The Annals of Mathematical Statistics
1971, Vol. 42, No. 2, 643–649

OPTIMAL DESIGNS WITH A TCHEBYCHEFFIAN SPLINE REGRESSION FUNCTION

BY V. N. MURTY
Pennsylvania State University

0. Summary. Studden (1968) showed that the optimal design for estimating any specific regression coefficient or parameter is supported by one of two sets of points for Tchebycheff systems with certain symmetry properties. In this paper we consider a Tchebycheffian Spline Regression Function, defined on an interval, and show that the optimal design for estimating any specified regression coefficient is supported on the same set of points. Familiarity with the notation and terminology used in the paper of Studden referred to above is assumed.

1. Definition of a Tchebycheffian spline regression function (TSF). Starting with $(n+1)$ functions $w_0, w_1, \cdots, w_n$ which are strictly positive on $[a, b]$ and such that w_k is of continuity class $C^{n-k}[a, b]$ we form the system:

$$\begin{aligned} u_0(x) &= w_0(x), \\ u_1(x) &= w_0(x)\textstyle\int_a^x w_1(\xi_1)\,d\xi_1, \\ &\vdots \\ u_n(x) &= w_0(x)\textstyle\int_a^x w_1(\xi_1)\int_a^{\xi_1} w_2(\xi_2)\cdots\int_a^{\xi_{n-1}} w_n(\xi_n)\,d\xi_n\cdots d\xi_1. \end{aligned} \tag{1}$$

It is shown (see Karlin and Studden (1966) page 379, Theorem 1.2) that the functions $u_0, u_1, \cdots, u_n$ in (1) comprise an Extended Complete Tchebycheff (ECT) system on $[a, b]$, obeying the boundary conditions:

$$u_k^{(p)}(a) = 0; \qquad p = 0, 1, \cdots, k-1;\ k = 1, 2, \cdots, n. \tag{2}$$

A function $s(x)$ is said to be a Tchebycheffian Spline Function (TSF) on $[a, b]$ of order $(n+1)$ or degree n, with k knots $\{\eta_i\}_1^k$,

$$\eta_0 = a < \eta_1 < \eta_2 < \cdots < \eta_k < b = \eta_{k+1}$$

provided (i) $s(x)$ reduces to a u-polynominal in the ECT system $\{u_i\}_0^n$ in each of the intervals (η_i, η_{i+1}); $i = 0, 1, \cdots, k$; and (ii) $s(x)$ has $(n-1)$ continuous derivatives.

The class of TSF's of degree n with k prescribed knots $\{\eta_i\}_1^k$ will be designated by $S_{n,k}(\eta_1, \eta_2, \cdots, \eta_k)$. Lemma 9.1, page 437 of Karlin and Studden (1966) shows that $S_{n,k}(\eta_1, \eta_2, \cdots, \eta_k)$ is precisely the set of functions

$$s(x) = \textstyle\sum_{i=0}^n a_i u_i(x) + \sum_{j=1}^k a_{n+j}\Phi_n(x; \eta_j) \tag{3}$$

Received August 14, 1969; revised October 2, 1970.

[1] This forms part of the author's dissertation submitted in partial fulfillment of the requirements for the Ph.D. degree in Mathematical Statistics at Purdue University.

where

$$(4)\qquad \Phi_n(x;\eta) = w_0(x)\int_\eta^x w_1(\xi_1)\int_\eta^{\xi_1} w_2(\xi_2)\cdots\int_\eta^{\xi_{n-1}} w_n(\xi_n)\,d\xi_n\cdots d\xi_1 \qquad \text{if } \eta \leqq x \leqq b,$$

$$= 0 \qquad \text{if } a \leqq x \leqq \eta.$$

Notice that $\Phi_n(x;a) = u_n(x)$.

A few theorems on best approximation in the uniform norm by a TSF and the zero structure of TSF, which are needed in the proof of our main theorems, are stated in Sections 2 and 3 for ready reference.

