cube

	Design Point	Weight
$n = 3$	(1, 1)	0.2606/4
	(1, 0.3680)	0.4665/8
	(0.5207, 0.5207)	0.2729/4
$n = 4$	(1, 1)	0.1596/4
	(1, 6170)	0.3382/8
	(1, 0)	0.1516/4
	(0.6876, 0.6876)	0.1814/4
	(0.7453, 0)	0.0891/4
	(0, 0)	0.0801/1
$n = 5$	(1, 1)	0.1089/4
	(1, 7336)	0.2263/8
	(1, 0.2775)	0.2265/8
	(0.7951, 0.7951)	0.1406/4
	(0.3393, 0.3393)	0.1521/4
	(0.7829, 0.1922)	0.1456/8

In each case we considered a perturbed symmetric product design. For example, with $q = 2$ and $n = 4$ we use a design with a set of typical points $\{(1, 1), (1, a), (1, 0), (b, b), (c, 0), (0, 0)\}$. For $n = 5$, we use $\{(1, 1), (1, a), (1, b), (c, c), (d, d), (e, f)\}$. In each case the symmetry allows us to block the information matrix according to the parity of the power of each component. For $q = 2$, we divide f into 4 groups while we get 8 groups for $q = 3$. For $q = 2$ and $n = 4$,

$$f'_{(1)} = (1, x_1^2, x_2^2, x_1^2x_2^2, x_1^4, x_2^4),$$

$$f'_{(2)} = (x_1, x_1x_2^2, x_1^3),$$

$$f'_{(3)} = (x_2, x_2x_1^2, x_2^3)$$

and

$$f'_{(4)} = (x_1x_2, x_1x_2^3, x_1^3x_2).$$

The determinant in each case was maximized on the CDC 6500 by using the Newton–Raphson algorithm as a function of the eight or ten parameters involved which gave the design ξ^* in Table 2. $\sup_x d(x, \xi^*)$ was computed numerically and found to be less than or equal to 15 or 21 to five decimal places. As n increases, numerical problems increase dramatically. For $n = 5$, an initial starting design was even hard to obtain. For this a program ACED [Algorithms for the Construction of Experimental Designs, see Welch (1985), page 146] was used to distribute 30 observations on a grid of 1681 candidate points on $[-1, 1] \times [-1, 1]$. For $n = 6$, the ACED seemed to give an excellent starting design. However, due to ill conditioning of high-degree polynomial models, our optimization algorithm failed to produce an optimal design.

TABLE 4
Numerical symmetric D-optimal design for $n = 3$ and $q = 3$

Design Point	Weight
(1, 1, 1)	0.3142/8
(1, 1, 0.2970)	0.3942/24
(1, 0.4215, 0.4215)	0.2649/24
(0.5012, 0.5012, 0.5012)	0.0267/8

TABLE 5
Numerical symmetric D-optimal design for the two highest order coefficients for $n = 3$ and $q = 2$

Design Point	Weight
(1, 1)	0.3241/4
(1, 0.3360)	0.4490/8
(0.4579, 0.4579)	0.2269/4

Similarly, we get numerical D_s-optimal designs for the highest order terms for $n = 3, 4, 5$ and $q = 2$ and those are listed in Table 3. Comparing Table 3 with Table 2, we note that the design points inside the 2-cube move toward the 4 corner points and the weights shift toward the inside design points.

Two further cases were considered. The D-optimal design for $n = 3$ and $q = 3$ and the D_s-optimal design for the two highest order coefficients for $n = 3$ and $q = 2$ are given in Tables 4 and 5.

We remark that a symmetric numerical D-optimal design ξ^* for $q = 2$ and $n = 3$ is unique. As in Farrell, Kiefer and Walbran (1967), this can be shown by checking that $\{x\colon d(x, \xi^*) - 10 = 0\}$ is exactly the support of ξ^* and a 27×16 matrix $\|\phi_i(\mathbf{x}_j)\|$, where $\phi_i(x)$ is of the form $\prod_{j=1}^{q} x_j^{m_j}$ with $1 \le \sum_{j=1}^{q} m_j \le 6$, $m_j \ge 0$ and $\mathbf{x}_j \in$ support ξ^*, has full column rank. But for $n = 4$ and 5, the D-optimal design may not be unique since the matrix $\|\phi_i(\mathbf{x}_j)\|$ does not have full column rank.

