Minimal Point Second Order Designs

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ABSTRACT. This paper deals with the problem of finding nearly D-optimal designs for multivariate quadratic regression on a cube which take as few observations as possible and still allow estimation of all parameters. It is shown that among the class of all such designs taking as many observations as possible on the corners of the cube there is one which is asymptotically efficient as the dimension of the cube increases. Methods for constructing designs in this class, using balanced arrays, are given. It is shown that the designs so constructed for dimensions ≤ 6 compare well with existing computer generated designs, and in dimensions 5 and 6 are better than those in the literature prior to 1978.

Key Words: Optimum designs, quadratic regression, saturated designs, D-optimality, efficiency, balanced arrays.

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1. INTRODUCTION. Let $I = [-1,+1]$ and let I^k be the k-fold Cartesian product of the closed interval I. Suppose on the basis of n obervations $\underline{x}(m) = (x_1(m),x_2(m),\ldots,x_k(m))' \in I^k$ (primes on vectors and matrices denote transposes), where $m = 1,2,\ldots,n$, we wish to fit by least squares a second order model

$$(1.1) \qquad y(\underline{x}(m)) = b_0 + \sum_{i=1}^{k} b_i x_i(m) + \sum_{1\le i<j\le k} b_{ij}x_i(m)x_j(m)$$

$$+ \sum_{i=1}^{k} b_{ii}x_i^2(m) + e_m \ , \ m = 1,\ldots,n \ .$$

Here the b's are unknown real-valued parameters that we wish to estimate and the $\{e_m\}$ are uncorrelated random variables with mean 0 and finite variance σ^2.

Let $q = {}^{(k+1)(k+2)}/2$. For $\underline{x} \in I^k$ define

$$(1.2) \quad f(\underline{x}) = (1,x_1,\ldots,x_k,x_1x_2,x_1x_3,\ldots,x_{k-1}x_k,x_1^2,\ldots,x_k^2)'$$

and let $\underline{b}$ be the corresponding qx1 column vector so that

$$(1.3) \qquad y(\underline{x}(m)) = \underline{b}'f(\underline{x}(m)) + e_m \quad , \quad m = 1,2,\ldots,n$$

Let X be the qxn matrix whose m-th column is $f(\underline{x}(m))$. Let $\underline{Y}$ be the nx1 column vector whose m-th entry is $y(\underline{x}(m))$. If XX' is non-singular, which implies $n \geq q$, the unique best linear unbiased estimator (B.L.U.E.) $\hat{\underline{b}}$ of $\underline{b}$ is

$$(1.4) \qquad \hat{\underline{b}} = (XX')^{-1}XY$$

which has covariance matrix

$$(1.5) \qquad \mathrm{cov}(\hat{\underline{b}}) = \sigma^2(XX')^{-1} \quad .$$

Let ξ be the probability measure on I^k defined by

(1.6) $\xi(\underline{x})$ = (number of $\underline{x}(m)$ which equal $\underline{x}$)/n .

Then we can write

(1.7) $$XX' = n\int_{I^k} f(\underline{x})f(\underline{x})'d\xi(\underline{x})$$

where the integral is the lebesgue integral with respect to ξ. Define

(1.8) $$M(\xi) = \int_{I^k} f(\underline{x})f(\underline{x})'d\xi(\underline{x}) = XX'/n .$$

Notice $M(\xi)$ is a qxq matrix. ξ is called the design measure or the design and $M(\xi)$ is called the information matrix (per unit variance) of the design ξ. Since the left hand side of (1.8) makes sense for any probability measure ξ on I^k, we take it to be the definition of $M(\xi)$ when ξ is an arbitrary probability measure on I^k.

A design ξ which has the form of equation (1.6) for some integer $n>0$ is called an n-exact design for sample size n. Otherwise ξ is called an approximate design. An n-exact design can actually be implemented in practice by taking $n\xi(\underline{x})$ observations at $\underline{x} \in I^k$. Notice for all but a finite number of $\underline{x}$, $n\xi(\underline{x})$ is 0. An approximate design cannot be implemented in practice, only approximated closely by some n-exact design for large n.

