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Φ_p -Optimal Second Order Designs for Symmetric Regions

By L. Pesotchinsky

1. Introduction.

At first we must refer to the paper of Kiefer (1975), emphasizing the problem of examination of structure and performance of competing designs under various changes of criterion. As an illustration such a study was successfully completed in that paper for a family of Φ_p -optimality criteria, that included the three most commonly used criteria, those of D-, A- and E-optimality, with respect to quadratic regression on the m -simplex. In the papers of Galil and Kiefer (1977a,b) the study was also completed with respect to rotatable designs on a ball and optimal designs on a cube.

The family of criteria considered is produced by optimality functionals $\Phi_p(\xi)$, derived from the $N \times N$ information matrix

$$M(\xi) = \int_X f'(x) f(x) \xi(dx),$$

where N is the number of unknown parameters, ξ is the design, that is, in general, a probability measure over experimental region X , and f is the known regression function $(f_1(x), \dots, f_N(x))'$. The corresponding model is supposed to be of a linear form: $EY = \theta f'$, where Y is the response function and N coefficients θ are unknown. We also assume that the observations of Y are uncorrelated and with the equal variances. If in case of nonsingular information matrix $\mu_1(\xi), \dots, \mu_N(\xi)$ denote the eigenvalues of $M(\xi)$, then the functionals $\Phi_p(\xi)$ are defined as follows:

$$\Phi_p(\xi) = [N^{-1} \text{tr} \{M^{-p}(\xi)\}]^{1/p} = \{N^{-1} \sum_{i=1}^N \mu_i^{-p}(\xi)\}^{1/p}, \quad 0 < p < \infty,$$

$$(1.1) \quad \Phi_0(\xi) = \lim_{p \rightarrow 0+} \Phi_p(\xi) = \{\det M^{-1}(\xi)\}^{1/N},$$

$$\Phi_\infty(\xi) = \lim_{p \rightarrow +\infty} \Phi_p(\xi) = \max_{1 \leq i \leq N} \{\mu_i^{-1}(\xi)\};$$

Φ_0 , Φ_1 and Φ_∞ are the familiar D-, A- and E-optimality criteria.

A Φ_p -optimal design ξ_p^* is one that minimizes $\Phi_p(\xi)$.

In the above mentioned papers of Galil and Kiefer it was noticed in particular, that on the unit ball and the simplex the Φ_p -optimal designs (from a class of rotatable ones if on the ball) were fairly efficient relative to the other designs of the same family, which was not the fact on a cube.

We consider in this paper the same family of criteria with respect to quadratic regression on the unit ball, on a cube $C_m = [-1,1]^m$ and on a cube with the vertices, truncated by planes $\sum_{i=1}^m |x_i| \leq Q$, denoted further as a region

$$\Omega_m(k,a) = C_m \cap \{x \mid \sum_{i=1}^m |x_i| \leq k+a\},$$

where integer $k \in [1, m-1]$ and $0 \leq a < 1$. One of the reasons for the artificial in some sense choice of polyhedrons $\Omega_m(k,a)$ is that they can serve as an approach in experimental problems when a region, if presented as a cube, has unattainable vertices, because the trials at them or near them are either expensive or too complicated. The next reason is that the main details of study on $\Omega_m(k,a)$ follow from the study on a cube and

that Φ_p -optimum designs, as it is shown in sections 3 and 4, are often unique on $\Omega_m(k,a)$ with the same set of support for all p and are "good" even for a cube C_m . The same reasons hold for the regions

$$\Omega_m(k,a;n,b) = C_m \cap \{x \mid n-1+b \leq \sum_{i=1}^m |x_i| \leq k+a\}$$

when the center point is also unattainable.

In the paper the main attention is paid to the study of structure of the supports of the Φ_p -optimal designs over C_m , $\Omega_m(k,a)$ and the unit ball (in the latter case with respect to all the designs) both under variation of p and transformation of region (the latter mainly in the sense of variation of $k+a$ in $\Omega_m(k,a)$ with m fixed).

There is some regularity to be expected in behavior of the Φ_p -optimal supports under fixed experimental region and with p changing, so the study of both "extreme" cases $p = 0, \infty$ is of special interest, also because it can be done algebraically. By such direct methods we can obtain some general results for the case of a ball of arbitrary radius, as well as for the study of uniqueness and structure of the Φ_p -optimal supports for all p . These problems are considered in section 3. In other parts of this section we study the asymptotical robustness of the D- and E-optimum designs under changes of p with $m \rightarrow \infty$.

The numerical results on structure in the case $0 < p < \infty$ as well as the results on the performance of the designs ξ_p^* with respect to various criteria are illustrated in section 4.

In section 5 an attempt is made to construct some integer designs on the cube and the unit ball which are uniformly "good" with respect to the family of the Φ_p -optimality criteria.

As well as criteria of the Φ_p -family we consider here the criterion of G-optimality with the optimality functional

$$G(\xi) = N^{-1} \max_{x \in X} d(x, \xi) = N^{-1} \max_{x \in X} f(x)M^{-1}(\xi)f'(x)$$

where $d(x, \xi)$ for nonsingular $M(\xi)$ is the normalized variance function of the regression function fitted by least squares. The original equivalence theorem (Kiefer and Wolfowitz, 1960) asserts that G-optimality is equivalent to Φ_0 -optimality and that $\max_{x \in X} d(x, \xi_0^*) = N$. One of the conclusions of the study on the regions in this paper is that the high Φ_0 -efficiency of ξ_p^* 's (and especially of ξ_∞^*) does not imply the high G-efficiency, as it was in the case of the m -simplex (Kiefer, 1975).

2. Definitions and Notation.

For simplicity we shall define the Φ_p -efficiency of ξ as the ratio $\Phi_p(\xi_p^*)/\Phi_p(\xi)$, denoted further as $e_p(\xi)$; thus for $p = 0$ we obtain the D-efficiency of Atkinson (1973). The G-efficiency of ξ is defined as the ratio $g(\xi) = N/\bar{d}(\xi)$, where $\bar{d}(\xi) = \max_{x \in X} d(x, \xi)$.

We will consider mainly the values of $e_q(\xi_p^*)$ and $g(\xi_p^*)$, so for brevity they will be denoted as $e_q(p)$ and $g(p)$ correspondingly.

