

Optimal Designs On Tchebycheff Points*

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§0. Summary. Kiefer and Wolfowitz (1959) proved that the optimal design for estimating the highest coefficient in polynomial regression is supported by certain Tchebycheff points. Hoel and Levine (1964) showed that the optimal designs for extrapolation in polynomial regression were all supported by the Tchebycheff points. These results were extended by Kiefer and Wolfowitz (1965) to cover nonpolynomial regression problems involving Tchebycheff systems and the large class of designs supported by the Tchebycheff points was characterized. In the present paper it is shown that the optimal design for estimating any specific parameter is supported by one of two sets of Tchebycheff points. Different proofs of the Kiefer-Wolfowitz results are also presented.

§1. Introduction. Let $f = (f_0, f_1, \dots, f_n)$ denote $n + 1$ linearly independent continuous functions on a compact set \mathcal{X} . For each $x \in \mathcal{X}$ an experiment can be performed. The outcome is a random variable $y(x)$ with mean value $\sum_{i=0}^n \theta_i f_i(x)$ and a common variance σ^2 . The functions f_0, f_1, \dots, f_n , called the regression functions, are assumed known while $\theta_0, \theta_1, \dots, \theta_n$ and σ^2 are unknown. An experimental design is a probability measure ξ on \mathcal{X} . The problem concerned with here is that of estimating

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a linear form $(c, \theta) = \sum_{i=0}^n c_i \theta_i$. It will always be assumed that $\sum_{i=0}^n c_i^2 > 0$.

For a given design ξ let $m_{ij} = m_{ij}(\xi) = \int f_i f_j d\xi$ and $M(\xi) = ||m_{ij}(\xi)||_{i,j=0}^n$.

A linear form (c, θ) is called estimable with respect to ξ if c is contained in the range of the matrix $M(\xi)$. If c is estimable with respect to ξ let

$$V(c, \xi) = \sup \frac{(c, d)^2}{(d, M(\xi)d)}$$

where the sup is taken over the set of vectors d such that the denominator is nonzero. If c is not estimable with respect to ξ we define $V(c, \xi) = \infty$.

Suppose ξ concentrates mass ξ_i at the points $x_i, i=1, 2, \dots, r$ and $\xi_i N = n_i$ are integers. If N uncorrelated observations are made, taking $N\xi_i$ observations at x_i , then the variance of the best linear unbiased estimate of (c, θ) is given by $\sigma^2 N^{-1} V(c, \xi)$. An arbitrary measure or design ξ is called c-optimal if ξ minimizes $V(c, \xi)$. For a more complete discussion of the above model see Kiefer (1959) or Karlin and Studden (1966b).

We assume throughout that $X = [-1, 1]$. Hoel and Levine showed that if $f_i(x) = x^i, i = 0, 1, \dots, n$ and $c = f(x_0)$ with $|x_0| > 1$ then the c-optimal design is supported on the Tchebycheff points $s_v = \cos \frac{v\pi}{n}, v = 0, 1, \dots, n$. These are the points where $|T_n(x)| = 1, T_n(x)$ being the nth Tchebycheff polynomial of the 1st kind.

Kiefer and Wolfowitz consider more general systems of regression of functions and a related set of Tchebycheff points. Let T^* denote the set of all c such that a c-optimal design is supported on the entire set of Tchebycheff points. The set T^* is divided into 2 different sets R^* and $S^* = T^* - R^*$ which they explicitly characterize. Moreover they show that

the set R^* includes the set A^* of all vectors c for which (c, θ) is not estimable for any design on fewer than $n+1$ points. The set A^* may be characterized by stipulating that $c \in A^*$ if and only if the determinants

$$(1.1) \quad \begin{vmatrix} f_0(x_1) & \dots & f_0(x_n) & c_0 \\ f_1(x_1) & & f_1(x_n) & c_1 \\ \cdot & & & \\ \cdot & & & \\ f_n(x_1) & & f_n(x_n) & c_n \end{vmatrix}$$

do not vanish whenever the x_i are all distinct.

In Sections 2 and 3 we offer different proofs of the Kiefer-Wolfowitz results and more emphasis is placed on the fact that their sets S^* and R^* can be characterized in a manner similar to the determinant characterization of A^* . More explicitly the set R^* is precisely the set of c for which the determinants (1.1) are of one strict sign for x_1, x_2, \dots, x_n an order subset of the Tchebycheff points $s_0 < s_1 < \dots < s_n$ and S^* consists of those vectors c for which the determinants (1.1) alternate in sign as we progressively omit successive s_i . The proofs offered here rely heavily on the elegant result of Elfving which is stated in Theorem 2.1. A close inspection of the analysis used by Kiefer and Wolfowitz and the analysis used here shows certain similarities, however much of the preliminary discussion and game theory has been eliminated using the Elfving result.

In Section 4 it is shown that the vectors $c_p = (0, \dots, 0, 1, 0, \dots, 0)$ (a one only in the $p+1$ st component) are in R^* if $n-p$ is even while if $n-p$ is odd the c_p -optimal design is supported on the Tchebycheff points

of one lower order. The case $p = n$ was originally proven in Kiefer and Wolfowitz (1959). The above shows that in the case of ordinary polynomial regression the optimum design for estimating θ_p is supported by the set $s_v = -\cos \frac{v\pi}{n}$, $v = 0, 1, \dots, n$, when $n-p$ is even and by the set $t_v = -\cos \frac{v\pi}{n-1}$, $v = 0, 1, \dots, n-1$, when $n-p$ is odd.

Section 5 contains some additional remarks which show that certain linear combinations of the vector c_p are also supported by the Tchebycheff points while Section 6 contains a simple counterexample which shows the minimax design is not necessarily supported by the minimal number of $n+1$ points when f_0, f_1, \dots, f_n form a Tchebycheff system.