One rationale for choosing a design is to make the covariance matrix of the B.L.U.E.s $\hat{\underline{b}}$ as "small" as possible. Recall

(1.9) $$\text{cov}(\hat{\underline{b}}) = \sigma^2(XX')^{-1} = \sigma^2M^{-1}(\xi_n)/n$$

when we use an n-exact design ξ_n. There are numerous ways of defining a measure of smallness for the matrix $\text{cov}(\hat{\underline{b}})$. The one we shall use is called the D-criterion, namely to examine $\det M^{-1}(\xi_n)$. We seek to minimize $\det M^{-1}(\xi_n)$, or equivalently, maximize $\det M(\xi_n)$. A design which does this is called D-optimum. For a brief discussion of the rationale behind the choice of the D-criterion in the setting of second order regression as examined here, see Box and Draper (1974).

If we restrict ourselves to using only exact designs, finding a D-optimum design may be difficult due to the discrete nature of exact designs. Finding D-optimum designs over the set of both approximate and exact designs is often easier owing to the continuous nature of approximate designs. Techniques such as calculus can then be employed to yield D-optimal approximate designs in many cases. Furthermore a "reasonably" efficient n-exact design can often be obtained from a D-optimum approximate design ψ for large n. For each $\underline{x}$ we approximate $\psi(\underline{x})$ by a rational number $j(\underline{x})/n$, $j(\underline{x})$ an integer between 0 and n, and define $\xi(\underline{x}) = j(\underline{x})/n$. The $j(\underline{x})$ must sum to n for ξ to be a probability measure.

Define

(1.10) $\Xi(k) = \{$all designs ξ on I^k such that $\det M(\xi) \neq 0\}$

(1.11) $\Xi(k,n) = \{\xi \in \Xi(k);\ \xi$ is n exact$\}$

The condition $\det M(\xi) \neq 0$ is equivalent to requiring that $\underline{b}$ be estimable for the design ξ. In general one seeks a D-optimum design over $\Xi(k,n)$ (i.e. a design $\xi_0 \in \Xi(k,n)$ such that

$$\det M(\xi_0) = \sup_{\xi \in \Xi(k,n)} \det M(\xi)$$

or since the calculations are usually intractable, a D-optimum design over $\Xi(k)$. Since I^k is compact, a D-optimum design (not necessarily unique) will exist.

Using this idea, Farrell, Kiefer, and Walbran (1965) have found D-optimal approximate designs over the class $\Xi(k)$ for second order regression as in (1.1). The number of points in the support of their designs is shown to be greater than or equal to $(k+1)(k^3+9k^2-10k+48)/24$ which is on the order of $q^2/6$. These designs give rise to reasonably efficient n-exact designs for $n > q^2/6$, but are hard to implement as n-exact designs for n near q.

In general, exactly what the minimal number of points needed to support a D-optimal design over $\Xi(k)$, is unknown. Pesotchinsky (1975) has studied this problem for small k ($k \leq 7$) and has found approximate designs which are D-optimum over $\Xi(k)$. These do not necessarily give rise to reasonably efficient n-exact designs for n near q, though.

A minimal point design ξ, is one whose support contains the minimal number of points such that $M(\xi)$ is nonsingular ($\det M(\xi) \neq 0$). In our case this number is q. It is easy to show that the D-optimal design over the set of all minimal point designs puts equal mass in each of the q points on its support and hence is q-exact. Such a design is also called a saturated design. It is therefore sufficient to restrict attention to q-exact (saturated) designs if we seek a D-optimum minimal point design. If the number of observations in an experiment is limited for some reason (e.g. cost, time, space) minimal point or nearly minimal point exact designs may be of interest. It is the purpose of this paper to find designs which are nearly D-optimum over the class of all q-exact designs, Ξ (k,q)

If Ξ is a given class of designs and ξ_0 is some given design, we define the D-efficiency of ξ_0 with respect to Ξ to be

$$(1.12) \qquad e_k(\xi_0,\Xi) = (\det M(\xi_0) \,/\, \sup_{\xi\in\Xi} \det M(\xi))^{1/q}$$

for our setting of second order regression. For a more general definition and a discussion of why this gives the correct notion of efficiency, see Atwood (1969).