4. Canonical moments. In this section we describe some results concerning canonical moments used in the next section.

For any arbitrary measure ξ on $[-1, 1]$, let $c_k = \int_{-1}^{1} x^k \, d\xi(x)$. For a given finite set of moments $c_0, \dots, c_{i-1}$, let c_i^+ denote the maximum of the ith moment $\int_{-1}^{1} x^i \, d\xi(x)$ over the set of all measures ξ having the given set of moments $c_0, \dots, c_{i-1}$. Similarly, let c_i^- denote the corresponding minimum. The canonical moments are defined by

$$p_i = \frac{c_i - c_i^-}{c_i^+ - c_i^-}, \qquad i = 1, 2, \dots . \tag{4.1}$$

The canonical moments p_i range freely over $[0,1]$ and permit easy maximization of $|M(\xi)|$ when $q = 1$. The remainder of the problem is converting the optimum p_i to the support points and the weights in the corresponding design. Most of the proofs of the following lemmas are in either Studden (1982a, b) or Lau (1983).

LEMMA 4.1. *The design ξ is symmetric iff $p_{2i+1} = \frac{1}{2}$ for all i.*

Let $p_0 = 0$ and define $q_i = 1 - p_i$, $i \geq 0$. Also define

$$\zeta_i = q_{i-1}p_i, \qquad i = 1, 2, \ldots. \tag{4.2}$$

Let a sequence of polynomials $W_l(x)$, $l \geq 0$, be defined by taking them orthogonal to $d\xi$. Then the recursive relation for the orthogonal polynomials $W_l(x)$ with leading coefficient 1 is given in Lemma 4.2.

LEMMA 4.2. *Let $W_0(x) = 1$ and $W_1(x) = x$. Then the orthogonal polynomials $W_l(x)$ for $l \geq 2$ satisfy the recursive relations*

$$W_l(x) = (x + 1 - 2\zeta_{2l-2} - 2\zeta_{2l-1})W_{l-1}(x) - 4\zeta_{2l-3}\zeta_{2l-2}W_{l-2}(x). \tag{4.3}$$

Lemma 4.3 expresses the L_2 norm of an orthogonal polynomial $W_l(x)$ in terms of the canonical moments.

LEMMA 4.3. *For $l \geq 1$,*

$$\int_{-1}^{1} W_l^2(x)\,dx = 2^{2l}\zeta_1\zeta_2 \cdots \zeta_{2l-1}\zeta_{2l}. \tag{4.4}$$

Using Lemma 4.3, it can be easily shown that

$$|M(\xi)| = \prod_{l=0}^{n} \int_{-1}^{1} W_l^2(x)\,d\xi(x) = 2^{n(n+1)} \prod_{l=1}^{n} (\zeta_{2l-1}\zeta_{2l})^{n-l+1} \tag{4.5}$$

for $q = 1$.

There is a considerable amount of literature concerning the relationship between the sequence of canonical moments $\{p_i\}$ and the corresponding design ξ. [See Studden (1982a, b) and Lau (1983).] We state here only those results that are pertinent to some of the D_s-optimal product design problems. Lemma 4.4 follows from similar arguments to Lemma 2.3 in Studden (1982a).

LEMMA 4.4. (a) *The design corresponding to $(\frac{1}{2}, p_2, \frac{1}{2}, 1)$ concentrates mass $\alpha, 1 - 2\alpha, \alpha$ on the points $-1, 0, 1$, respectively, where $\alpha = p_2/2$.*

(b) *The design corresponding to $(\frac{1}{2}, p_2, \frac{1}{2}, p_4, \frac{1}{2}, 1)$ concentrates mass α, $\frac{1}{2} - \alpha, \frac{1}{2} - \alpha, \alpha$ on the points $-1, \sqrt{t}, \sqrt{t}, 1$, respectively, where $\alpha = p_2p_4/(2(q_2 + p_2p_4))$, $t = p_2q_4$.*

(c) *The design corresponding to $(\frac{1}{2}, p_2, \frac{1}{2}, p_4, \frac{1}{2}, 1)$ concentrates mass α_1, α_2, $1 - 2\alpha_1 - 2\alpha_2, \alpha_2, \alpha_1$ on the points $-1, \sqrt{t}, 0, \sqrt{t}, 1$, respectively, where $\alpha_1 = p_2p_4p_6/(2(1 - t))$, $\alpha_2 = p_2q_2q_4/(2t(1 - t))$, $t = p_2q_4 + p_4q_6$.*