§2. Designs Supported by Tchebycheff Points. The following result due to Elfving (1952) characterizes the c-optimal designs ξ and will be frequently employed throughout the paper.

Theorem 2.1. Let $R_+ = \{f(x) = (f_0(x), \dots, f_n(x)) \mid x \in X\}$, $R_- = \{-f(x) \mid x \in X\}$ and $R =$ the convex hull of $R_+ \cup R_-$. A design ξ_0 is c-optimum if and only if there exists a measurable function $\varphi(x)$ satisfying $|\varphi(x)| \equiv 1$ such that (i) $\int \varphi(x) f(x) \xi(dx) = \beta c$ for some β and (ii) βc is a boundary point of R . Moreover βc lies on the boundary of R if and only if $\beta^2 = v_0^{-1}$ where $v_0 = \min_{\xi} V(c, \xi)$.

Every vector $c \in R$ can be put in the form

$$(2.1) \quad c = \sum_{v=1}^k \epsilon_v p_v f(x_v)$$

where $\epsilon_v = \pm 1$, $p_v > 0$ and $\sum_1^k p_v = 1$. The integer k may always be taken

to be at most $n+2$ and at most $n+1$ if c is a boundary point of R .

The following simple lemma will be needed.

Lemma 2.1. A vector c of the form (2.1) lies on the boundary of \mathcal{R} if and only if there exists a nontrivial 'polynomial' $u(x) = \sum_{\nu} a_{\nu} f_{\nu}(x)$ such

that $|u(x)| \leq 1$ for $x \in [-1,1]$, $\epsilon_{\nu} u(x_{\nu}) = 1$, $\nu = 1, 2, \dots, k$, and $\sum_{\nu} a_{\nu} c_{\nu} = 1$.

Proof. If the required polynomial exists and $a = (a_0, a_1, \dots, a_n)$ then $(a, c) = \sum_{\nu} \epsilon_{\nu} p_{\nu} (a, f(x)) = \sum_{\nu} p_{\nu} \epsilon_{\nu} u(x_{\nu}) = 1$ and $(a, y) \leq 1$ for all $y \in \mathcal{R}$. The vector a defines a supporting plane to \mathcal{R} at c so that c is a boundary point of \mathcal{R} .

If c is a boundary point of \mathcal{R} then a supporting plane exists, i.e. there exists a vector $a \neq 0$ such that $(a, c) = 1$ and $(a, y) \leq 1$ for all $y \in \mathcal{R}$. (Note that the origin is in the interior of \mathcal{R} .) Therefore $1 = (a, c) = \sum_{\nu=1}^k p_{\nu} \epsilon_{\nu} (a, f(x_{\nu}))$ and $|(a, f(x))| = |u(x)| \leq 1$ for all $x \in [-1,1]$.

In this case $\epsilon_{\nu} (a, f(x_{\nu})) = 1$ for $\nu = 1, \dots, k$ since we have assumed $p_{\nu} > 0$.

Remark 2.1. For an arbitrary vector $c \neq (0, \dots, 0)$, βc lies on the boundary of \mathcal{R} for some $\beta > 0$ and hence $\beta c = \sum_{\nu=1}^{n+1} \epsilon_{\nu} p_{\nu} f(x_{\nu})$ for some $\{\epsilon_{\nu} p_{\nu}\}$

and $\{x_{\nu}\}$. If $(a, f) = \sum_{i=0}^n a_i f_i$ denotes the polynomial of Lemma 2.1 then

the minimal value of $V(c, \xi)$ is $\beta^{-2} = \left(\sum_0^n a_i c_i \right)^2 = (a, c)^2$ since

$(\beta c, a) = 1$. Moreover

$$\begin{aligned} \inf_{\xi} V(c, \xi) &= \inf_{\xi} \sup_b \frac{(c, b)^2}{\int (b, f(x))^2 \xi(dx)} \\ &\geq \sup_b \inf_{\xi} \frac{(c, b)^2}{\int (b, f(x))^2 \xi(dx)} \\ &\geq (c, a)^2. \end{aligned}$$

Since the first and last terms are equal

$$\inf_{\xi} \sup_b \frac{(c,b)^2}{\int (b, f(x))^2 \xi(dx)} = \sup_b \inf_{\xi} \frac{(c,b)^2}{\int (b, f(x))^2 \xi(dx)} .$$

We shall assume throughout the paper that the set of functions f_0, f_1, \dots, f_n form a Tchebycheff system or a T-system on $[-1, 1]$ and that $U(x) = \sum_i a_i f_i(x) \equiv 1$ for some set $\{a_i\}_0^n$. A T-system f_0, f_1, \dots, f_n is such that every linear combination $\sum_i a_i f_i(x)$ ($\sum_i a_i^2 > 0$) has at most n distinct zeros on $[-1, 1]$ or equivalently the determinants

$$(2.2) \quad F \begin{matrix} 0, 1, \dots, n \\ x_0, x_1, \dots, x_n \end{matrix} = \begin{vmatrix} f_0(x_0) & f_0(x_1) & \dots & f_0(x_n) \\ f_1(x_0) & f_1(x_1) & \dots & f_1(x_n) \\ \vdots & \vdots & & \vdots \\ \vdots & \vdots & & \vdots \\ f_n(x_0) & f_n(x_1) & \dots & f_n(x_n) \end{vmatrix}$$

are of one strict sign provided $-1 \leq x_0 < x_1 < \dots < x_n \leq 1$. For definiteness we shall assume that the determinants are positive. We shall call any linear combination $\sum_{i=0}^n a_i f_i(x)$ a polynomial. The classical example of a T-system consists of the ordinary powers $f_i(x) = x^i$, $i = 0, 1, \dots, n$. In this case the determinant (2.2) reduces to the classical Vandermonde determinant. A simple constructive method of generating more general T-systems will be given in Section 4.