We examine here second order regression on symmetric regions, so the limiting arguments similar to those in papers of Kiefer (1974,1975) and Farrell et al. (1967) may be implemented to reduce the problem and consider only invariant Φ_p -optimum designs; that is in our case, designs invariant under permutations of indices and changes of signs of the design points coordinates. In general, even on a ball, orthogonal transformations preserve only D-optimality of the designs; thus we shall consider only the above invariance.

If ξ is an invariant second order design, then $M(\xi)$ depends only on the even moments

$$\lambda_2 = E(x_i^2), \lambda_3 = E(x_i^2 x_j^2), \lambda_4 = E(x_i^4) \quad (1 \leq i, j \leq m)$$

and the odd moments are zero. These conditions on moments are also valid for noninvariant second order symmetric designs, as defined by Kono (1962), so we shall not further underline the difference between invariant and non-invariant designs with the same information matrix, and shall call both types of them "symmetric designs". E.g., the second order symmetric D-optimum designs on the cube in the papers of Kiefer (1961) and Kono (1962) are invariant and the same designs in the papers of Farrell et al. (1967) and Pesotchinsky (1975) are noninvariant with $m > 3$.

Throughout this paper E denotes the set of points of the 3^m factorial, divided into $m+1$ sets E_k with the k -th set consisting of all $2^k m! / k! (m-k)!$ points with k nonzero coordinates; and for the unit ball E_k denotes the set of all points with k coordinates equal to $\pm 1/\sqrt{k}$ and $m-k$ equal to zero; $E = \bigcup_{k=0}^m E_k$. We can note that if $A_k (A_k \subset E_k)$ is the set of

support of a second order symmetric design on a cube, then the corresponding set of a ball also supports some symmetric design, because both sets differ only in value of levels of factors. Thus the problem of study of structure of supports of the designs over points of E on a ball can be reduced to the same problem over points of E on a cube, though the optimal weights are different.

In the following E_0^k will denote $\bigcup_{i=0}^k E_i$ and $E_m(k,a)$ - the set of vertices of the polyhedron $\Omega_m(k,a)$ - the points with k coordinates equal to $\underline{+1}$, one equal to $\underline{+a}$, and $m-k-1$ equal to zero, and $B_m(k,a)$ - the set of points with all coordinates equal to $\underline{+(k+a)/m}$. (If $k+a = m$, then $B_m(k,a) = E_m(k,a) = E_m$ and if $a = 0$, then the set $E_m(k,a)$ coincides with E_k). The union of all the above sets will be denoted as

$$R_m(k,a); R_m(k,a) = E_0^k \cup E_m(k,a) \cup B_m(k,a).$$

3. Main Theoretical Results.

3.1 The sets of support and uniqueness of Φ_p -optimal designs.

It follows from the General Equivalence Theorem (G.E.T.) (Kiefer, 1974), that ξ is Φ_p -optimal for $0 \leq p < \infty$ if and only if for all $x \in X$

$$(3.1) \quad d_\xi(x) = f(x) M^{-p-1} f'(x) \leq \text{tr} \{M^{-p}(\xi)\}$$

and that an optimal ξ assigns measure one to the set of x for which equality holds in (3.1). $d_\xi(x)$ in (3.1) is a quartic in x , and for symmetric second order ξ

$$(3.2) \quad d_{\xi}(x) = A + B \sum_{i=1}^m x_i^2 + C \sum_{i=1}^m x_i^4 + D \left(\sum_{i=1}^m x_i^2 \right)^2$$

where A, B, C, D are the functions of p .

It can be proved in the same way as for D -optimum designs in the paper of Farrell et al. (1967), that with all $p < \infty$ Φ_p -optimum second order designs on a ball must be supported by points of the sphere of the same radius and the center point. As to $X = \Omega_m(k, a)$, then the maximizing points of (3.2) must belong to the set $R_m(k, a)$.

Moreover, suppose that the points of three sets E_{k_i} , $i = 1, 2, 3$, give maximum to $d_{\xi}(x)$ for some fixed p . (These sets can belong to the supports of different Φ_p -optimal designs, not necessarily to the same). Then we have in the case of quadratic regression that

$$(3.3) \quad A + Bk_i + Ck_i + Dk_i^2 = A + Bk_j + Ck_j + Dk_j^2, \quad i \neq j, \quad i, j \leq 3$$

and thus $D(k_1 - k_2)(k_3 - k_1) = 0$, $B + C = -D(k_1 + k_j)$. So $D = 0$ and $B = -C$ and this fact implies that all the points of E have the same property as those of E_{k_i} . From this fact we can derive that:

- 1) A Φ_p -optimal design ξ_p^* for $\Omega_m(k, a)$ is also Φ_p -optimal for cube C_m , because in this case $d_{\xi}(x) = A$ in points of E , where all the possible supports of Φ_p -optimal designs must be contained. By G.E.T. it means that the design ξ_p^* is Φ_p -optimal for cube;
- 2) $\xi_p^*\{E_m(k, a)\} = \xi_p^*\{B_m(k, a)\}$, this follows from p. 1) because both $E_m(k, a)$ and $B_m(k, a)$ must not be contained in the supports of Φ_p -optimal designs for cube;

3) A Φ_p -optimal design on a cube is nonunique if $m \geq 3$, that is at least two "basic" Φ_p -optimal designs exist supported by different groups of at most three sets $E_{k_1} \cup E_{k_2} \cup E_{k_3}$. It simply follows from the fact that the system of three linear equations for the moments of Φ_p -optimal measure, the same system as in the paper of Pesotchinsky (1975), includes $m+1$ weights α_k of sets E_k , $k = 0, 1, \dots, m$, and thus the existence of one solution implies the existence of the others.

On the other hand, if $k+a < m$ and only two sets E_{k_1}, E_{k_2} belong to the support of the Φ_p -optimum design, then we can show as above in (3.3) that for any integer r , $r < k$, $D(k_1-r)(k_2-r) < 0$, thus $k_1 = 0$ and $k_2 = k$ and the Φ_p -optimum design is unique on $\Omega_m(k, a)$. (We do not consider here the possibility of reduction of number of points of support with the help of noninvariant designs.)