In general it is not known what designs are D-optimum over the class $\Xi(k,q)$ or even what are efficient saturated designs with respect to $\Xi(k,q)$ for second order regression on I^k. Recent research on the subject has dealt with constructing designs which appear good but without any general optimality results. Some, such as Mitchell and Bayne (1976) (using their Detmax computer search on 3^k lattice points, which are all the points in I^k whose coordinates are +1,-1, or 0) and Dubova and Federov (1972) (a computer search not restricted to lattice points) have used large amounts of computer time to find what appear to be good designs for $k \leq 5$. For $k > 5$, searches require too much computer time to be feasible. Others, such as Hoke (1974) (on lattice points), Rechtschaffner (1967) (also on lattice points), and Box and Draper (1974) (not restricted to lattice points) have proposed designs using clever methods of construction. Hoke's results are only for some special values of k. Rechtschaffner and Box and Draper propose designs for general k, but it can be shown that their results have an asymptotic D-efficiency of 0 with respect to $\Xi(k,q)$ as $k\to\infty$.

In section 2 we shall exhibit a finite class of saturated designs on the 3^k lattice, for each k, such that the best designs in these classes have an asymptotic D-efficiency of 1 with respect to $\Xi(k,q)$. The problem of constructing these designs will be examined in section

3 and results for k = 2,3,4,5, and 6 will be compared with the results of the studies mentioned above.

2. EFFICIENCY RESULTS. Suppose ξ is an n-exact design. We shall write X as $X(\xi)$ to indicate the dependence on ξ. Notice if $\xi \in \Xi(k,q)$ then n=q and $X(\xi)$ is a square matrix.

Let $\xi \in \Xi(k,q)$. Since $M(\xi) = X(\xi)X'(\xi)/q$ we have

$$\det M(\xi) = (1/q)^q \det^2 X(\xi) \tag{2.1}$$

Our objective is to determine ξ so as to make det $M(\xi)$ large, or equivalently, to make $\det^2 X(\xi)$ large. To do this we shall partition $X(\xi)$ in a convenient manner and then consider a class of designs which enables us to calculate det $X(\xi)$ in terms of the partition. This technique will allow us to construct designs which are asymptotically D-efficient.

Partition $X(\xi)$ so that

$$X(\xi) = \begin{pmatrix} Z_1(\xi) \\ Z_2(\xi) \end{pmatrix} = \begin{pmatrix} Y_{11}(\xi) & Y_{12}(\xi) \\ Y_{21}(\xi) & Y_{22}(\xi) \end{pmatrix} \tag{2.2}$$

where $Z_1(\xi)$ is (q-k)xq , $Z_2(\xi)$ is kxq, $Y_{11}(\xi)$ is (q-k)x(q-k), $Y_{12}(\xi)$ is (q-k)xk, $Y_{21}(\xi)$ is kx(q-k), and $Y_{22}(\xi)$ is kxk.

Let $\{-1, +1\}^k$ denote the k-fold Cartesian product of the two point set $\{-1, +1\}$ and let $\{0, 1\}^k$ denote the k-fold Cartesian product of the two point set $\{0, 1\}$.

Define

(2.3) $\Psi(k) = \{\psi \in \Xi(k,q)$; q-k points in the support of ψ are in $\{-1, +1\}^k$ and k points in the support of ψ are in $\{0, 1\}^k$ with at least one coordinate being 0$\}$

The D-optimum design in $\Psi(k)$ will be shown to have an asymptotic D-efficiency of 1 with respect to $\Xi(k,q)$ as $k \to \infty$.

It should be mentioned that the designs of Rechtschaffner (1967) are of this form, although he does not choose the best designs on $\Psi(k)$ for $k > 4$ but rather an asymptotically inefficient sequence of designs.

For $\psi \in \Psi(k)$ we may assume its support set is so ordered that the first q-k points are in $\{-1, +1\}^k$ and the last k points are in $\{0,1\}^k$ with at least one coordinate being 0 as the ordering of the support set does not change det $M(\psi)$. We shall call this standard form

Suppose $\psi \in \Psi(k)$ is in standard form. Notice $Y_{21}(\psi) = J_{q-k,k}$ where ~~$J_{m,n}$ denotes the m×n matrix all of whose entries are +1.~~ If we subtract the first row of $X(\psi)$ (a row of +1s) from the last k rows we eliminate $Y_{21}(\psi)$ and hence

(2.4) $$\det X(\psi) = \det (Y_{11}(\psi)) \det (Y_{22}(\psi) - J_{k,k}).$$

Notice that $Y_{11}(\psi)$ depends only on the first q-k points in the support of ψ (the points from $\{-1, +1\}^k$) and $Y_{22}(\psi)$ depends only on the last k points in the support of ψ (the points in $\{0,1\}^k$ with at least one coordinate being 0), so that these two collections of points can be chosen independently to maximize $\det^2(Y_{11}(\xi))$ and $\det^2(Y_{22}(\psi) - J_k)$ and thus $\det^2 X(\psi)$.