The following important property of T-systems will be used (see Karlin and Studden (1966a), Theorem II. 10.1). If $\{f_i\}_0^n$ is a T-system on $[-1, 1]$ then there exists a unique polynomial $W(x) = \sum_{i=0}^n a_i^* f_i(x)$ satisfying the properties

$$(i) \quad |W(x)| \leq 1$$

(ii) there exists $n+1$ points $-1 \leq s_0 < s_1 < \dots < s_n \leq 1$ such that $W(s_i) = (-1)^{n-i}$, $i = 0, 1, \dots, n$. Moreover when $U(x) \equiv 1$ is a polynomial equality occurs in (i) only for $x = s_0, s_1, \dots, s_n$ and $s_0 = -1$ and $s_n = +1$.

For any vector $c = (c_0, \dots, c_n)$ considerable use will be made of the determinants

$$(2.3) \quad D_v(c) = \begin{vmatrix} f_0(s_0) & \dots & f_0(s_{v-1}) & f_0(s_{v+1}) & \dots & f_0(s_n) & c_0 \\ f_1(s_0) & \dots & f_1(s_{v-1}) & f_1(s_{v+1}) & \dots & f_1(s_n) & c_1 \\ \vdots & & \vdots & & & \vdots & \\ f_n(s_0) & \dots & f_n(s_{v-1}) & f_n(s_{v+1}) & \dots & f_n(s_n) & c_n \end{vmatrix}$$

The sign of $D_v(c)$ will be denoted by $d_v(c)$; if $D_v(c) = 0$ the sign may be defined as -1 or $+1$. We further let $L_v(x) = \sum_i a_{vi} f_i(x)$ denote the Lagrange interpolation polynomial defined by requiring that $L_v(s_j) = \delta_{vj}$, $v, j = 0, 1, \dots, n$. In terms of the determinants (2.2) $L_v(x)$ has the more explicit form

$$L_v(x) = \frac{F \left(\begin{matrix} 0, \dots, v-1, v, v+1, \dots, n \\ s_0, \dots, s_{v-1}, x, s_{v+1}, \dots, s_n \end{matrix} \right)}{F \left(\begin{matrix} 0, \dots, n \\ s_0, \dots, s_n \end{matrix} \right)}.$$

For any vector c and any polynomial $u(x) = \sum_i a_i f_i(x)$ we shall use the notation $u(c) = \sum_i a_i c_i$. In this case we have

$$(-1)^{n-v} D_v(c) = L_v(c) F \left(\begin{matrix} 0, \dots, n \\ s_0, \dots, s_n \end{matrix} \right).$$

Now for any polynomial $u(x)$ we have

$$u(x) = \sum_{v=0}^n u(s_v) L_v(x).$$

Since the coefficients of f_i on either side are equal we find that

$$u(c) = \sum_{v=0}^n u(s_v) L_v(c).$$

Letting $u(x)$ be successively the polynomials f_0, f_1, \dots, f_n we find that

$$\begin{aligned} c &= \sum_{v=0}^n f(s_v) L_v(c) \\ &= \sum_{v=0}^n (-1)^{n-v} d_v(c) |L_v(c)| f(s_v). \end{aligned}$$

Therefore

$$(2.4) \quad \beta c = \sum_{v=0}^n (-1)^{n-v} d_v(c) p_v f(s_v)$$

where

$$p_v = \frac{|L_v(c)|}{\sum_{j=0}^n |L_j(c)|} = \frac{|D_v(c)|}{\sum_{j=0}^n |D_j(c)|} \quad v = 0, 1, \dots, n$$

and

$$\beta = \left(\sum_{j=0}^n |L_j(c)| \right)^{-1} = F(s_0, \dots, s_n) \left(\sum_{j=0}^n |D_j(c)| \right)^{-1}.$$

Let R denote the class of vectors c such that $\epsilon D_\nu(c) \geq 0$ for $\nu = 0, 1, \dots, n$ where ϵ is fixed to be $+1$ or -1 for a given c (i.e. the $D_\nu(c)$ $\nu = 0, 1, \dots, n$ all have the same sign in a weak sense) and let S denote those c for which $\epsilon(-1)^\nu D_\nu(c) \leq 0$, $\nu = 0, 1, \dots, n$. The following theorem is a slight generalization of Theorem 3.1 of Karlin and Studden (1966) and Theorem 3 of Kiefer and Wolfowitz (1965).

Theorem 2.2. Suppose that $\{f_i\}_0^n$ is a T-system such that $U(x) \equiv 1$ is a polynomial.

(a) For any design ξ

$$(2.5) \quad d(c, \xi) \geq \begin{cases} [W(c)]^2 & c \in R \\ [U(c)]^2 & c \in S \end{cases}$$

where $W(x)$ is the oscillatory polynomial defined above.

(b) Equality occurs in (2.5) for $\xi = \xi_0$ concentrating mass

$$p_\nu = \frac{|L_\nu(c)|}{\sum_{\nu=0}^n |L_\nu(c)|} = \frac{|D_\nu(c)|}{\sum_{\nu=0}^n |D_\nu(c)|}$$

at the points s_ν , $\nu = 0, 1, \dots, n$.

(c) The design ξ_0 is the only design supported on $s_0 < \dots < s_n$ attaining equality in (2.5). If $c \in R$ then ξ_0 is the only design attaining equality in (2.5).