The above reasoning suggest the procedure of theoretical or numerical study of Φ_p -optimal designs for $\Omega_m(k, a)$ with $0 \leq p < \infty$: for each m we shall find the "basic" Φ_p -optimal designs for the cube C_m ; let $k_m(p)$ be the minimum of k_3 's for "basic" Φ_p -optimal designs supported by at most three sets E_{k_1}, E_{k_2} and E_{k_3} , $k_1 \leq k_2 \leq k_3$; then the main result for the study is given in the following Lemma.

Lemma. If $k \geq k_m(p)$, then the Φ_p -optimal design on $\Omega_m(k, a)$ can be presented by at least one of the Φ_p -optimal designs on a cube, and if $k < k_m(p)$, then the Φ_p -optimal design on $\Omega_m(k, a)$ is unique and its set of support is contained in $E_0 \cup E_m(k, a) \cup E_k \cup B_m(k, a)$; moreover, the optimal weights of E_0 and $E_m(k, a)$ are both nonzero.

This result will be used further in 3.2 and 3.3 for the study of D- and E-optimum designs.

We can also note, that if $n_m(p)$ denotes the maximum of k_1 's for "basic" Φ_p -optimal designs on a cube, then the Φ_p -optimal design for region $\Omega_m(k, a; n, b)$ is unique provided that the condition $n_m(p) < n < k < k_m(p)$ does not occur and the set of support of such design is contained in $B_m(n-1, b) \cup E_k \cup E_m(k, a)$.

All the results above were valid for $0 \leq p < \infty$, the case of $p = \infty$, that is the E-optimality of the designs, is studied algebraically later in this section to remove some difficulties arising for $p = \infty$ in an analogue of (3.1) (Kiefer, 1974).

3.2 D-optimum designs.

Our considerations here are limited to the case $X = \Omega_m(k, a)$, because both the D-optimum designs on a cube and a ball were studied in papers of Kiefer (1961) and Farrell et al. (1967).

For the D-optimum designs on a cube we have that $k_m(0) = m$ (Farrell et al., 1967); thus the D-optimum designs are unique on $\Omega_m(k, a)$ for $k+a < m$. For $p = 0$ the left-hand side of (3.1) is the variance of the estimate of the regression function and the right-hand side is the number of unknown parameters, that is $N = (m+1)(m+2)/2$. The coefficients A, B, C, D in (3.2) can be found algebraically as functions of moments λ_2, λ_3 and λ_4 , so the condition (3.1) is easy to verify.

We can start the search of the D-optimum designs on $\Omega_m(k, a)$ with the D-optimum designs $\xi_0^*(k, a)$ from the class of designs supported by

points of $E_m(k,a)$ and the center point. Maximizing the value of the information matrix determinant, we obtain the weight α_0 of the center point: $\alpha_0 = N^{-1}$ for all m, k, a . Then we verify the condition (3.1) at points of E_k and $B_m(k,a)$, thus obtaining that the designs $\xi_0^*(k,a)$ are D-optimum for the regions $\Omega_m(k,a)$ with $2 \leq k \leq m-2$ ($m \geq 4$) and $0 \leq a < 1$. Verification of (3.1) for the designs $\xi_0^*(k,a)$ with $k = 1$ or $m-1$ discloses the existence of such "critical" values a'_m and a''_m that:

- 1) for $k = 1$ and $a \geq a'_m$ the designs $\xi_0^*(1,a)$ are still D-optimum for $\Omega_m(1,a)$ and
- 2) for $k = m-1$ and $a \leq a''_m$ these designs are D-optimum for $\Omega_m(m-1,a)$.

The values of a'_m and a''_m are independent for $m \geq 3$, but for $m = 2$ we have $(1-a'_2)/(1+a'_2) = a''_2$; this can be proved even geometrically because the 45° turning of $\Omega_2(1,a)$ with suitable normalization gives us the region $\Omega_2(1,b)$ where a, b are in the same relation as a'_2 and a''_2 above.

a'_m can be found by solving the equation $d_\xi(x) = N$ at $x \in B_m(1, a'_m)$, $\xi = \xi_0^*(1, a'_m)$, and a''_m - by solving the same equation at $x \in E_{m-1}$, $\xi = \xi_0^*(m-1, a''_m)$. Both the left-hand sides of the equations can be reduced respectively to polynomials of powers 12 and 8 with at most one root on $(0,1)$. In particular, from the second of them we have

$$(a''_m)^2(-m^2+7m-9) + \sum_{k=2}^4 \beta_k (a''_m)^{2k} = 0,$$

where β_k 's depend only on m ; that gives us $a''_m = 0$ for $m \geq 6$.

a'_m and a''_m are listed in table 1.

Table 1. The critical values a'_m (for $\Omega_m(1,a)$) and a''_m (for $\Omega_m(m-1,a)$).

m	2	3	4	5	6	7	8
a'_m	0.234	.171	.169	.163	.157	.151	.145
a''_m	0.621	.476	.332	.150	0	0	0

To complete the study of the D-optimum designs on $\Omega_m(k,a)$ we can note that in the case $k = m-1$ and for a increasing beyond a''_m the set of support of the D-optimum design must be supplemented by the set E_{m-1} , and in the case $k = 1$ and $0 < a < a'_m$ by the set $B_m(1,a)$; thus the following theorem holds.

Theorem 1. The D-optimum designs for quadratic regression on $\Omega_m(k,a)$ are supported by the center point and with respect to values of k,a by the following sets:

- 1) $E_m(k,a)$: (i) for $k = 1$ and $a \geq a'_m$, (ii) $2 \leq k \leq m-2$,
(iii) $k = m-1$ and $a \leq a''_m$;
- 2) $E_m(1,a)$ and $B_m(1,a)$: for $k = 1$ and $0 < a < a'_m$;
- 3) $E_m(m-1,a)$ and E_{m-1} : for $k = m-1$ and $a''_m < a < 1$.

We should note that the optimal moments λ_2, λ_3 and λ_4 are the functions of weights of sets $B_m(1,a), E_m(m-1,a)$ and E_{m-1} , so these weights under m, k, a fixed could be found by direct maximization of $\det M_{\xi}$.

We can note that the points of $E_m(k,a)$ belong to a sphere of radius $k+a$ and $\xi_0^*(k,a)$ assigns to this sphere the same measure $m(m+3)/\{(m+1)(m+2)\}$ as the D-optimum design on a ball (Kiefer, 1961). Hence we expect that the designs $\xi_0^*(k,a)$ have good D-efficiencies relative to a ball.