These observations plus the lemmas below are what will yield the desired efficiency result.

LEMMA 2.1. Suppose $M = \binom{A}{B}$ is a partitioned matrix where M is nxn, A is (n-m)xn, B is mxn, and m < n. Then

$$\det{}^2 M \leq \binom{n}{m}^2 \det{}^2 A^* \det{}^2 B^* \tag{2.5}$$

where A* is the (n-m)x(n-m) submatrix of A having largest absolute value of its determinant and B* is the mxm submatrix of B having largest absolute value of its determinant.

PROOF. By the Theorem of Corresponding Minors (see Householder (1964)) we have

$$\begin{aligned} \det AA' &= \sum \det{}^2 (A_{n-m}) \\ \det BB' &= \sum \det{}^2 (B_m) \end{aligned} \tag{2.6}$$

where $\sum \det{}^2(A_{n-m})$ is over all (n-m)x(n-m) submatrices A_{n-m} of A and $\sum \det{}^2(B_m)$ is over all mxm submatrices B_m of B. Then we have

$$\begin{aligned} \det{}^2 M &= \det MM' \\ &\leq \det (AA') \det (BB') \\ &= (\sum \det{}^2 (A_{n-m}))(\sum \det{}^2 (B_m)) \\ &\leq (\tbinom{n}{n-m} \det{}^2 A^*)(\tbinom{n}{m} \det{}^2 B^*) \\ &= \tbinom{n}{m}^2 \det{}^2 A^* \det{}^2 B^* \quad . \quad \square \end{aligned}$$

LEMMA 2.2. Suppose $g_1, g_2, \ldots, g_N$ are N real valued affine linear functions on R^k. Let a and b be real numbers and suppose for j=1,...,N, i=1,...,k that $a \leq x_i(j) \leq b$. Let P be the NxN matrix whose r,j^{th} entry is $g_r(x_1(j),\ldots,x_k(j))$. Then | det P | can be maximized over all possible values of the $x_i(j)$ by restricting the $x_i(j)$ to be a or b.

PROOF. This lemma follows from the linearity of det P in each of its entries (expand det P by minors of the appropriate column) and from the multilinearity of the g_n. □

We can now prove an asymptotic efficiency result using the above discussion and lemmas.

THEOREM 2.1. For each $k \geq 1$ let $\psi_k^* \in \Psi(k)$ be such that $\det M(\psi_k^*) = \sup_{\psi_k \in \Psi(k)} \det M(\psi_k)$ (such a ψ_k^* exists since for each k, $\Psi(k)$ is a finite set). Then we have

(2.7) $$1 \geq e_k(\psi_k^* , \Xi(k,q)) \geq (1/\binom{q}{k}^2)^{1/q}$$

and hence $\lim_{k\to\infty} e_k(\psi_k^*, \Xi(k,q)) = 1$.

PROOF. Let $\xi \in \Xi(k,q)$. Using equations (2.1) and (2.2) if we subtract the first row of $Z_1(\xi)$ (a row of +1s) from all the rows of $Z_2(\xi)$ we have

$$q^q \det M(\xi) = \det{}^2 \begin{pmatrix} Z_1(\xi) \\ Z_2(\xi) - J_{k,q} \end{pmatrix}$$

Applying Lemma 2.1 gives

(2.8) $$q^q \det M(\xi) \leq \binom{q}{k}^2 \det{}^2[(Z_1(\xi))^*] \det{}^2[(Z_2(\xi) - J_{k,q})^*]$$

where $(Z_1(\xi))^*$ is the (q-k)x(q-k) submatrix of $Z_1(\xi)$ having largest absolute value of its determinant and $(Z_2(\xi) - J_{k,q})^*$ is the kxk submatrix of $Z_2(\xi) - J_{k,q}$ having largest absolute value of its determinant.