2. Best approximation in the uniform norm by a TSF. In view of the representation (3) spline approximation problem with fixed knots $\{\eta_i\}_1^k$ reduces to the standard linear approximation problem of determining the best approximation of a given continuous function, in the uniform norm, by a linear combination of $(n+k+1)$ functions $\{u_i\}_0^n U\{\Phi_n(x;\eta_j)\}_1^k$.

By the general linear theory (see Meinardus, G. (1967), page 1) we have the following:

THEOREM 2.1. *Let $a < \eta_1 < \eta_2 \cdots < \eta_k < b$ be fixed. Suppose $f(x) \in C[a, b]$. Then there exists a best approximation $s^*(x) \in S_{n,k}(\eta_1, \cdots, \eta_k)$,* i.e., *$s^*(x)$ satisfies*

$$\|s^*-f\| \leqq \|s-f\| = \max_{a\leqq x\leqq b}|s(x)-f(x)|$$

for every $s(x) \in S_{n,k}(\eta_1, \cdots, \eta_k)$.

Theorems 2.2 and 2.3 stated below are due to Schumaker (1967a and 1967b).

THEOREM 2.2. *Let $f \in C[a, b]$. Then there exists an $s(x) \in S_{n,k}(\eta_1, \cdots, \eta_k)$ such that $f-s$ alternates at least $(n+k+1)$ times on $[a, b]$,* i.e., *there exist $\{x_i\}_1^{n+k+2}$ points $a \leqq x_1 < x_2 \cdots < x_{n+k+2} = b$, such that*

$$f(x_i)-s(x_i) = \varepsilon(-1)^i \max_{a\leqq x\leqq b}|f(x)-s(x)|$$

where $\varepsilon = \pm 1$ and $i = 1, 2, \cdots, n+k+2$.

THEOREM 2.3. *Suppose $f \in C[a, b]$. Then $s(x) \in S_{n,k}(\eta_1, \cdots, \eta_k)$ is the unique best approximation of f, if there exist points $a \leqq t_1 < t_2 \cdots < t_{n+k+2} \leqq b$ satisfying*

$$t_{i+1} < \eta_i < t_{n+i+1}; \qquad i = 1, 2, \cdots, k,$$

and

$$f(t_i)-s(t_i) = (-1)^i\zeta A_{n,k}; \qquad i = 1, 2, \cdots, (n+k+2),$$

where

$$A_{n,k} = \min_{s\in S_{n,k}(\eta_1,\cdots,\eta_k)}\|f-s\|, \qquad \zeta = \pm 1.$$

3. Zero structure of TSF's. The following lemma on the simple zeros of a TSF is due to Schumaker (1967b).

LEMMA 3.1. *Suppose* $s(x) \in S_{n,k}(\eta_1, \cdots, \eta_k)$ *possesses the zeros* $x_1 < x_2 \cdots < x_{n+k}$ *and does not vanish identically on any interval containing two of these zeros.*

$$x_i < \eta_i < x_{n+i};\ i = 1, 2, \cdots, k. \tag{5}$$

Moreover, $s \in S_{n,k}$ *can have at most* $(n+k)$ *distinct zeros provided s does not vanish identically between any two of them.*

One of the perversities of TSF's is that it is possible for a non-null TSF to vanish on an interval. When counting zeros of a TSF the following conventions are used. (See Karlin and Schumaker (1967) and Studden and Van Arman (1968).)

(a) No zeros are counted on any open interval (η_i, η_j) if $s(x) \equiv 0$ there.

(b) The multiplicity of a zero $z \neq \eta_i$ $i = 1, 2, \cdots, k$ is r if

$$s^{(j)}(z) = 0; \qquad j = 0, 1, \cdots, (r-1); \qquad s^{(r)}(z) \neq 0.$$

(c) If $s(x) \equiv 0$ on (η_{i-1}, η_i) and $\not\equiv 0$ on (η_i, η_{i+1}) the zero at η_1 is counted as in (b) using the right-hand derivatives. Similarly, we use the left-hand derivatives for $s(x) \not\equiv 0$ on (η_{i-1}, η_i) and $\equiv 0$ on (η_i, η_{i+1}).