For instance the D-efficiency of $\xi_0^*(k,0)$ on a ball of radius k (this efficiency is denoted further by $f_m(k)$) varies as a function of $k \in [2, m-1]$ from $f_m(2)$ up to 1 (at $k = (m+2)/3$) and then to $f_m(m-1)$. We have that $f_m(2) \downarrow 1/2$ and $f_m(m-1) \uparrow 1$ as $m \rightarrow \infty$; the minimum value of $f_m(m-1)$ is 0.787 at $m = 11$ and $f_m(2) > 0.829$ for $m \leq 11$. Also the estimations show that the D-efficiency of $\xi_0^*(k,0)$ relative to the "larger" region $\Omega_m(n,0)$ ($k < n \leq m$) is more than k/n and that $\xi_0^*(1,a)$ is fairly D-efficient even in cases when $0.05 \leq a < a'_m$. It turns out from these remarks, as well as from the evident remark that $\xi_0^*(k,a)$ is invariant under truncation of cube vertices in points of $E_m(k,a)$ by any concave (to the center point) surface, that the designs $\xi_0^*(k,a)$ are somewhat robust in their D-efficiency under variation of experimental region.

3.3 E-optimum designs.

The result for cube was independently obtained by V.K. Denisov and A. A. Popov of Novosibirsk (not yet published), Galil and Kiefer (1977b) and the author. For details we can refer to the paper of Galil and Kiefer (1977b), and here we can mention briefly that the E-optimum design on a cube has moments $\lambda_2 = \lambda_4 = 2/5$, $\lambda_3 = 1/5$ (independently of m).

We can easily find that the basic solution of the equations for moments exists for the weights of sets E_{k_i} , $i = 1, 2, 3$, iff

$$(3.4) \quad \begin{aligned} 0 \leq k_1 \leq \{2mk_3 - m(m+1)\}/(5k_3 - 2m) \leq k_2 \leq \\ \leq \{m(m+1) - 2mk_1\}/(2m - 5k_1) \leq k_3, \end{aligned}$$

so we can find that for the E-optimum design ($p = \infty$) $k_m(\infty) = (m+1)/2$ for odd m and $m/2+1$ for even m and $n_m(\infty)$ is the integer part of $(m-1)/3$. It is also of interest that basic solutions with two nonzero components exist, as, e.g., with $k_1 = k_2 = 0$ and $k_3 = k_m(\infty)$ with odd m .

Taking into account the fact that $k_m(p)$ decreases with p , we can note that all Φ_p -optimum designs are unique on $\Omega_m(k, a)$ iff $k \leq (m+1)/2$. On the other hand, it means that for good (in the sense of Φ_p -optimality) designs on a cube the minimum of maximal distance of the design points from the center point should never be less than $(m+1)/2$.

In the case $k < k_m(\infty)$ the E-optimum designs on $\Omega_m(k, a)$ can be found by the same reasoning as for the cube. E.g., if $a = 0$, we have that ξ_∞^* is supported by points of $E_0 \cup E_k$ with $\xi_\infty^*(E_k) = m(m-1)(km-2k+1)/[k\{(k-1)(km-2k+1) + m(m-1)^2\}]$.

For the study on the unit ball we shall note that the moments of invariant measure obey the following equalities:

$$(3.5) \quad \lambda_4 + (m-1)\lambda_3 = \lambda_2 = \alpha_s/m,$$

where α_s denotes the measure of the unit sphere. For the proof of

(3.5) we can consider the chain of equalities:

$$\begin{aligned}
\lambda_2 &= \left\{ \sum_{i=1}^m E(x_i^2) \right\} / m = \left\{ E \left(\sum_{i=1}^m x_i^2 \right) \right\} / m = \alpha_s / m = \\
&= \left\{ E \left(\sum_{i=1}^m x_i^2 \right)^2 \right\} / m = \left\{ E \left(\sum_{i=1}^m x_i^4 \right) + E \left(\sum_{i \neq j} x_i^2 x_j^2 \right) \right\} / m = \\
&= \{ m\lambda_4 + m(m-1)\lambda_3 \} / m = \lambda_4 + (m-1)\lambda_3 .
\end{aligned}$$

Thus we have for the only five distinct eigenvalues of $M(\xi)$:

$$\begin{aligned}
\mu_1 &= \lambda_3, \quad \mu_2 = \lambda_4 - \lambda_3 = \lambda_2 - m\lambda_3, \quad \mu_3 = \{ 1 + \lambda_2 - \sqrt{(1 - \lambda_2)^2 + 4m\lambda_2^2} \} / 2, \\
\mu_4 &= 1 + \lambda_2 - \mu_3 \quad \text{and} \quad \mu_5 = \lambda_2,
\end{aligned}$$

and, taking into account the uniqueness of solutions of the equations $\mu_i = \mu_j$ ($1 \leq i, j \leq 3$), we obtain in the same way as for the cube the E-optimum values of λ_2, λ_3 :

$$\lambda_2 = (m+1)/(m^2+2m+2), \quad \lambda_3 = \lambda_2/(m+1).$$

Now we have for the ball that

$$(3.6) \quad \max \min \{ \mu_i \} = \lambda_3 = (m^2+2m+2)^{-1}$$

and the E-optimum measure of the unit sphere is $\alpha_s(\infty) = m(m+1)/(m^2+2m+2)$.

The existence and structure of finite supports over points of E of the E-optimum measure follow from the more general result (theorem 2), proved later in this section.

3.4 Φ_p -optimum designs on a ball.