If one considers the form of the entries of $(Z_1(\xi))^*$ (the entries are multilinear functions of the $x_i(j)$), it follows from Lemma 2.2 that there is a $\psi' \in \Psi(k)$, with ψ' in standard form, such that

$$(2.9) \qquad \det {}^2 Y_{11}(\psi') = \sup_{\xi \in \Xi(k,q)} \det {}^2(Z_1(\xi))^*$$

where $Y_{11}(\psi')$ is as in equation (2.2).

If we let $u_i(j) = x_i^2(j) - 1$, $i = 1,2,\ldots,k, j = 1,\ldots,q$, one sees that the entries of $(Z_2(\xi) - J_{k,q})^*$ are multilinear functions of the $u_i(j)$. The $u_i(j)$ can take on any values between -1 and 0 and hence $\sup_{\xi \in \Xi(k,q)} \det^2(Z_2(\xi) - J_{k,q})^*$ occurs for some set of values of the $u_i(j)$ such that $u_i(j) = 0$ or $u_i(j) = -1$ by Lemma 2.2. This means that the $x_i(j)$ must be +1,0, or -1 for all i,j and it suffices to just consider the $x_i(j)$ to be either +1 or 0. Hence there is a $\psi'' \in \Psi(k)$, with ψ'' in in standard form, such that

$$(2.10) \quad \det {}^2[Y_{22}(\psi'') - J_{k,q}] = \sup_{\xi \in \Xi(k,q)} \det {}^2(Z_2(\xi) - J_{k,q})^*.$$

Recall that $Y_{11}(\psi')$ depends only on the first q-k points in the support of ψ' and $Y_{22}(\psi'')$ depends only on the last k points in the support of ψ''. Let ψ be that element of $\Psi(k)$ whose first q-k support points are the same as those of ψ' and whose last k support points are the same as those of ψ''. Then $Y_{11}(\psi) = Y_{11}(\psi')$ and $Y_{22}(\psi) = Y_{22}(\psi'')$. Using equations (2.8), (2.9), and (2.10) we have for any $\xi_0 \in \Xi(k,q)$

$$\begin{aligned}(2.11) \quad q^q \det M(\xi_0) &\le \binom{q}{k}^2 \det {}^2[(Z_1(\xi_0))^*] \det {}^2[(Z_2(\xi_0) - J_{k,q})^*] \\ &\le \binom{q}{k}^2 [\sup_{\xi \in \Xi(k,q)} \det {}^2[Z_1(\xi)]] \, [\sup_{\xi \in \Xi(k,q)} \det^2[Z_2(\xi) - J_{k,q}]] \\ &= \binom{q}{k}^2 \det {}^2 Y_{11}(\psi) \det {}^2(Y_{22}(\psi) - J_{k,q})\end{aligned}$$

By equations (2.1) and (2.4) we have

$$(2.12) \qquad \det {}^2 Y_{11}(\psi) \det {}^2(Y_{22}(\psi) - J_{k,q}) = q^q \det M(\psi).$$

Combining equations (2.11) and 2.12) we have

(2.13) $$\det M(\xi_0) \leq \binom{q}{k}^2 \det M(\psi)$$

for any $\xi_0 \in \Xi(k,q)$. If $\psi_k^* \in \Psi(k)$ is as defined in the statement of the Theorem, equation (2.13) implies

(2.14) $$\det M(\xi_0) \leq \binom{q}{k}^2 \det M(\psi_k^*) = \binom{q}{k}^2 \sup_{\psi \in \Psi(k)} M(\psi)$$

for any $\xi_0 \in \Xi(k,q)$. Equation (2.7) now follows from (2.14) and the definition (1.12) of $e_k(\psi_k^*, \Xi(k,q))$. One can show $\lim_{k\to\infty} e_k(\psi_k^*, \Xi(k,q)) = 1$ from (2.7) and Stirling's approximation. □

The lower bound on $e_k(\psi_k^*, \Xi(k,q))$ is crude. One can show that $(1/\binom{q}{k}^2)^{1/q}$ is about .481 for k = 1, takes on its minimum value of .382 at k =4, is .454 at k = 10, .827 at k = 100, .972 at k = 1000. It increases slowly for $k \geq 4$. In the next section we shall see these bounds are not sharp.