(d) If $s(x) \not\equiv 0$ on (η_{i-1}, η_i) or (η_i, η_{i+1}) and

$$s^{(j)}(\eta_i -) = s^{(j)}(\eta_i +) = 0; \qquad j = 0, 1, \cdots, (r-1),$$
$$A = s^{(r)}(\eta_i -); \qquad B = s^{(r)}(\eta_i +); \qquad \text{and} \qquad A \neq B,$$

then η_i is a zero of order

(i) r if $AB > 0$,

(ii) $r+1$ if $AB < 0$,

(iii) $r+1$ if $AB = 0$ and $B-A > 0$,

(iv) $r+2$ if $AB = 0$ and $B-A < 0$.

Let $Z(s)$ denote the number of zeros of $s(x)$ according to the above conventions. The following lemma due to Studden and Van Arman (1968) and Karlin and Schumaker (1967) gives an upper bound to $Z(s)$.

LEMMA 3.2. *A non-trivial* TSF $s(x) \in S_{n,k}(\eta_1, \cdots, \eta_k)$ *has* $Z(s) \leqq n+k$.

4. Uniqueness and existence of the oscillatory polynomial $W(x)$. Utilizing the theorems and lemmas stated in Sections 2 and 3, we now state and prove:

THEOREM 4.1. *Let* $n \geqq 2$ *and* $w_0(x)$ *in the system* (1) be $\equiv 1$. *There exists a unique* $W(x)$ *(unique up to* $\pm W(x)$*) belonging to* $S'_{n,k}(\eta_1, \cdots, \eta_k)$ *satisfying*

(i) $|W(x)| \leqq 1\ \forall\, x \in [a, b]$,

(ii) *The set* $\{x: |W(x)| = 1\}$ *consists of precisely* $(n+k+1)$ *points* $\{x_i\}_1^{n+k+1}$, *where* $x_1 = a$, $x_{n+k+1} = b$ *and* $x_1 < x_2 \cdots < x_{n+k+1}$.

(iii) $W(x_i) = \varepsilon(-1)^i$ *where* $\varepsilon = \pm 1$; $i = 1, 2, \cdots, n+k+1$.

(iv) $x_{i+1} < \eta_i < x_{n+i}$; $i = 1, 2, \cdots, k$.

PROOF. Consider $f = \Phi_n(x; \eta_k) \in C[a, b]$. Theorem 2.2 assures the existence of an $s^*(x)$ belonging to $S_{n,k-1}(\eta_1, \eta_2, \cdots, \eta_{k-1})$ such that s^* is a best approximation of f with respect to the class $S_{n,k-1}(\eta_1, \cdots, \eta_{k-1})$, and $f - s^*$ alternates at least $(n+k)$ times. Hence there exist $(n+k+1)$ points $\{x_i\}_1^{n+k+1}$ where $a \leqq x_1 < x_2 \cdots < x_{n+k+1} \leqq b$ and

$$f(x_i) - s^*(x_i) = \varepsilon(-1)^i \max_{a \leqq x \leqq b} |f(x) - s^*(x)| \qquad i = 1, 2, \cdots, n+k+1.$$

Set

$$W(x) = \frac{1}{||f - s^*||}[f(x) - s^*(x)]$$
$$= \textstyle\sum_{i=0}^n a_i^* u_i(x) + \sum_{j=1}^k a_{n+j}^* \Phi_n(x; \eta_j).$$