In this case the more detailed description of the Φ_p -optimal designs and their properties can be found algebraically. For the case of the unit ball we shall consider now the two "free" parameters λ_2 and λ_3 remaining from (3.5) (both depending on p for the Φ_p -optimal design), denoting the ratio of them by $r = \lambda_3/\lambda_2$. Thus the functional $\Phi_p(\xi)$ may be considered as depending only on values of λ_2 and r , and the formal differentiation of Φ_p with $0 < p < \infty$ gives us the equations $\frac{\partial \Phi_p}{\partial r} = \frac{\partial \Phi_p}{\partial \lambda_2} = 0$ for the Φ_p -optimal values of r and λ_2 . From the first of them we have $r = \{m+2^{1/(p+1)}\}^{-1}$ (and this is also valid for $p = 0, \infty$), and the second can be easily solved now algebraically (as for $p = 1$) or numerically. We can prove that the solution $\lambda_2(p)$ as a function of p monotonically decreases from $(m+3)/\{(m+1)(m+2)\}$ at $p = 0$ to $(m+1)/(m^2+2m+2)$ at $p = \infty$ and the approximate solution (to order m^{-4}) of the equation for $\lambda_2(p)$ is $\lambda_2(p) = 1/m - \{2^{1/(p+1)}\}/\{m^{2+1/(p+1)}\}$; thus the Φ_p -optimal measure of the unit sphere $\alpha_s(p)$ is approximately (to order m^{-3}) equal to

$$1 - \{2^{1/(p+1)}\}/\{m^{1+1/(p+1)}\}$$

for $0 \leq p \leq \infty$.

If we want to represent the Φ_p -optimal (for any p) measure over points of E , then we can find the equations for the moments

$$\begin{aligned} \lambda_2(p) &= \alpha_s(p)/m = \left(\sum_{k=1}^m \alpha_k(p) \right) / m, \\ (3.7) \quad \lambda_3(p) &= \left[\sum_{k=2}^m \{ \alpha_k(p) k(k-1)/k^2 \} \right] / \{m(m-1)\} = \\ &= \{ \alpha_s(p) - \sum_{k=2}^m (\alpha_k(p)/k) \} / \{m(m-1)\}, \end{aligned}$$

where $\alpha_k(p)$ denotes the Φ_p -optimal weight of the set E_k , $0 \leq k \leq m$. For basic solutions of (3.7), say $\alpha_k(p), \alpha_j(p)$, we have for each p (with $\lambda_3(p) = \lambda_2(p) r(p)$) that

$$\alpha_i(p) = i\alpha_s(p) \frac{\{m-l-2^{1/(p+1)}(l-1)\}}{\{(i-l)(m+2^{1/(p+1)})\}},$$

where i, l are equal, respectively, to k, j or j, k . By positivity of the solution we obtain that

$$k \geq \frac{\{m+2^{1/(p+1)}\}}{\{1+2^{1/(p+1)}\}} \geq j.$$

The latter condition on k, j does not depend on the value of the unit sphere measure $\alpha_s(p)$; thus all the Φ_p -optimal designs can be supported by points of E .

The formal result is given in the following Theorem.

Theorem 2. All the Φ_p -optimum designs for quadratic regression on a ball are second order symmetric ones and can be supported by points of E ; if A denotes the set of support of such a design, then the vector

$$P = \{\xi(A_m), \dots, \xi(A_0)\},$$

where $A_k = A \cap E_k$, may be represented as a linear convex combination of the basic solutions of (3.7).

In particular, all such designs can be supported by points of $E_0 \cup E_1 \cup E_m$ with the Φ_p -optimal weights, respectively, as follows:

$1 - \alpha_s(p)$, $\alpha_s(p)\{1 - r(p)m\}$, $\alpha_s(p)r(p)m$. We can note that for basic D- and E-optimum solutions we have, respectively, that $k \geq (m+2)/3 \geq j$ and $k \geq (m+1)/2 \geq j$; thus basic D- or E-optimum designs exist over points of $E_0 \cup E_k$, where k is equal to $(m+2)/3$ (with $m = 3n+1$, $n = 0, 1, \dots$) or $(m+1)/2$ (with odd m). Moreover, only these designs can be supported by points of one set E_k and the center point.

The D-optimum designs supported by points of $E_0 \cup E_1 \cup E_m$ were constructed in the paper of Farrell et al. (1967), and for $m = 7$ such a design over points of $E_0 \cup E_{(m+2)/3}$ can be constructed with the help of simplex-sum design of Box and Behnken (1960a).

It is interesting to compare the above results with those of Galil and Kiefer (1977a), where the Φ_p -optimum designs from the class of rotatable designs, say $\eta_p^*(R)$, were considered on a ball of arbitrary radius R . Substituting (3.7) for a ball of radius R for

$$(3.8) \quad \lambda_4 + (m-1)\lambda_3 = R^2\lambda_2$$

and denoting by r the ratio $\lambda_3/R^2\lambda_2$, we can prove that Φ_p -optimal $r(p) = 1/\{m+2^{1/(p+1)}\}$ for all R . This fact implies that the structure of the Φ_p -optimal designs over points of E is also the same for all R . (E denotes now the sets of points with the coordinates $\pm R/\sqrt{k}$, $k = 1, 2, \dots, m$); that is that Theorem 2 is valid as well as the remark after it. The only value that changes with R is $\alpha_s(p)$. E.g., we can find $\alpha_s(\infty)$:

$$\alpha_s(\infty) = \begin{cases} \frac{m(m+1)}{(m+1)^2 + R^4} & \text{if } R^2 \leq m+1 \\ \frac{m(R^2-1)}{(m+R^2-1)R^2} & \text{if } R^2 > m+1 . \end{cases}$$

Compared with the corresponding result from the paper of Galil and Kiefer (1976a) it gives us the estimate of the Φ_∞ -efficiency of $\eta_\infty^*(R)$ of order m^{-2} :

$$\text{eff}(\eta_\infty^*(R)/\xi_\infty^*(R)) = \begin{cases} 1-1/m & \text{if } R < m+2 \\ 1 & \text{if } R \geq m+2 . \end{cases}$$

Thus the rotatable designs $\eta_\infty^*(R)$ are nearly E-optimum for all R . For $p < \infty$ we can expect the result of the same order, because the designs $\eta_0^*(R)$ are D-optimum for all R , so a good performance is provided for both the extreme cases $p = 0, \infty$.

We should note also, that the representation of the Φ_p -optimal measures over points of E is not the unique possible way; e.g., the D-optimum designs with $m = 2$ can be supported by the vertices of a regular polygon (with the number of sides more than 4) and the center point, and, for arbitrary m , by any orthogonal transformation of any D-optimum design over points of E . (The latter is not valid for Φ_p -optimal designs with $p > 0$, except the trivial cases of permutation of factors or change of signs of them).