3. CONSTRUCTION OF DESIGNS AND NUMERICAL RESULTS. From equations (2.1) and (2.4) we have that for any $\psi \in \Psi(k)$ in standard form

(3.1) $$\det M(\psi) = (1/q)^q \det {}^2Y_{11}(\psi) \det {}^2(Y_{22}(\psi) - J_{k,k}).$$

We recall that $Y_{11}(\psi)$ depends only on the first q-k points in the support of ψ (the points from $\{-1, +1\}^k$) and that $Y_{22}(\psi)$ depends only on the last k points in the support of ψ (the points from $\{0,1\}^k$ with at least one coordinate being 0). The two collections of points can be chosen separately so as to maximize first $\det {}^2Y_{11}(\psi)$, then $\det {}^2(Y_{22}(\psi) - J_{k,k})$, and hence $\det M(\psi)$. We utilize this idea to construct D-optimal and nearly D-optimal designs in $\Psi(k)$ for k = 2,3,4,5, and 6. The techniques used in these cases can be applied to other values of k to yield what appear to be good designs in $\Psi(k)$.

First, let us outline how to choose the last k points in the support of ψ so as to maximize $\det^2(Y_{22}(\psi) - J_{k,k})$. Recalling the form of $Y_{22}(\psi) - J_{k,k}$ and using some elementary row operations and properties of the determinant we obtain:

$$(3.2)\quad \det^2(Y_{22}(\psi)-J_{k,k}) = \det^2 \begin{bmatrix} x_1^2(q-k+1) - 1 & \cdots & x_1^2(q) - 1 \\ \vdots & & \vdots \\ x_k^2(q-k+1) - 1 & \cdots & x_k^2(q) - 1 \end{bmatrix}$$

$$= (1/2^{2k}) \det^2 \begin{bmatrix} 1 & 1 & \cdots & 1 \\ 1 & 2x_1^2(q-k+1)-1 & \cdots & 2x_1^2(q) - 1 \\ \vdots & \vdots & & \vdots \\ 1 & 2x_k^2(q-k+1)-1 & \cdots & 2x_k^2(q) - 1 \end{bmatrix}$$

Since $\psi \in \Psi(k)$ the $x_i(j)$, $1 \leq i \leq k$, $q-k+1 \leq j \leq q$, can take on the values 0 and 1 arbitrarily. Hence the last matrix in equation (3.2) is a $(k+1)\times(k+1)$ matrix whose first row and column consists of +1s, and whose remaining entries are arbitrary +1s and -1s. The problem of maximizing the square of the determinant of such a matrix has been studies in detail for many values of k. See, for example, Ehlich (1964a), Ehlich (1964b), Yang (1966), Yang (1968), and sections 17.4 and 17.6 of Raghavarao (1971). When $k+1 \equiv 0 \pmod 4$, the matrix which maximizes the square of the determinant on the last line of equation (3.2) is commonly called a Hadamard matrix in standard form.

Once the matrix which maximizes the square of the determinant in the last line of equation (3.2) has been found, the $x_i(j)$, $1 \le i \le k$ and $q-k+1 \le j \le q$, can be determined. The solutions will be either 0 or +1, and these solutions determine the last k points in the support of the D-optimal design in $\Psi(k)$.

The above provides a method for choosing the last k points in the support of a good design in $\Psi(k)$. We now outline a method for choosing the first q-k points in the support of a good design in $\Psi(k)$. Our object (see equation (3.1)) is to make det ${}^2Y_{11}(\psi)$ as large as possible. The first q-k points in the support of a design $\psi \in \Psi(k)$ must be elements of $\{-1, +1\}^k$. If ψ is in standard form, then the j^{th} column of $Y_{11}(\psi)$, $1 \le j \le q-k$, looks like

(3.3) $(1, x_1(j), \ldots, x_k(j), x_1(j)x_2(j), x_1(j)x_3(j), \ldots, x_{k-1}(j)x_k(j))'$

The problem of maximizing the square of the determinant of a (q-k)x(q-k) matrix whose j^{th} column is of the form given in equation (3.3) and where the $x_i(j)$ are restricted to be ± 1, is in general unsolved. Srivastava and Chopra (1971a), Srivastava and Chopra (1971b), and Srivastava (1972) have studied this problem using balanced arrays of strength 4 on two symbols and have constructed matrices of the form of $Y_{11}(\psi)$ which have large absolute value of their determinant, at least for smaller values of k ($k \le 10$). We next define balanced arrays of strength 4 on two symbols and present some of the results of Srivastava and Chopra.