Proof. (a) For $c \in R \cup S$ the quantity βc in (2.4) is a boundary point of R . Moreover for $c \in R$, $\beta W(c) = 1$ so that the minimum value of

$V(c, \xi)$ is $\beta^{-2} = [W(c)]^2$. Similarly $[U(c)]^2$ is the minimal value of $V(c, \xi)$ for $c \in S$.

(b) The design ξ_0 is c -optimal in each case by Lemma 2.1 and the properties of U and W .

(c) For $c \in S$ and any c -optimal design supported on s_0, s_1, \dots, s_n , equation (2.4) holds for some set $(-1)^{n-v} d_v(c) p_v$, $v = 0, 1, \dots, n$, where $\beta^{-2} = (U(c))^2$. However this set of linear equations has a unique solution since $F\left(\begin{smallmatrix} 0, \dots, n \\ s_0, \dots, s_n \end{smallmatrix}\right) \neq 0$. For $c \in R$ we have

$$\begin{aligned} V(c, \xi) &= \sup_d \frac{(c, d)^2}{(d, M(\xi)d)} \\ &\geq \frac{(W(c))^2}{\int (W(x))^2 d\xi} \\ &\geq (W(c))^2. \end{aligned}$$

The last inequality is strict unless ξ is supported on s_0, s_1, \dots, s_n since $|W(x)| < 1$ for $x \neq s_0, s_1, \dots, s_n$. The last sentence in (c) now follows since the c -optimum design supported by s_0, s_1, \dots, s_n is again unique.

Remark 2.1. As observed by Kiefer and Wolfowitz the above theorem is a consequence of the fact that the convex hulls A and B of the two sets $\{f(s_v)\}_0^n$ and $\{(-1)^{n-v} f(s_v)\}_0^n$ both lie in boundary faces of the set \mathcal{R} defined by Theorem 2.1. It is easily seen that the B is the entire face since $|W(x)| = 1$ only for $x = s_0, s_1, \dots, s_n$, i.e. the intersection of \mathcal{R} and the hyperplane defined by $W(c) = 1$ is precisely B . The union of B and its symmetric image is the set R .

The set A is properly contained in the face of \mathcal{R} determined by $U(c) = 1$. The complete face in this case is the convex hull of the whole curve $\{f(x) | x \in [-1, 1]\}$, so that with the assumption that $W(x) \equiv 1$ is a polynomial every vector $c = \sum_{\nu} p_{\nu} f(x_{\nu})$ is a boundary point of \mathcal{R} . The usefulness of S will be apparent in the next section.

§3. The Kiefer-Wolfowitz Theorems. Kiefer and Wolfowitz (1965) define five sets of vectors T^*, R^*, S^*, A^*, H^* . The first set T^* consists of those c such that a c -optimal design exists on the full set of Tchebycheff points s_0, s_1, \dots, s_n . The next two sets R^* and S^* consist of those c which for some $\beta \neq 0$ are of the form

$$\beta c = \sum_{\nu=0}^n \epsilon_{\nu} p_{\nu} f(s_{\nu}) \quad p_{\nu} > 0, \quad \sum_0^n p_{\nu} = 1$$

where the ϵ_{ν} alternate in sign for $c \in R^*$ while the ϵ_{ν} are the same sign for the vectors in S^* . The set A^* consists of those c for which

$$(3.1) \quad \begin{vmatrix} f_0(x_1) & \dots & f_0(x_n) & c_0 \\ f_1(x_1) & \dots & f_1(x_n) & c_1 \\ \vdots & & & \\ f_n(x_1) & \dots & f_n(x_n) & c_n \end{vmatrix} \neq 0.$$

provided the x_i are distinct and lie in $[-1, 1]$. The set A^* is shown to consist of those c such that (c, θ) is only estimable for designs supported by at least $n+1$ points. Finally to define H^* it is assumed that the regression functions f_0, f_1, \dots, f_n are defined on some interval containing $[-1, 1]$ and $c \in H^*$ if and only if $c = \beta f(x_0)$ for some $|x_0| > 1$ and $\beta \neq 0$.

With suitable further assumptions (see below) on f_0, f_1, \dots, f_n it is shown that:

- (i) R^* contains a neighborhood of $c = (0, \dots, 0, 1)$
- (ii) $H^* \subset A^* \subset R^*$
- (iii) The vectors $c \in R^*$ have unique optimal designs while the vectors $c \in S^*$ have unique designs among those supported by s_0, \dots, s_n .
- (iv) R^* and S^* are disjoint and $R^* \cup S^* = T^*$

In Section 2 we have formulated our sets R and S entirely in terms of the determinants (2.3) or (3.1) using only the points s_0, s_1, \dots, s_n . If we define R_0 and S_0 as the subsets of R and S respectively such that the determinants $D_v(c) \neq 0, v = 0, 1, \dots, n$ then it can readily be seen that $R_0 = R^*$ and $S_0 = S^*$. Moreover the sets R_0 and S_0 are simply the interiors of the sets R and S respectively. The majority of the results (i)-(iv) above follow from Theorem 2.2.

- (i) To prove (i) it suffices to assume that the determinants

$$(3.2) \quad \begin{vmatrix} f_0(s_0) & \dots & f_0(s_{v-1}) & f_0(s_{v+1}) & \dots & f_0(s_n) \\ \vdots & & \vdots & & & \vdots \\ f_{n-1}(s_0) & \dots & f_{n-1}(s_{v-1}) & f_{n-1}(s_{v+1}) & \dots & f_{n-1}(s_n) \end{vmatrix}$$

for $v = 0, 1, \dots, n$ are all nonzero and of the same sign. This will be true whenever the functions f_0, f_1, \dots, f_{n-1} form a T-system on $[-1, 1]$.