Clearly $||W|| = 1$; hence (i) of Theorem 4.1 is proved. Since $n \geqq 2$, $W'(x) = (d/dx)W(x)$ exists, it belongs to $S_{n-1,k}(\eta_1, \cdots, \eta_k)$ and has at least $(n+k-1)$ distinct zeros $\{x_i\}_2^{n+k}$ and does not vanish identically between any two of them. Hence, from Lemma 3.1 we have:

$$(6) \qquad x_{i+1} < \eta_i < x_{n+1}; \qquad i = 1, 2, \cdots, k.$$

This establishes (iv) of the Theorem. We have thus seen the existence of a polynomial belonging to $S_{n,k}(\eta_1, \eta_2, \cdots, \eta_k)$ possessing properties (i) to (iv). To show that this is inique, let $W_1(x) = \sum_{i=0}^n b_i u_i(x) + \sum_{j=1}^k b_{n+j} \phi_n(x; \eta_j)$ be another polynomial having properties (i) to (iv) of Theorem 4.1. From Lemma 3.4, page 251 of [2] and since W_1 has (iii), it follows that each $b_i (i = 0, 1, \cdots, n+k)$ is different from zero and in particular $b_{n+k} \neq 0$.

Consider
$$s_1(x) = -\sum_{i=0}^n \frac{b_i}{b_{n+k}} u_i(x) - \sum_{j=1}^{k-1} \frac{b_{n+j}}{b_{n+k}} \phi_n(x; \eta_j).$$

Clearly s_1 belongs to $S_{n,k-1}(\eta_1, \eta_2, \cdots, \eta_{k-1})$. If $s \in S_{n,k}$ alternates $n+j+1$ times on any subinterval $[x_m, x_{m+j+1}] \subset [a, b]$, then s is a best approximation of f in the class $S_{n,k}$. (See Schumaker 1967a.) Since $s_1 \in S_{n,k-1}$, and W_1 satisfies (iii) of Theorem 4.1, $f - s_1$ does alternate $n+k$ times and hence s_1 is a best approximation of f. Since W_1 also satisfies (iv) of Theorem 4.1, from Theorem 2.3 we conclude that s_1 is the unique best approximation of f, thus establishing the uniqueness of W.

If the set $\{x: |W(x)| = 1\}$ has at least $(n+k+2)$ points, the additional point, say x_0, cannot be such that the function $W(x)$ attains its maximum absolute value with alternating signs at each of these $(n+k+2)$ points. That is, this additional point x_0 and the $(n+k+1)$ points $\{x_i\}_{i=1}^{n+k+1}$ cannot form an alternant of $W(x)$, for then $W'(x) \in S_{n-1,k}$ must vanish at every such interior point so that W' will have at least $(n+k)$ distinct zeros, which is a contradiction, since W' cannot have more than $(n+k-1)$ such zeros. Hence W' may vanish identically in (x_0, x_1) if the additional point x_0 at which $|W(x_0)| = 1$ is in $[a, x_1)$, or it may vanish identically in (x_{n+k+1}, x_0) if x_0 is in $(x_{n+k+1}, b]$, or it may vanish identically in (x_i, x_0) if

$x_0 \in (x_i, x_{i+1})$. In each case it is easily seen that $Z(W') \geqq n+k$, which is a contradiction. Hence the set $\{x: |W(x)| = 1\}$ consists of precisely $(n+k+1)$ points $\{x_i\}_1^{n+k+1}$. Moreover, $x_1 = a$ and $x_{n+k+1} = b$.

This completes the proof of Theorem 4.1.

5. Optimal designs of individual regression coefficients with a TSF as regression function.

THEOREM 5.1. *Let $n \geqq 2$ and*

$$E(y \mid x) = \textstyle\sum_{i=0}^{n} \theta_i u_i(x) + \sum_{j=1}^{k} \theta_{n+j} \Phi_n(x; \eta_j)$$

where $x \in [a, b]$ and $\{u_i\}_0^n$ is the ECT-*system* (1) *with $w_0(x) \equiv 1$. Then the optimal design for estimating any $\theta_l (1 \leqq l \leqq n+k+1)$ is unique and is supported on the full set of extreme points of $W(x)$ obtained in Theorem* 4.1 *and the unique optimal design for estimating θ_0 concentrates its entire mass at the point $x_1 = a$.*

Before we give the proof of Theorem 5.1 we recall some of the definitions given in Studden's paper (1968), so as to facilitate ready reference and easy understanding of the proof.