5. D_s-optimal product designs. Let

$$\Xi_1 = \{\xi_1 \times \xi_2 \times \cdots \times \xi_q: \xi_i \text{ is a design on } [-1,1]\}.$$

Consider an arbitrary design $\eta = \xi_1 \times \cdots \times \xi_q$ in Ξ_1. For each $j = 1, \dots, q$, let $W_{i(j)}(x)$ be the orthogonal polynomial of degree i with the leading coefficient 1 with respect to ξ_j. Define

$$N_{l,m} = \binom{l+m}{m}. \tag{5.1}$$

Also denote $M_n(\eta)$ by the information matrix of a design η for the nth degree polynomial regression model on the q-cube.

LEMMA 5.1.

$$|M_n(\eta)| = 2^{K_{n,q}} \prod_{j=1}^{q} \prod_{i=1}^{n} \left[\int_{-1}^{1} W_{i(j)}^2(x)\, d\xi_j(x) \right]^{N_{q-1,n-i}}, \tag{5.2}$$

where $K_{n,q} = 2q\sum_{i=1}^{n} iN_{q-1,n-i}$.

PROOF. Recall that $f(x)$ is the vector of $N_{n,q}$ monomials $x_1^{l_1} \cdots x_q^{l_q}$, $\sum_{j=1}^{q} l_j \le n$. Let $g(x)$ be the vector of length $N_{n,q}$ monomials $W_{l_1(1)}(x_1) \cdots W_{l_q(q)}(x_q)$, $\sum_{j=1}^{q} l_j \le n$. Then it can be easily checked that there exists an $N_{q,n} \times N_{q,n}$ lower triangular matrix A with $|A| = 1$ such that $g(x) = Af(x)$. So

$$|M_n(\eta)| = \left| \int f(x) f(x)'\, d\eta(x) \right| = \left| \int g(x) g(x)'\, d\eta(x) \right|. \tag{5.3}$$

Note that $\int g(x)g(x)'\, d\eta(x)$ is a diagonal matrix since

$$\int_{-1}^{1} W_{i(j)}(x_j) W_{l(j)}(x_j) \xi_j(dx_j) = 0$$

for any j and $l \ne i$. Also there exist $N_{q-1,n-i}$ components of $g(x)$ like $W_{i(j_0)}(x_{j_0}) \prod_{j \ne j_0} W_{l_j(j)}(x_j)$ since $\prod_{j \ne j_0} W_{l_j(j)}(x_j)$ is a monomial of degree less than or equal to $n - i$ with $q - 1$ variables. Thus

$$\begin{aligned} |M_n(\eta)| &= \prod_{\sum_{i=1}^{q} l_i \le n} \prod_{j=1}^{q} 2^{2l_j} \int_{-1}^{1} W_{l_j(j)}^2(x_j)\, d\xi_j(x_j) \\ &= \prod_{j=1}^{q} \prod_{i=1}^{n} \left[2^{2i} \int_{-1}^{1} W_{i(j)}^2(x_j)\, d\xi_j(x_j) \right]^{N_{q-1,n-i}} \\ &= 2^{2q\sum_1^q iN_{q-1,n-i}} \prod_{j=1}^{q} \prod_{i=1}^{n} \left[\int_{-1}^{1} W_{i(j)}^2(x)\, d\xi_j(x) \right]^{N_{q-1,n-i}}. \qquad \square \end{aligned}$$

THEOREM 5.1. *The D-optimal product design over the class of product designs* Ξ_1 *is*

$$\eta_{n,q}^* = \xi_{n,q}^* \times \cdots \times \xi_{n,q}^*, \tag{5.4}$$

in which the canonical moments of $\xi^*_{n,q}$ *are given by*

$$(5.5)\qquad \begin{aligned} p_{2i-1} &= \frac{1}{2}, \qquad i = 1,\dots,n,\\ p_{2i} &= \frac{q+n-i}{q+2(n-i)}, \qquad i = 1,\dots,n-1,\\ p_{2n} &= 1. \end{aligned}$$