- (ii) That $A^* \subset R^*$ is clear while $H^* \subset A^*$ provided f_0, f_1, \dots, f_n is a T-system on $(-\infty, \infty)$. In fact $c = \beta f(x_0) \in A^*$ for fixed $x_0 \notin [-1, 1]$ provided f_0, f_1, \dots, f_n is a T-system on $[-1, 1] \cup \{x_0\}$.

- (iii) This follows directly from Theorem 2.2.

(iv) That R^* and S^* are disjoint and both are contained in T^* is immediate once we note their identification with R_0 and S_0 . For completeness we will now prove that $R^* \cup S^* = T^*$ (or $R^* \cup S^* \supset T^*$) with the

aid of Assumption 2 in Kiefer and Wolfowitz (1965). Assumption 2 states that every polynomial $\sum_{i=0}^n a_i f_i(x)$ either has less than or equal to $n-1$ changes of direction on $(-1,1)$ or else is constant on $(-1,1)$. (A function $u(x)$ changes direction at $y \in (-1,1)$ if $u(x)$ has a local maximum or minimum at y . In particular if $u(x)$ is constant on an open subinterval of $(-1,1)$ it is said to have infinitely many changes of direction). With this assumption we may prove that $R^* \cup S^* \supset T^*$ (and hence that $R^* \cup S^* = T^*$) as follows. If $c \in T^*$ then

$$\beta c = \sum_{v=0}^n \epsilon_v p_v f(s_v)$$

for some $\beta \neq 0$, $\epsilon_v = \pm 1$, $p_v > 0$ and $\sum_{v=0}^n p_v = 1$. Moreover by Lemma 2.1 there exists a polynomial $u(x) = \sum_{i=0}^n a_i f_i(x)$ such that $|u(x)| \leq 1$ for $x \in [-1,1]$ and $\epsilon_v u(s_v) = 1$, $v = 0, 1, \dots, n$. Now if $c \notin R^* \cup S^*$ then the ϵ_v are not constant (hence $u(x) \neq \text{constant}$) and do not alternate in sign so that there exists a j such that $\epsilon_j \epsilon_{j+1} > 0$. Then $u(x)$ has a change of direction at s_1, s_2, \dots, s_{n-1} and at least one in the open interval (s_j, s_{j+1}) . We therefore have a contradiction since $u(x)$ has n changes of direction and is nonconstant.

§4. Optimal Designs for the Individual Regression Coefficients.

Let $c_p = (0, \dots, 0, 1, 0, \dots, 0)$ denote the vector with a one in the p -th component and zeros elsewhere. In this case $(c_p, \theta) = \theta_p$. For $p=n$ it follows from Theorem 2.2 that if f_0, \dots, f_{n-1} is a T -system then the unique c_n -optimal design is supported by the full set of Tchebycheff points $s_0 < s_1 < \dots < s_n$. This result was first proven in Kiefer and Wolfowitz (1959). The purpose of this section is to show that under

suitable assumptions the unique c_p -optimal design ($p > 0$) is supported by this same full set of Tchebycheff points if $n-p$ is even and by the full set of Tchebycheff points of one lower order if $n-p$ is odd. For $p = 0$, $n \geq 2$ the unique c_p optimal design is supported entirely on $x = 0$. This result is motivated by certain extremal properties of the ordinary Tchebycheff polynomial $T_n(x) = \cos n\theta$, $x = \cos \theta$. The assumptions to be made on the regression functions will be such that they resemble to a very large extent the ordinary powers $1, x, \dots, x^n$ on $[-1, 1]$.

We shall assume the following:

- (i) $\{f_i\}_0^k$ for $k=n-2, n-1, n$, are T-systems on $[-1, 1]$
- (ii) $f_0(x) \equiv 1$
- (iii) $f_i(x) = (-1)^i f_i(-x)$ $i = 0, 1, \dots, n$
- (iv) for every subset i_1, i_2, \dots, i_k of $0, 1, \dots, n$ the system $f_{i_1}(x), f_{i_2}(x), \dots, f_{i_k}(x)$ is a T-system on the half open interval $(0, 1]$, i.e. every linearly combination of f_{i_1}, \dots, f_{i_k} has at most $k-1$ distinct zeros in $(0, 1]$.
- (v) every polynomial $\sum_0^n a_i f_i$ either has fewer than n changes of direction on $(-1, 1)$ or else is constant on $(-1, 1)$.

Since $\{f_i\}_0^n$ and $\{f_i\}_0^{n-1}$ are both T-systems, the polynomials $W_n(x) = W(x)$ and $W_{n-1}(x)$ exist. (W_{n-1} is defined in terms of $\{f_i\}_0^{n-1}$). Denote the Tchebycheff points for W_n by $s_0 = -1 < s_1 < \dots < s_n = 1$ as before and the Tchebycheff points for $W_{n-1}(x)$ by $t_0 = -1 < t_1 < \dots < t_{n-1} = 1$. From the uniqueness properties of W_n and W_{n-1} both of the sets $\{s_i\}_0^n$ and $\{t_i\}_0^{n-1}$ are symmetric about zero as in the case of the ordinary powers.