Starting with $(n+1)$ regression functions $f_0, f_1, \cdots, f_n$, and the $(n+1)$ Tchebycheff points $s_0, s_1, \cdots, s_n$ (see page 1438 of Studden (1968)), for any vector $c \neq (0, 0, \cdots, 0)$

$$D_\nu(c) = \begin{vmatrix} f_0(s_0) & f_0(s_1)\cdots f_0(s_{\nu-1}) & f_0(s_{\nu+1})\cdots f_0(s_n) & c_0 \\ f_1(s_0) & f_1(s_1)\cdots f_1(s_{\nu-1}) & f_1(s_{\nu+1})\cdots f_1(s_n) & c_1 \\ \vdots & \vdots \qquad \vdots & \vdots \qquad \vdots & \vdots \\ f_n(s_0) & f_n(s_1)\cdots f_n(s_{\nu-1}) & f_n(s_{\nu+1})\cdots f_n(s_n) & c_n \end{vmatrix}$$

$\nu = 0, 1, 2, \cdots, n.$

If $D_\nu(c) = 0$, the sign of $D_\nu(c)$ may be defined as -1 or $+1$. $c_p = (0, 0, \cdots, 0, 1, 0, \cdots, 0)$ is an $(n+1)$ component vector with a one only in the $(p+1)$st component, $p = 0, 1, 2, \cdots, n$. R denotes the class of vectors $c = (c_0, c_1, \cdots, c_n)$ such that $\varepsilon D_\nu(c) \geqq 0$ for $\nu = 0, 1, 2, \cdots, n$ where ε is fixed to be $+1$ or -1 for a given vector c (i.e., the $D_\nu(c)$, $\nu = 0, 1, 2, \cdots, n$, all have the same sign in a weak sense).

Now in our case we start with $(n+k+1)$ functions $\{u_i\}_0^n$ and $\{\phi_n(x; \eta_j)\}_1^k$, and the Tchebycheff points $\{s_i\}_0^n$ of Studden are replaced by the $(n+k+1)$ points $\{x_i\}_1^{n+k+1}$. In Studden's notation we have

$$u_i(x) = f_i(x), \qquad i = 0, 1, 2, \cdots, n,$$

$$\phi_n(x; \eta_j) = f_{n+j}(x), \qquad j = 1, 2, \cdots, k,$$

and Studden's s_i will be our x_{i+1}.

Note that

$$f_0(s_0) = u_0(x_1) = 1,$$

$$f_1(s_0) = u_1(x_1) = u_1(a) = 0, \qquad f_{n+1}(s_0) = \phi_n(x_1; \eta_1) = \phi_n(a; \eta_1) = 0,$$

$$f_2(s_0) = u_2(x_1) = u_2(a) = 0, \qquad f_{n+2}(s_0) = \phi_n(x_1; \eta_2) = \phi_n(a; \eta_2) = 0,$$

$$\vdots \qquad\qquad\qquad \vdots$$

$$f_n(s_0) = u_n(x_1) = u_n(a) = 0, \qquad f_{n+k}(s_0) = \phi_n(x_1; \eta_k) = \phi_n(a; \eta_k) = 0.$$

PROOF OF THEOREM 5.1. Let

$$K(x, i) = u_i(x), \qquad i = 0, 1, 2, \cdots, n,$$
$$= \Phi_n(x; \eta_{i-n}), \qquad i = n+1, n+2, \cdots, n+k,$$

so that $K(x, i) = f_i(x)$, $i = 0, 1, 2, \cdots, n+k$.