Suppose T is a kxn (+1, -1) matrix. Such a matrix will be called _a balanced array of strength 4 on two symbols_ with index set $\underline{m}' = (m_0,m_1,m_2,m_3,m_4)$ if every 4xn submatrix T_0 of T satisfies the following: let $\underline{y}$ be any one of the 16 possible 4x1 (+1,-1) column vectors. Then $\underline{y}$ occurs as a column of T_0 m_i times, where i is the number of +1s in $\underline{y}$. This holds for all possible choices of $\underline{y}$.

Suppose T is a kx(q-k) matrix and is a balanced array of strength 4 on two symbols with index set $\underline{m}' = (m_0,m_1,m_2,m_3,m_4)$. Let

(3.5)
$$u_1 = m_0 + 4m_1 + 6m_2 + 4m_3 + m_4$$
$$u_2 = (m_4 - m_0) + 2(m_3 - m_1)$$
$$u_3 = m_4 - 2m_2 + m_0$$
$$u_4 = (m_4 - m_0) - 2(m_3 - m_1)$$
$$u_5 = m_0 - 4m_1 + 6m_2 - 4m_3 + m_4$$

Also let

(3.6)
$$\begin{aligned} c_3 = {} & u_1^3 - k(k-1)^2u_3^3/2 + (3k-5)u_1^2u_3 + (k-2)(k-3)u_1^2u_5/2 \\ & + (k-1)(3k-8)u_1u_3^2/2 + (k-1)(k-2)(k-3)u_1u_3u_5/2 \\ & - (3k-2)u_1u_2^2 - (k-1)(k-2)^2u_1u_4^2/2 - 2(k-1)(k-2)u_1u_2u_4 \\ & + 2ku_2^2u_3 - k(k-2)(k-3)u_2^2u_5/2 + k(k-1)(k-2)u_2u_3u_4 \end{aligned}$$
$$c_5 = (u_1-u_3)[u_1-(k-3)u_5 + (k-4)u_3] - (k-2)(u_2-u_4)^2 \ .$$

One can show, using the results of Srivastava and Chopra (1971a), that if $\psi \in \Psi(k)$ is in standard form and the first q-k points in the support of ψ are the columns of T, then

(3.7)
$$\det {}^2\Upsilon_{11}(\psi) = c_3c_5^{k-1}(16m_2)^{k(k-3)/2}.$$

Srivastava and Chopra have constructed kx(q-k) matrices T which are balanced arrays for several values of k and with several different index sets. These are tabulated in Srivastava and Chopra (1971b) and subsequent papers by these authors. Using equations (3.5), (3.6), and (3.7) and the tabulated balanced arrays of Srivastava and Chopra we can, by trial and error for a given k, find the kx(q-k) balanced array that gives rise to the largest value of det ${}^2Y_{11}(\psi)$, by testing each of the possible index sets given in the tables. This maximizing balanced array determines the first q-k points in the support of a design $\psi_0 \in \Psi(k)$, as mentioned above equation (3.7). For k = 2,3, and 5 it is possible to show this is indeed the design ψ_0 that maximizes det ${}^2Y_{11}(\psi)$ over all $\psi \in \Psi(k)$. For other values of k this is unclear, but for small values of k ($k \leq 10$) the designs produced from balanced arrays in this manner appear good. For $k \geq 10$ few balanced arrays have been constructed.

The techniques outlined above provide a method for choosing both the first q-k points and the last k points in the support of a design $\psi \in \Psi(k)$, and thus determine ψ completely. These techniques have been used for k = 1,2,3,4,5,and 6 to construct optimal or near optimal designs in $\Psi(k)$ so as to provide numerical results for comparison with known results in the literature. We now give the supports of the designs constructed using the above method and the values of the determinant of the information matrix of these designs.

k = 2: Support set is $\{(1,1)',(1,-1)',(-1,1)',(-1,-1)',(1,0)',(0,1)'\}$.

det $M(\psi) = 5.49\text{x}10^{-3}$

k = 3: Support set is $\{(1,1,1)',(1,1,-1)',(1,-1,1)',(-1,1,1)',(1,-1,-1)'$ $(-1,1,-1)',(-1,-1,1)',(1,0,0)',(0,1,0)',(0,0,1)'\}$.