In fact for n even, say $n=2m$, $W_n = \sum_{k=0}^m a_{2k} f_{2k}$; while for $n=2m+1$,

$$W_n = \sum_{k=0}^m a_{2k+1} f_{2k+1}.$$

The powers $1, x, \dots, x^n$ satisfy all of the conditions (i)-(v). A simple constructive method of obtaining further systems satisfying these conditions is as follows. Let w_1, w_2, \dots, w_n be any n strictly positive continuous functions on $[-1, 1]$ such that $w(x) = w(-x)$ and define

$$\begin{aligned} f_0(x) &= 1 \\ f_1(x) &= \int_0^x w_1(\xi_1) d\xi_1 \\ f_2(x) &= \int_0^x w_1(\xi_1) \int_0^{\xi_1} w_2(\xi_2) d\xi_2 d\xi_1 \\ &\vdots \\ &\vdots \\ f_n(x) &= \int_0^x w_1(\xi_1) \int_0^{\xi_1} w_2(\xi_2) \dots \int_0^{\xi_{n-1}} w_n(\xi_n) d\xi_n \dots d\xi_1 \end{aligned}$$

It can be shown (see Karlin and Studden (1966a), Ch. 11) that the above system satisfies conditions (i) - (v). The powers arise for the special case $w_i(\xi) \equiv 1$, $i = 1, 2, \dots, n$. The proofs for this special case can be found in Natanson (1964), p. 53.

Now for $p = 0$ and $n = 1$ it is clear that ξ is c_p -optimal if and only if ξ is symmetric about zero. For $p = 0$ and $n \geq 2$ it is easily seen that the unique c_p -optimum design concentrates mass one at $x = 0$. We shall therefore assume that $p \neq 0$ and $n \geq 2$.

Theorem 4.1. Let $\{f_i\}_0^n$ satisfy conditions (i) - (v) and suppose that $n \geq 2$ and $p \neq 0$.

(a) If $n - p$ is even then $c_p \in R_0 = R^*$, i.e. the unique c_p -optimal design is supported by the full set of Tchebycheff points s_0, s_1, \dots, s_n . The c_p -optimal design and the minimal value of $V(c_p, \xi)$ are explicitly characterized in Theorem 2.2.

(b) For $n-p$ odd the unique c_p -optimal design is supported by the full set of Tchebycheff points t_0, t_1, \dots, t_{n-1} and this design is obtained from Theorem 2.2 by considering the 1st n component of c_p . (The vector c_p is in fact, contained in the set $R_0^{(n-1)} = R^{*(n-1)}$ defined analogous to R_0 using $\{t_i\}_0^{n-1}$ instead of $\{s_i\}_0^n$.)

The above theorem relies on the following result. For the ordinary polynomial case the proof is given in Natanson (1964), p. 53. The proof for the more general systems follows essentially word for word and will therefore be omitted.

Theorem 4.2. If $n-p$ is even then of all polynomials $u = \sum_{i=0}^n a_i f_i$ in

which the coefficient of f_p is equal to unity the polynomial $W_n(x)/a_p^{(n)}$ minimizes

$$\sup_{-1 \leq x \leq 1} |u(x)|.$$

If $n-p$ is odd then the polynomial $W_{n-1}(x)/a_p^{(n-1)}$ has the above property. (The quantities $a_p^{(n)}$ and $a_p^{(n-1)}$ are the coefficients of f_p in W_n and W_{n-1} respectively).

With the aid of the above theorem we can prove

Lemma 4.1. For $n \geq 2$ the c_p -optimal design is supported by the Tchebycheff points s_0, s_1, \dots, s_n if $n-p$ is even and by the Tchebycheff points t_0, t_1, \dots, t_{n-1} if $n-p$ is odd.

Proof. By Remark 2.1 following Lemma 2.1 we have

$$\begin{aligned}
\inf_{\xi} V(c_p, \xi) &= \inf_{\xi} \sup_a \frac{(c_p, a)^2}{\int (a, f(x))^2 \xi(dx)} \\
&= \sup_a \inf_{\xi} \frac{(c_p, a)^2}{\int (a, f(x))^2 \xi(dx)} \\
&= \sup_a \frac{(c_p, a)^2}{\sup_{-1 \leq x \leq 1} (a, f(x))^2} \\
&= \begin{cases} (a_p^{(n)})^2 & n-p \text{ even} \\ (a_p^{(n-1)})^2 & n-p \text{ odd.} \end{cases}
\end{aligned}$$

Suppose that ξ_0 is c_p -optimal and $n-p$ is even. Then

$$\begin{aligned}
V(c_p, \xi_0) &= \sup_a \frac{(c_p, a)^2}{\int (a, f(x))^2 \xi_0(dx)} \\
&\geq \frac{(a_p^{(n)})^2}{\int (W_n(x))^2 \xi_0(dx)} \\
&\geq (a_p^{(n)})^2.
\end{aligned}$$

Since $|W_n(x)| = 1$ only for s_0, s_1, \dots, s_n strict inequality holds at the last step unless ξ_0 is supported by s_0, s_1, \dots, s_n . The argument for $n-p$ odd is the same.

Proof of Theorem 4.1. Suppose that $n-p$ is even, $n \geq 2$ and $p \neq 0$. Since any c_p -optimal design is supported by s_0, s_1, \dots, s_n there must exist a solution $\{\epsilon_{\nu p_{\nu}}\}$ to the system of equations

$$(4.1) \quad \beta c_p = \sum_{v=0}^n \epsilon_v p_v f(s_v), \quad \beta^{-1} = |a_p^{(n)}|.$$

It suffices to show that $p_v \neq 0$ since in this case our assumption (v) together with the Kiefer-Wolfowitz result (iv) described in Section 3 tells us that either the ϵ_v alternate in sign or they are constant. However since $p \neq 0$ the first component of (4.1) reveals that ϵ_v cannot be all of one sign. Therefore $c_p \in R_0 = R^*$.