PROOF. By Lemma 5.1,

$$|M_n(\eta)| = 2^{K_{nq}} \prod_{j=1}^{q} \prod_{i=1}^{n} \left[\int_{-1}^{1} W^2_{i(j)}(x)\, d\xi_j(x)\right]^{N_{q-1,n-i}}.$$

Note that

$$\max_{\xi_1,\dots,\xi_q} \prod_{j=1}^{q} \prod_{i=1}^{n} \left[\int_{-1}^{1} W^2_{i(j)}(x)\, d\xi_j(x)\right]^{N_{q-1,n-i}}$$
$$= \left[\max_{\xi} \prod_{i=1}^{n} \left[\int_{-1}^{1} W_i^2(x)\, d\xi(x)\right]^{N_{q-1,n-1}}\right]^q.$$

So it suffices to find a design $\xi^*_{n,q}$ which maximizes $\Pi_1^n[\int W_i^2(x)\, d\xi(x)]^{N_{q-1,n-i}}$ and then the D-optimal product design is

$$\eta^*_{n,q} = \xi^*_{n,q} \times \cdots \times \xi^*_{n,q}.$$

It can be easily checked that $N_{q,i} = \Sigma_{j=0}^{i} N_{q-1,j}$ [Scheffé (1958)]. Using this and (4.4), we get

$$(5.6)\qquad \begin{aligned} &\prod_{i=1}^{n} \left[\int_{-1}^{1} W_i^2(x)\, d\xi(x)\right]^{N_{q-1,n-i}}\\ &= (\zeta_1\zeta_2)^{N_{q-1,n-1}} (\zeta_1\zeta_2\zeta_3\zeta_4)^{N_{q-1,n-2}} \cdots (\zeta_1\zeta_2 \cdots \zeta_{2n-1}\zeta_{2n})^{N_{q-1,0}}\\ &= (\zeta_1\zeta_2)^{N_{q,n-1}} (\zeta_3\zeta_4)^{N_{q,n-2}} \cdots (\zeta_{2n-1}\zeta_{2n})^{N_{q,0}}\\ &= (p_1 q_1 p_2)^{N_{q,n-1}} (q_2 p_3 q_3 p_4)^{N_{q,n-2}} \cdots (q_{2n-2} p_{2n-1} q_{2n-1} p_{2n})^{N_{q,0}}. \end{aligned}$$

Simple algebra shows that (5.6) is maximized at

$$\begin{aligned} p_{2i-1} &= \frac{1}{2}, \qquad i = 1,\dots,n,\\ p_{2i} &= \frac{N_{q,n-i}}{N_{q,n-i} + N_{q,n-(i+1)}} = \frac{q+n-i}{q+2(n-i)}, \qquad i = 1,\dots,n-1,\\ p_{2n} &= 1. \end{aligned}$$

The uniqueness of the D-optimal product design comes from $p_{2n} = 1$. □

For the $q = 2$ case, we get $p_{2i} = (n - i + 2)/2(n - i + 1)$, $p_{2i-1} = \frac{1}{2}$ and $p_{2n} = 1$ from Theorem 5.1. In the following examples we illustrate the D-optimal product design for $2 \le n \le 4$ and $q = 2$ by using Lemma 4.4.

EXAMPLE 5.1. Suppose $n = 2$. Then $p_2 = \frac{3}{4}$ and $p_4 = 1$. By Lemma 4.4, the corresponding design is

$$\xi_{2,2}^* = \begin{bmatrix} -1 & 0 & 1 \\ \frac{3}{8} & \frac{1}{4} & \frac{3}{8} \end{bmatrix}$$

and $\eta_{2,2}^* = \xi_{2,2}^* \times \xi_{2,2}^*$ is the D-optimal product design.

EXAMPLE 5.2. Suppose $n = 3$. Then $p_2 = \frac{2}{3}$, $p_4 = \frac{3}{4}$ and $p_6 = 1$. By Lemma 4.4,

$$\xi_{3,2}^* = \begin{bmatrix} -1 & \dfrac{-1}{\sqrt{6}} & \dfrac{1}{\sqrt{6}} & 1 \\ 0.3 & 0.2 & 0.2 & 0.3 \end{bmatrix}$$

and $\eta_{3,2}^* = \xi_{3,2}^*$ is the D-optimal product design.