3.5 Remarks on the efficiency behavior.

We shall estimate now the values of $e_0(\infty)$, $g(\infty)$ and $e_\infty(0)$ for large m on a cube or $\Omega_m(k,a)$, thus obtaining some information about the "extreme" cases of $g(p)$ and $e_q(p)$ behavior.

For the D-optimum designs on a cube or $\Omega_m(k,a)$ the minimum eigenvalue is

$$\mu_3 = N^{-1} + O(m^{-3}),$$

thus $e_\infty(0) \rightarrow 0$ as $m \rightarrow \infty$. For simplicity the calculation of $e_0(\infty)$ is given in case of odd m , when ξ_∞^* exists supported by $E_{(m+1)/2} \cup E_0$. The D-efficiency ξ_∞^* relative to the D-optimum design on $\Omega_m\{(m+1)/2, 0\}$ is approximately (to order m^{-2}) the ratio of weights on the set $E_{(m+1)/2}$, that is $4(m+2)/\{5(m+3)\}$. The D-efficiency of the D-optimum design on $\Omega_m\{(m+1)/2, 0\}$ relative to that on a cube is approximately (to order m^{-1}) $(m+1)/\{2(m-2)\}$, thus $e_0(\infty) \rightarrow 0.4$ as $m \rightarrow \infty$. Also we have for ξ_∞^* on a cube that

$$g(\infty) = (m+1)(m+2)(m+5)/\{5(m^3+5m^2+4m+2)\} \rightarrow 0.2$$

as $m \rightarrow \infty$.

These calculations exhibit the difficulties arising in the problem of choice of "uniformly good" design on a cube. One of the possible ways of solving such a problem with respect to the family $\{\Phi_p, 0 \leq p \leq \infty\}$ is the search of the design ξ which maximizes $\min\{e_q(\xi)\}$ over q in a subset $R \subseteq R_+ = [0, \infty) \cup \{\infty\}$; the value of $g(\xi)$ may be also considered.

For $R = R_+$ we can find approximate (to order m^{-1}) values of moments of the solution for $\max_{q \in R_+} \min\{e_q(\xi)\}$; the moments of such $\hat{\xi}$ are as follows:

$\lambda_3 = 25/54$, $\lambda_2 = 7\lambda_3/5$ and $\min\{e_q(\hat{\xi})\} = e_0(\hat{\xi}) = \lambda_3$ ($q \in \mathbb{R}_+$). Though for moderate values of m the results are more favorable, as one can see in sections 4, 5, the use of a compound criterion (Kiefer, 1974) may be more promising; an example is given in section 4.

In case of a ball we can use the approximate solution for λ_2 from section 3.4 to estimate G-, D- and E-efficiencies. Thus, we have that, to order m^{-2} , for p fixed, $0 \leq p < \infty$, $e_\infty(p) = (2/m)^{1/(p+1)} \rightarrow 0$ as $m \rightarrow \infty$ (and $e_\infty(p) \rightarrow 1$ with m fixed and $p \rightarrow \infty$; this is quite natural because $\xi_\infty^* = \lim \xi_p^*$ as $p \rightarrow \infty$). In the same manner we find that, for p fixed, $0 < p \leq \infty$, $e_0(p) = 1 - c(p)/m \rightarrow 1$ as $m \rightarrow \infty$, where $c(p)$ depends on p .

For $g(p)$ the result is less favorable: $g(p) = 2^{1/(p+1)-1}$ (to order m^{-1}); thus $g(p) \downarrow 1/2$ as $p \rightarrow \infty$. This result could be considered as somewhat strange because $e_0(p) \rightarrow 1$, but in the general case, with the help of estimations for $\det M(\xi)/\det M(\xi_0^*)$ (Kiefer, 1961; Fedorov, 1972, section 2.6) we can prove that

$$(3.9) \quad e_0^N \leq g \leq \{\ln(e/e_0)\}^{-1},$$

where $e_0 = \{\det M(\xi)/\det M(\xi_0^*)\}^{1/N}$ and $g = N/\bar{d}(\xi)$, so the convergence of e_0 to one with departure of order, say $m^{-2-\beta}$ with $\beta > 0$, would be sufficient for the convergence of g to one.

The estimations above show that for the ball the efficiency behavior is much better than for the cube and we can expect that with m fixed the performance of ξ_p^* improves with p increasing and that with large p , or $p = \infty$, the Φ_p -optimum designs on the ball would be fairly efficient,

or even robust, with respect to family $\{\Phi_p, 0 \leq p \leq \infty\}$; thus the problem of choice of "good" design would not cause any difficulty.

4. Numerical Results.

The qualitative study of the behavior of structure of Φ_p -optimal designs was presented in section 3, so we shall underline here some main conclusions.

The common features of the study on the m -simplex (Kiefer, 1975) and in other cases are the changes in structure of the designs with p increasing, although in the case of the cube the value of $k_m(p)$ decreases, increasing for the case of the m -simplex, and we have the regularity of behavior of optimal weights for p fixed and m increasing. Some results can be obtained algebraically for $p = 0, \infty$; e.g., the weight of E_k for the D-optimum designs on a cube with support on $E_k \cup E_{m-1} \cup E_m$ is equal to

$$[m(m-1)/\{(m-k)(m-k-1)\}][4/\{(m+2)(2m+3)\} + O(m^{-4})],$$

the weight of E_0 for the D-optimum designs of $\Omega_m(k, a)$ with $k+a \leq m-1+a_m$ is N^{-1} , and for the E-optimum designs with support on $E_{(m+1)/2} \cup E_0$ (with odd m) $\xi_\infty^*(E_0) = (m+5)/\{5(m+1)\}$.

As an example of structure behavior the optimal weights $\alpha_k = \xi_p^*(E_k)$ for the cube were listed in Table 2 by Galil and Kiefer (1977b).

Of interest for us is the computation of such values $p_{\text{crit}}(m, k)$ that for $p \geq p_{\text{crit}}(m, k)$ Φ_p -optimum designs on $\Omega_m(k, a)$ are also

Φ_p -optimum on a cube, or on the other hand, for $p < p_{crit}(m,k)$
 Φ_p -optimum designs on $\Omega_m(k,a)$ are unique. The values of $k_m(p)$
 can be found now from the conditions $p_{crit}\{m, k_m(p)\} \leq p < p_{crit}\{m, k_m(p)-1\}$.
 The values of $p_{crit}(m,k)$ for $3 \leq m \leq 8$ are given in Table 2.