Now suppose that $p_i = 0$ for some fixed i . From equation (4.1) the determinant with column vectors $f(s_0), \dots, f(s_{i-1}), c_p, f(s_{i+1}), \dots, f(s_n)$ is zero. Therefore there exists a polynomial $P(x) = \sum_0^n a_i f_i(x)$ such that $\sum_0^n a_i^2 > 0$, $a_p = 0$ and $P(s_v) = 0$ for $v \neq i$. Since $n-p$ is even, two cases may arise (a) n and p are both even or (b) n and p are odd. If n and p are even and $n=2m$ we note, with the aid of condition (iii), that

$$\begin{aligned} Q(x) &= P(x) + P(-x) \\ &= \sum_{k=0}^m a_{2k} f_{2k}(x), \quad a_p = 0. \end{aligned}$$

The polynomial $Q(x)$ has at most m terms since $a_p = 0$ and hence has at most $m-1$ zeros on $(0,1]$ by condition (iv). Note that $s_m = 0$ and $s_i = -s_{2m-i}$ $i = 0, 1, \dots, m-1$. If $i=m$, $Q(x)$ vanishes at s_{m+1}, \dots, s_{2m} implying that $a_{2k} = 0$ $k = 0, 1, \dots, m$. If $i \neq m$ we suppose that $i > m$. In this case $Q(s_m) = 0$ and Q now has $m-1$ terms and vanishes at $x = s_j$, $j = m+1, \dots, 2m$, $j \neq i$ again implying that $a_{2k} = 0$, $k = 0, 1, \dots, m$. Therefore

$$P(x) = \sum_{k=1}^m a_{2k-1} f_{2k-1}$$

vanishes at s_0, s_1, \dots, s_{m-1} and hence at s_{m+1}, \dots, s_{2m} . We conclude that $P(x) \equiv 0$ which is a contradiction. The case (b) where n and p are odd is handled in a similar manner using $Q(x) = P(x) - P(-x)$. The proof is omitted.

Now when $n-p$ is odd the c_p -optimal design is supported by t_0, t_1, \dots, t_{n-1} and hence there exists a solution $\{\epsilon_\nu, p_\nu\}$ of

$$(4.2) \quad \beta c_p = \sum_{\nu=0}^{n-1} \epsilon_\nu p_\nu f(t_\nu) \quad \beta^{-1} = |a_p^{(n-1)}|.$$

Omitting the last component the resulting system of equations reduces to the case $n-p$ even so that $p_\nu \neq 0$ and as before the ϵ_ν alternate in sign.

For the ordinary polynomials the explicit values of $\inf_{\xi} V(c_p, \xi)$ can be readily obtained from the coefficients of $W_n(x)$ or $W_{n-1}(x)$. Thus if $n-p$ is even and $k = 0, 1, \dots, \lfloor \frac{n}{2} \rfloor$ then

$$\inf_{\xi} V(c_{n-2k}, \xi) = \left\{ \frac{n}{n-k} \binom{n-k}{k} 2^{n-2k-1} \right\}^2$$

while for $n-p$ odd and $k = 0, 1, \dots, \lfloor \frac{n-1}{2} \rfloor$ we have

$$\inf_{\xi} V(c_{n-1-2k}, \xi) = \left\{ \frac{n-1}{n-1-k} \binom{n-1-k}{k} 2^{n-2k-2} \right\}^2.$$

We observe that for fixed k the minimal variance for estimating θ_k is equal when $n = k+2i$ and $n = k+2i+1$, $i=0, 1, \dots$.

§5. Remarks. We observe that the vectors $\sum_{v=0}^n \epsilon_v p_v f(s_v) = \beta c$ with ϵ_v alternating or ϵ_v of one sign form two sets of opposing n -dimensional convex faces in the boundary of Ω . Now each of these faces determines a convex cone such that any vector c in the cone has a c -optimal design supported on the Tchebycheff points. The simple property we wish to utilize is that a cone is closed under linear combinations with nonnegative coefficients. Each of these faces is, of course, the convex hull of the extreme points which are known; however it is of interest to determine, for example, in which face each of the vector c_p lie. For this purpose we consider the two cones

$$C_n = \{c | \beta c = \sum_{v=0}^n (-1)^{n-v} p_v f(s_v), \beta > 0\}$$

and

$$C_{n-1} = \{c | \beta c = \sum_{v=0}^{n-1} (-1)^{n-1-v} q_v f(t_v), \beta > 0\}$$

where $p_v, q_v \geq 0$ and $\sum_v p_v = 1$ and $\sum_v q_v = 1$.

Suppose that $\{f_i\}_0^n$ is a T-system on $[-1, \infty)$ such that

$$(5.1) \quad F \begin{pmatrix} 0, 1, \dots, n \\ x_0, x_1, \dots, x_n \end{pmatrix} > 0$$

whenever $-1 \leq x_0 < x_1 < \dots < x_n$. In this case $f(x) \in C_n$ for $x \geq 1$ and hence

$$\sum_{i=1}^k \lambda_i f(x_i) \in C_n$$

for $x_i \geq 1$ and $\lambda_i \geq 0$. In fact

$$(5.2) \quad \int f(x) d\mu(x) \in C_n$$

for any nonnegative measure μ on $[1, \infty)$ for which the integral is defined. The optimal designs for such linear combinations can easily be obtained using Theorem 2.2. For example the optimal design for the vector in (5.2) places mass

$$\alpha_\nu \left(\sum_{j=0}^n \alpha_j \right)^{-1} \text{ at } s_\nu \quad \text{where} \quad \alpha_\nu = \int |L_\nu(x)| d\mu(x), \quad \nu = 0, 1, \dots, n.$$

In order to determine in which face each of the vectors c_p lies we shall assume that for $k = n-2, n-1$, and n

$$(5.3) \quad F \begin{pmatrix} 0, 1, \dots, k \\ x_0, x_1, \dots, x_k \end{pmatrix} > 0$$

whenever $-1 \leq x_0 < \dots < x_k \leq 1$.