If we look at the determinants

$$D_\nu(c_0) \quad \text{for} \quad \nu = 0, 1, 2, \cdots, n+k$$

the first and the last columns in each of the determinants $D_1(c_0)$, $D_2(c_0)$, $\cdots$, $D_{n+k}(c_0)$ are identical as $(f_0(s_0), f_1(s_0), \cdots, f_{n+k}(s_0)) = c_0$, and hence these are all equal to zero, and in view of (6), $D_0(c_0) \neq 0$. Thus all the $D_\nu(c_0)$; $\nu = 0, 1, \cdots, n+k$ have the same sign, i.e., $c_0 \in R$.

Now let $p > 0$, and consider the determinants $D_0(c_p)$, $D_1(c_p)$, $\cdots$, $D_\nu(c_p)$, $\cdots$, $D_{n+k}(c_p)$. The determinants $D_\nu(c_p)$, $\nu = 1, 2, \cdots, n+k$, each of which is a $(n+k+1)$th order determinant, can each be immediately reduced by deleting the first row and first column and $(p+1)$th row and last column, since the first column of each of the determinants is $(1, 0, 0, \cdots, 0)$ and the last column is $c_p = (0, 0, \cdots, 0, 1, 0, \cdots, 0)$. These deletions do not change the value or the sign of these determinants. The determinant $D_0(c_p)$ can be reduced to the determinant obtained by deleting the last column and the $(p+1)$th row. It is now easily seen that these reduced determinants have the same form as $K(x, i)$ in the Theorem 2.2 page 514 of Karlin (1968) implying that all of them have the same sign.

Hence $c_p \in R$ for $p = 1, 2, \cdots, n+k$.

Using Theorem (2.2) page 1439 of Studden (1968), we conclude that the design $\xi = \xi_0$ concentrating mass

$$p_\nu = |D_\nu(c_p)| / \textstyle\sum_{\nu=0}^{n+k} |D_\nu(c_p)|$$

at the points $x_{\nu+1}$; $\nu = 0, 1, \cdots, n+k$ is the unique optimal design for estimating $\theta_l (1 \leqq l \leqq n+k)$, and that the unique optimal design for estimating θ_0 concentrates its entire mass at $x_1 = a$.

6. Acknowledgments. The author wishes to thank Professor W. J. Studden, Purdue University, for suggesting this problem and for his constant encouragement and guidance throughout the course of this investigation. Comments made by a referee were very helpful in giving a clearer presentation of some of the proofs.

REFERENCES

[1] KARLIN, S. (1968). *Total Positivity* **1**. Stanford Univ. Press.

[2] KARLIN, S. and SCHUMAKER, L. L. (1967). The fundamental theorem of algebra for Tchebycheffian mono splines. *J. Analyse Math.* **20** 233–270.

[3] KARLIN, S. and STUDDEN, W. J. (1966). *Tchebycheff Systems: With Applications in Analysis and Statistics*. Interscience, New York.

[4] MEINARDUS, G. (1967). *Approximation of Functions: Theory and Numerical Methods* (translated by Larry L. Schumaker). Springer-Verlag, New York.

[5] MURTY, V. N. (1969). Optimal designs of individual regression coefficients with a Tchebycheffian spline regression function. Mimeograph Series No. 191, Department of Statistics, Purdue Univ.

[6] SCHUMAKER, L. L. (1967a). Uniform approximation by Tchebycheffian spline functions-I, fixed Knots. Mathematics Research Center Summary Report No. 768, Madison, Wisconsin.

[7] SCHUMAKER, L. L. (1967b). Uniform approximation by Tchebycheffian spline functions-II, free Knots. Mathematics Research Center Summary Report No. 810, Madison, Wisconsin.

[8] STUDDEN, W. J. (1968). Optimal designs on Tchebycheff points. *Ann. Math. Statist.* **39** 1435–1447.

[9] STUDDEN, W. J. and VAN ARMAN, D. J. (1968). Admissible designs for polynomial spline regression. *Ann. Math. Statist.* **40** 1557–1569.