Table 2. The values of $P_{crit}(m,k)$.

		m					
		3	4	5	6	7	8
k	m-1	∞	1.7	0.89	0.46	0.38	0.29
	m-2		∞	∞	6.0	2.4	1.8
	m-3				∞	∞	7.0
	m-4						∞

As a typical illustration of the efficiency behavior in our problem on a cube the matrix of $e_q(p)$ and $g(p)$ efficiencies is presented in Table 3.

Table 3. The matrix of efficiencies (%) for cube when $m=5$.

P	g(p)	e_0	$e_{0.1}$	$e_{0.5}$	e_1	e_2	e_{10}	e_∞
0	100	100	99.6	91	73	48	25	19
0.1	95	99.6	100	95	81	57	26	24
0.5	81	95	97	100	96	82	45	41
1	69	88	91	97	100	95	61	56
2	57	79	81	90	96	100	77	72
10	45	68	70	79	87	95	100	88
∞	31	52	54	61	68	76	89	100

The numerical solution of the equation for s : $e(s) = \min_q \{e_q(s)\} = \max_p \min_q \{e_q(p)\}$ ($p, q \in R_+$) gives us for $m = 4, 5, 6, 7$ the values of s and $e(s)$ respectively as follows: 2.06, 2.25, 2.45, 2.54 and 0.80, 0.77, 0.73, 0.71.

Thus the performance of ξ_s^* is probably the best of what we can obtain on a cube with respect to family $\{\Phi_p, 0 \leq p \leq \infty\}$ if no particular reasons for the choice of criterion are given and we restrict considerations to designs of the form ξ_p^* .

If the value of $g(p)$ must be taken into account, then $e(s)$ coincides with $e_\infty(s)$ and, e.g., with $m = 5$, we have that $s = 1.4$ and $e(s) = 0.64$.

We can compare the results for the cube with the results for the region $\Omega_5(3,0)$, for which all Φ_p -optimum designs are unique with the support on $E_3 \cup E_0$. In Table 4 the optimal weights of the center point are given, and in Table 5 are the efficiencies with respect to both $\Omega_5(3,0)$ and cube.

Table 4. The optimal weights α_0 of the center point on $\Omega_5(3,0)$.

P	0	0.1	0.5	1	2	5	10	∞
α_0	1/21	.059	.102	.143	.196	.259	.291	1/3

Table 5. Some efficiencies (%) of Φ_p -optimal designs on $\Omega_5(3,0)$.

P	g(p)	$e_0(p)$	$e_1(p)$	$e_2(p)$	$e_\infty(p)$
0	100,38	100,66	83,56	51,43	15,15
1	81,38	95,63	100,79	96,81	45,45
2	75,36	91,61	98,77	100,84	61,61
10	61,33	82,55	90,71	94,79	88,88
∞	57,31	78,52	86,68	90,76	100,100

The left-hand number is the efficiency for $\Omega_5(3,0)$ and the right-hand number is the efficiency of the same design for the cube.

Such comparison exhibits the fact that the Φ_p -optimum designs on $\Omega_5(3,0)$ are relatively constant in their efficiency $e_q(p)$ firstly with small q and secondly with large p . Also of interest is the fact that the efficiencies of these designs for the cube are less variable than for $\Omega_m(k,0)$.

All the Φ_p -optimum designs on $\Omega_m(k,0)$ with k/m "far" from one are fairly efficient with respect to any compound criterion based on a convex average of Φ_p -optimality criteria. For example in the case $\Omega_5(3,0)$ all ξ_p^* with $p \geq 2$ have efficiency more than 0.99 relative to the Φ -criterion, defined as follows: $\Phi(\xi) = \{\Phi_0(\xi) + \Phi_1(\xi) + \Phi_\infty(\xi)\}/3$, and the minimum of Φ -efficiency is equal to 0.85 with $p = 0$. Thus an integer design can be chosen with 80 trials at points of E_3 and with such a number of trials at the center point that both the exact Φ_p -optimality for some p and "average goodness" are provided.

These results can be obtained algebraically because all the ϕ_p -optimum designs on $\Omega_m(k,0)$ with $k \leq (m+1)/2$ have the same simple structure; in general, the performance of the designs on $\Omega_m(k,0)$ improves as k decreases, or as the region "approaches" the m -simplex.

As it was expected, the ball exhibits much more regularity. The values of optimal weights α_0, α_1 and α_m were computed as well as the efficiencies for some values of p . With m fixed α_0 is monotonically increasing from $2/\{(m+1)(m+2)\}$ (at $p = 0$) to $(m+2)/(m^2+2m+2)$ (at $p = \infty$) and α_1 decreases from $2m(m+3)/\{(m+1)(m+2)^2\}$ (at $p = 0$) to $m/(m^2+2m+2)$ (at $p = \infty$). The value of α_m increases from $m^2(m+3)/\{(m+1)(m+2)^2\}$ (at $p = 0$) to some maximum (near $p = 1$) and then decreases to $m^2/(m^2+2m+2)$ (at $p = \infty$); the behavior of α_k 's with respect to m is also strongly regular.

The designs ξ_∞^* appeared to be remarkably robust in their efficiency; the value of $e_q(\infty)$ monotonically increases with q from $e_0(\infty)$ to 1, and it was shown in section 3.5 that $e_0(\infty) \rightarrow 1$ as $m \rightarrow \infty$; $e_0(\infty)$ is already equal to 0.871 at $m = 3$.

The characteristics of the designs ξ_p^* are given in Table 6 for the ball of dimension 5.

Table 6. The Characteristics of ϕ_p -optimum Designs on a Ball when $m = 5$.