Theorem 5.1. Let $\{f_i\}_0^n$ satisfy conditions (i) - (v) of Section 4 and suppose that (5.3) holds. If $n-p$ is even then

$$(5.4) \quad (-1)^k c_{n-2k} \in C_n, \quad k = 0, 1, \dots, \left[\frac{n}{2} \right]$$

and if $n-p$ is odd then

$$(-1)^k c_{n-1-2k} \in C_{n-1}, \quad k = 0, 1, \dots, \left[\frac{n-1}{2} \right].$$

Note that we have normalized the system $\{f_i\}_0^{n-1}$ in such a way that c_n is always in C_n . If $n = 4$ then $c_4, -c_2, c_0$ lie in C_n so that $\lambda_4 c_4 - \lambda_2 c_2 + \lambda_0 c_0 \in C_n$ when $\lambda_0, \lambda_2, \lambda_4$ are nonnegative and hence $\lambda_4 \theta_4 - \lambda_2 \theta_2 + \lambda_0 \theta_0$ is optimally estimated by a design on the points s_0, \dots, s_4 .

Proof of Theorem 5.1. The arguments are somewhat similar to that given in Theorem 4.1. We shall consider only the case where $n-p$ is even and $p \neq 0$. The remaining cases are similar.

Observe that $c_p \in C_n$ when $D_n(c_p) > 0$ and $-c_p \in C_n$ if $D_n(c_p) < 0$. Now the sign of $D_n(c_p)$ is the same as the sign of the coefficient of f_p in the polynomial

$$P(x) = F \begin{pmatrix} 0, 1, \dots, n-1, n \\ s_0, s_1, \dots, s_{n-1}, x \end{pmatrix}$$

$$= \sum_{i=0}^n a_i f_i(x).$$

For $n = 2m$ the polynomial

$$Q(x) = 2^{-1}(P(x) + P(-x)) = \sum_{k=0}^m a_{2k} f_{2k}(x)$$

vanishes at $s_m = 0$ (so that $a_0 = 0$) and at the $m-1$ points s_{m+1}, \dots, s_{2m-1} .

Now the system $\{f_{2k}\}_1^m$ satisfies Descartes Rule of Signs (see Theorem 4.4, p. 25 in Karlin and Studden (1966a)). That is, the number of zeros of $Q(x)$ on $(0, 1]$ is bounded above by the number of sign changes in the sequence a_2, a_4, \dots, a_{2m} where zero terms are omitted if there are any. Since $Q(x)$ has $m-1$ zeros the sequence a_2, a_4, \dots, a_{2m} must alternate in sign.

Since $a_{2m} > 0$ we have $(-1)^k a_{n-2k} > 0$, $k = 0, \dots, m$. Therefore $(-1)^k c_{n-2k} \in C_n$, for $k = 0, 1, \dots, m$.

§6. A Counterexample. From the papers of Hoel-Levine, Kiefer-Wolfowitz and Karlin-Studden it is apparent that the assumption that the functions $\{f_i\}_0^n$ form a T-system provides enough structure to analyze certain design problems. Now in the case where $f_i(x) = x^i$, $i = 0, 1, \dots, n$ on $[-1, 1]$ it is known that the minimax design, which minimizes $\max_{-1 \leq x \leq 1} V(x, \xi)$, is supported by $n+1$ points, namely the zeros of $(1-x^2) P_n'(x) = 0$ where P_n is the nth Legendre polynomial. In fact in the ordinary polynomial case all admissible designs (see Kiefer (1959)) use only $n-1$ points in the open interval $(-1, 1)$. The purpose of this section is to exhibit a simple example of a T-system for which any minimax design must be supported by more than $n+1$ points. We shall utilize the theorem of Kiefer and Wolfowitz (1960) which states that ξ_0 minimizes $\max_{-1 \leq x \leq 1} V(x, \xi)$ if and only if ξ_0 maximizes the determinant of $M(\xi)$, $\max_{-1 \leq x \leq 1} V(x, \xi) \leq n+1$ for all $x \in [-1, 1]$.

Consider the functions f_0, f_1, f_2 on $[-1, 1]$ where $f_0 \equiv 1$, $f_1(x) = x$ and f_2 is such that $f_2(x) \geq 0$, $f_2(0) = 0$, $f_2(\pm 1) = 1$ and f_2 is convex. With these assumptions the design which minimizes $\max_{-1 \leq x \leq 1} V(x, \xi)$, among

those concentrating all mass on 3 points, has equal mass at the points $-1, 0, 1$. This is geometrical clear after noting that for a design ξ with weights $\lambda_0, \lambda_1, \lambda_2$ on x_0, x_1, x_2 we have

$$|M(\xi)| = \lambda_0 \lambda_1 \lambda_2 [\det |f_i(x_j)|_{i,j=0}^2]^2$$

and that the above determinant is the volume of the parallelepiped spanned by $f(x_0)$, $f(x_1)$, $f(x_2)$.

Now if the design ξ_0 with equal mass on $-1, 0, 1$ is minimax then

$$(6.1) \quad (f(x), M^{-1}(\xi_0)f(x)) \leq 3 \quad \text{for } x \in [-1, 1].$$

However the quadratic form

$$(1, y, z) M^{-1}(\xi_0) \begin{pmatrix} 1 \\ y \\ z \end{pmatrix} = 3$$

is given by

$$z = \frac{1}{3} \{2 \pm (4 - 3y^2)^{1/2}\}$$

which is strictly positive for $y \neq 0$. Thus (6.1) cannot hold when $f_2(x)$ is "sufficiently close" to zero. It can easily be verified that the system $\{1, x, x^4\}$ does not satisfy (6.1) and hence the minimax design is on at least four points. Further analysis in this particular case shows that four points actually suffices.

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