EXAMPLE 5.3. Suppose $n = 4$. Then $p_2 = \frac{5}{8}$, $p_4 = \frac{2}{3}$, $p_6 = \frac{3}{4}$ and $p_8 = 1$. By Lemma 4.4,

$$\xi_{4,2}^* = \begin{bmatrix} -1 & -\sqrt{\frac{9}{24}} & 0 & \sqrt{\frac{9}{26}} & 1 \\ \frac{1}{4} & \frac{1}{6} & \frac{1}{6} & \frac{1}{6} & \frac{1}{4} \end{bmatrix}$$

and $\eta_{4,2}^* = \xi_{4,2}^* \times \xi_{4,2}^*$ is the D-optimal product design.

We consider the usual D-efficiency defined by

$$D(\xi) = \left[\frac{|M(\xi)|}{|M(\xi^*)|} \right]^{1/K}, \tag{5.7}$$

where ξ^* is a D-optimal design, and the G-efficiency defined by

$$G(\xi) = \frac{K}{\sup_x d(x, \xi)} \tag{5.8}$$

to see how good D-optimal product designs are for $q = 2$.

Let $R_i(x)$ be the orthonormal polynomial of degree i with respect to $\xi_{n,2}^*$. By using (4.3) and (4.4), it can be easily checked that

$$\begin{aligned} R_0(x) &= 1, \\ R_1(x) &= \frac{1}{2\sqrt{\zeta_1\zeta_2}} x, \\ R_l(x) &= x \frac{1}{2} \frac{1}{\sqrt{\zeta_{2l-1}\zeta_{2l}}} R_{l-1}(x) - \sqrt{\frac{\zeta_{2l-3}\zeta_{2l-2}}{\zeta_{2l-1}\zeta_{2l}}} R_{l-2}(x), \qquad l \ge 2. \end{aligned} \tag{5.9}$$

From (4.2) and (5.5), $\zeta_1\zeta_2 = (n+1)/2n$ and $\zeta_{2l-1}\zeta_{2l} = \frac{1}{16}$ for $l \geq 2$. So

$$R_0(x) = 1,$$

$$R_1(x) = \sqrt{\frac{2n}{n+1}}\,x,$$

(5.10)

$$R_2(x) = 2\sqrt{\frac{2n}{n+1}}\,x^2 - 2\sqrt{\frac{n+1}{2n}},$$

$$R_l(x) = 2xR_{l-1}(x) - R_{l-2}(x), \qquad l \geq 3.$$

Since the variance function is invariant under linear nonsingular transformation of $f(x)$, $d(x, \eta^*_{n,2})$ can be written as

$$d(x, \eta^*_{n,2}) = \sum_{\substack{0 \leq i \leq j \leq n \\ i+j \leq n}} R_i^2(x_1)R_j^2(x_2), \tag{5.11}$$

which can be calculated easily by using the recursive relations (5.10). $\sup d(x, \eta^*_{n,2})$ was computed numerically on VAX 11/780. The D-efficiency for $3 \leq n \leq 5$ was based on a numerical D-optimal design which as found in Section 3. As mentioned in Section 3, the optimization algorithm would not produce numerical D-optimal designs for $5 \leq n \leq 12$. Therefore, we could not get values for the D-efficiency in these cases. However, by using the inequality

$$D(\xi) \geq \exp\left\{-\frac{1-G(\xi)}{G(\xi)}\right\} \tag{5.12}$$

in Kiefer (1962b), a lower bound of the D-efficiency for $6 \leq n \leq 12$ is given in Table 6.

In the case where interest is in only the $n-m$ highest order terms, i.e., $(m+1)$th, ..., nth degree terms, we give a similar analysis.

TABLE 6
Efficiency of D-optimal product designs when $q = 2$

Degree n	$(x^0_{1,n}, x^0_{2,n})$[a]	$d(x^0_{1,n}, x^0_{2,n})$	K	G-Efficiency	D-Efficiency
2	(0, 0)	7.000	6	0.8571	0.9952
3	(1, 0.3103)	10.2260	10	0.9779	0.9937
4	(0, 0)	17.2500	15	0.8696	0.9922
5	(1, 0.6989)	22.1270	21	0.9491	0.9928
6	(0, 0)	31.3333	28	0.8936	0.8878[b]
7	(1, 0.8366)	38.0338	36	0.9465	0.9451[b]
8	(0, 0)	49.3750	45	0.9114	0.9074[b]
9	(1, 8980)	58.0581	55	0.9473	0.9458[b]
10	(0, 0)	71.4000	66	0.9244	0.9214[b]
11	(1, 0.9303)	81.2191	78	0.9487	0.9596[b]
12	(0, 0)	97.4167	91	0.9341	0.9319[b]

[a] $d(x^0_{1,n}, x^0_{2,n}) = \sup_{x_1, x_2} d((x_1, x_2), \eta^*_{n,2})$.
[b] A lower bound.