P	Optimal weights			% efficiencies						
	α_0	α_1	α_m	$g(p)$	$e_0(p)$	$e_{0.5}(p)$	$e_1(p)$	$e_2(p)$	$e_5(p)$	$e_\infty(p)$
0	1/21	40/147	100/147	100	100	97.6	92.0	77.0	47.5	28.4
0.1	0.05594	0.25776	0.68630	96.0	99.9	98.7	94.7	83.2	55.2	33.1
0.5	.08278	.22103	.69619	85.2	98.7	100	99.2	95.0	77.3	48.0
1	.10442	.19746	.69812	77.9	97.2	99.5	100	98.9	90.0	59.5
2	.12786	.17553	.69661	70.8	95.1	98.0	99.3	100	97.6	71.5
5	.15456	.15498	.69037	63.8	92.5	95.6	97.3	99.0	100	84.4
∞	7/37	5/37	25/37	56.8	89.0	92.0	93.8	95.7	97.7	100

5. Integer Designs

Some of the results of sections 3 and 4 may be implemented for the construction of integer designs. On a cube for any p nearly Φ_p -optimum designs can be found approximating the moments λ_2, λ_3 of ξ_p^* ; e.g., we have with $m = 5$ nearly A-optimum design with 32 trials at points of E_5 and 40 trials at points of E_2 , its A-efficiency being equal to 0.996 and the other efficiencies being close to those of ξ_1^* . In the same way exact integer E-optimum designs can be constructed for any m ; e.g., with $m = 5$ such a design has 80 trials at points of E_3 and 40 trials at the center point; with $m = 7$ a design approximating ξ_∞^* of the same structure has 112 trials at points of a minimal second order symmetric set I_4 (such sets were defined in the paper of Pesotchinsky, 1975) and 48 trials at the center point. The set I_4 consists of seven subsets $E_4 \cap \{x \mid |x_{i_k}| = 1, 1 \leq k \leq 4\} = E_4(i_1, i_2, i_3, i_4)$; each of them is 2^4 -factorial, with the following groups of indices: 1,2,3,4; 1,4,5,6; 1,6,7,3; 2,4,6,7; 2,5,7,1; 3,4,7,5; and 3,5,6,2. The digits in groups are written in such a way that the first three of them correspond to the subsets $E_3(i_1, i_2, i_3)$ of the set I_3 with 56 points, used by Box and Behnken (1960b) for their three-level design.

The E-optimum designs over points of $E_0 \cup E_{(m+1)/2}$ on a ball have the same structure as on a cube.

For the search of designs on a cube, both practicable and "good" with respect to the family of G- and Φ_p -optimality criteria, we used the following procedure.

For each m by the study of known symmetric integer designs (Atkinson, 1974; Box and Behnken, 1960a,b; Nalimov, Golikova and Mikeskina, 1970;

Pesotchinsky, 1975) the "basic" sets were selected and the addition of some (sometimes duplicated) sets with a small number of points, such as E_0, E_1 , was considered. With $m = 4, 5, 6$ the basic sets were E_m, E_{m-1} and $I_{m,m-1}$ and the supplemented sets were E_0 and E_1 ; thus we started with the star point designs (Atkinson, 1973; Nalimov et al., 1970) and DP, DB designs (Pesotchinsky, 1975).

For $m = 4$ the best were the star point designs with the set E_1 duplicated two or three times, and for $m = 5, 6$ the best were the designs with the basic sets $I_{m,m-1}$ and the supplemented sets E_1 and E_0 .

For the integer construction on a ball we can note that the values of α_s (the measure of the sphere) and $r = \lambda_3/\lambda_2$ are "independent"; thus we can have $\lambda_2 = \alpha_s/m$ close to the E-optimum value, and r close to the D-optimum one, providing both the E- and D- goodness of the design (and, consequently, Φ_p -goodness for any p). This reasoning can be supported by theoretical arguments, because $\Phi_0(\xi)$ depends mainly on r , and $\Phi_\infty(\xi)$ on λ_2 . Thus we considered the star point designs for $4 \leq m \leq 6$ and the designs over points of $E_0 \cup E_{(m+2)/3}$ for $m = 4, 7$.

The characteristics of integer designs on a cube and on a ball are listed in Table 7. (I_m for a ball denotes a half-replica of the 2^m factorial with levels $\pm 1/\sqrt{m}$ and I_3 the minimal second order symmetric subset of E_3 ($m=7$), constructed by Box and Behnken (1960a)).

It is interesting to note that the minimum of Φ_p - and G-efficiencies of optimal designs ξ_s^* from section 4 is less than that of integer designs constructed above, but the latter are not Φ_p -optimum for any p . Also we may note that the variation of an additional set or number of duplications

Table 7. Characteristics of Integer Designs on a Cube and on a Ball.

Dimension	Structure of the Design	Number of Trials	% efficiencies				
			e_0	e_1	e_2	e_∞	
<u>Cube</u>							
4	$\left\{ \begin{array}{l} E_4 \cup \{E_1 \times 2\} \\ E_4 \cup \{E_1 \times 3\} \end{array} \right\}$	32 40	74 61	91 94	84 95	63 78	
5	$\left\{ \begin{array}{l} I_{5,5-1} \cup E_1 \cup \{E_0 \times 7\} \\ I_{5,5-1} \cup \{E_0 \times 12\} \end{array} \right\}$	65 60	69 74	98 95	94 86	76 67	
6	$I_{6,6-1} \cup E_1 \cup \{E_0 \times 4\}$	80	80	95	82	63	
<u>Ball</u>							
4	$\left\{ \begin{array}{l} E_4 \cup E_1 \cup \{E_0 \times 6\} \\ E_2 \cup \{E_0 \times 6\} \end{array} \right\}$	30 30	86 86	96 96	95 95	87 87	
5	$\left\{ \begin{array}{l} I_5 \cup E_1 \cup \{E_0 \times 4\} \\ E_5 \cup E_1 \cup \{E_0 \times 8\} \end{array} \right\}$	30 50	78 88	87 96	82 95	74 87	
6	$I_6 \cup E_1 \cup \{E_0 \times 7\}$	51	87	95	92	87	
7	$I_3 \cup \{E_0 \times 8\}$	64	90	96	95	90	

enables one to construct integer designs with improved characteristics for a particular subset of a family of criteria.

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Designs for quadratic regression on a cube, cube with truncated vertices and on a ball are studied in terms of a family of criteria, introduced by Kiefer (1974, 1975), that includes those of A-, D- and E-optimality. Both theoretical and numerical results on structure and performance are presented. In particular, D- and E-optimum designs are described and a procedure of construction of nearly robust under variation of criterion integer designs is suggested. Some examples are given for the dimensions 4, 5 and 6.