det $M(\psi) = 1.05\text{x}10^{-4}$

k = 4: Support set is $\{(1,1,-1,-1)',(1,-1,1,-1)',(1,-1,-1,1)', (-1,1,1,-1)',(-1,1,-1,1)',(-1,-1,1,1)',(1,1,1,-1)',(1,1,-1,1)', (1,-1,1,1)',(-1,1,1,1)',(-1,-1,-1,-1)',(1,0,0,0)',(0,1,0,0)', (0,0,1,0)',(0,0,0,1)'\}$.

det $M(\psi) = 7.95\times10^{-7}$

k = 5: Support set is $\{(1,1,1,1,1)',(1,1,1,-1,-1)',(1,1,-1,1,-1)', (1,1,-1,-1,1)',(1,-1,1,1,-1)',(1,-1,1,-1,1)',(1,-1,-1,1,1)', (-1,1,1,1,-1)',(-1,1,1,-1,1)',(-1,1,-1,1,1)',(-1,-1,1,1,1)', (1,-1,-1,-1,-1)',(-1,1,-1,-1,-1)',(-1,-1,1,-1,-1)',(-1,-1,-1,1,-1)', (-1,-1,-1,-1,1)',(1,1,0,0,1)',(1,1,0,1,0)',(0,0,0,1,1,)', (0,1,1,0,0)',(1,0,1,0,0)'\}$

det $M(\psi) = 7.89\times10^{-8}$

k = 6: Support set is $\{(1,1,1,1,1,1)',(1,-1,-1,-1,-1,-1)', (-1,1,-1,-1,-1,-1)',(-1,-1,1,-1,-1,-1)',(-1,-1,-1,1,-1,-1)', (-1,-1,-1,-1,1,-1)',(-1,-1,-1,-1,-1,1)',(1,1,1,1,-1,-1)', (1,1,1,-1,1,-1)',(1,1,1,-1,-1,1)',(1,1,-1,1,1,-1)',(1,1,-1,1,-1,1)', (1,1,-1,-1,1,1)',(1,-1,1,1,1,-1)',(1,-1,1,1,-1,1)',(1,-1,1,-1,1,1)', (1,-1,-1,1,1,1)',(-1,1,1,1,1,-1)',(-1,1,1,1,-1,1)',(-1,1,1,-1,1,1)', (-1,1,-1,1,1,1)',(-1,-1,1,1,1,1)',(1,0,1,0,0,0)',(0,0,1,1,1,1)', (0,1,1,0,0,1)',(1,1,0,1,0,1)',(1,1,0,0,1,1)',(0,1,1,1,1,0)'\}$

det $M(\psi) = 1.53\times10^{-10}$

For purposes of comparison with other exact designs ξ in the literature we list values of $(\det M(\xi))^{1/q}$ for some of the designs in the literature. Here * denotes designs on the 3^k lattice.

$[\det M(\xi)]^{1/q}$

k	q	New Designs* (1978)	Box and Draper (1974)	Mitchell and Bayne* (1976)	Rechtschaffner* (1967)	Dubova and Federov (1972)
2	6	.420	.423	.420	.420	.423
3	10	.400	.423	.410	.400	.423
4	15	.392	.374	.425	.392	.432
5	21	.459	.317	.456	.450	No Design
6	28	.446	.268	No Design	.428	No Design

The new designs presented here compare favorably with other minimal point designs in the literature for small k. In fact for k = 5 and 6 the new designs are better than any proposed previously. It is important to emphasize that the construction of good designs in $\Psi(k)$ using the techniques presented above, is relatively easy. The computer searches of Mitchell and Bayne or of Dubova and Federov require large amounts of computer time and cannot be carried out for k > 5. The constructions of Box and Draper or Rechtschaffner are fine for small k but can be shown to have an asymptotic D-efficiency of 0 with respect to the class of all minimal point designs. For these reasons, the new designs and construction techniques appear to be an improvement over results presently in the literature.

4. REMARKS. Although we have only discussed the problem of multivariate second order regression, the same ideas can be applied to the problem of finding D-optimal saturated designs for multivariate polynomial regression of higher orders. Lemmas 2.1 and 2.2 can be

used, after performing some row and column operations on the design matrix, to show that asymptotically D-efficient designs can be found among the class of all non-singular saturated designs which take as many observations as possible from $\{-1,+1\}^k$. The problem of finding the best designs in this class for various values of k is a difficult combinatorial problem, though.

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