THEOREM 5.2. *The D_s-optimal product design for the $n - m$ highest order terms over the class of product designs Ξ_1 is*

$$\eta_s^* = \xi_s^* \times \cdots \times \xi_s^*,$$

in which the canonical moments of ξ_s^* are

$$(5.13)\quad \begin{aligned} p_{2i-1} &= \frac{1}{2}, \qquad i = 1, \dots, n, \\ p_{2i} &= \frac{N_{q,n-i} - N_{q,m-i}}{N_{q,n-i} - N_{q,m-i} + N_{q,n-i-1} - N_{q,m-i-1}}, \qquad i = 1, \dots, m, \\ p_{2i} &= \frac{q + n - i}{q + 2(n - i)}, \qquad i = m + 1, \dots, n - 1, \\ p_{2n} &= 1. \end{aligned}$$

Here $N_{l,m}$ is given by (5.1).

PROOF. Recall the computation formula for $|\Sigma(\eta)|$ and use (5.2). Then

$$(5.14)\quad \begin{aligned} |\Sigma(\eta)| &= 2^{K_n - K_m} \frac{|M_n(\eta)|}{|M_m(\eta)|} \\ &= 2^{K_n - K_m} \frac{\prod_{j=1}^{q} \prod_{i=1}^{n} \left[\int W_{i(j)}^2(x)\, d\xi_j(x) \right]^{N_{q-1,n-i}}}{\prod_{j=1}^{q} \prod_{i=1}^{m} \left[\int W_{i(j)}^2(x)\, d\xi_j(x) \right]^{N_{q-1,m-i}}} \\ &= 2^{K_n - K_m} \prod_{j=1}^{q} \left[\prod_{i=1}^{m} \left[\int W_{i(j)}^2(x)\, d\xi_j(x) \right]^{N_{q-1,n-i} - N_{q-1,m-i}} \right. \\ &\qquad \left. \times \prod_{i=m+1}^{n} \left[\int W_{i(j)}^2(x) \xi_j(dx) \right]^{N_{q-1,n-i}} \right]. \end{aligned}$$

The rest is analogous to the D-optimal product design case. □

As special cases, first we consider $m = n - 1$, i.e., all the highest order terms. By the substitution of $m = n - 1$ into (5.13) and then, simplification of the resulting expression, we get

$$(5.15)\quad \begin{aligned} p_{2i} &= \frac{q - 1 + n - i}{q - 1 + 2(n - i)}, \qquad 1 \le i \le n - 1, \\ p_{2n} &= 1. \end{aligned}$$

For the $q = 2$ case, interestingly the canonical moments correspond to the D-optimal design for the nth degree polynomial regression on $[-1, 1]$. For

$m = n - 2$, i.e., all the highest and second highest terms, (5.13) is simplified to

$$(5.16)\qquad \begin{aligned} p_{2i} &= \frac{2(n-i)^2 + 3(q-5)(n-i) + (q-1)(q-2)}{4(n-i)^2 + 4(q-2)(n-i) + (q-1)(q-2)}, \quad 1 \le i \le n-2, \\ p_{2(n-1)} &= \frac{q+1}{q+2}, \\ p_{2n} &= 1. \end{aligned}$$

For the $q = 2$ case, (5.16) reduces to $p_{2i} = (2(n-i)+1)/4(n-i), 1 \le i \le n-1$ and $p_{2n} = 1$.

The D_s-efficiency of the product design for $q = 2$, $m = n - 1$, $3 \le n \le 5$ are 0.9727, 0.9569, 0.9605, respectively. Also the D_s-efficiency for $q = 2$, $m = 1$, $n = 3$ is 0.9902. All the D_s-efficiency are based on numerical D_s-optimal designs in Section 3.

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