OPTIMAL DESIGNS WITH RESPECT TO ELFVING'S PARTIAL MINIMAX CRITERION IN POLYNOMIAL REGRESSION

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Abstract. For the polynomial regression model on the interval [a, b] the optimal design problem with respect to Elfving's minimax criterion is considered. It is shown that the minimax problem is related to the problem of determining optimal designs for the estimation of the individual parameters. Sufficient conditions are given guaranteeing that an optimal design for an individual parameter in the polynomial regression is also minimax optimal for a subset of the parameters. The results are applied to polynomial regression on symmetric intervals [-b, b] ($b \leq 1$) and on nonnegative or nonpositive intervals where the conditions reduce to very simple inequalities, involving the degree of the underlying regression and the index of the maximum of the absolute coefficients of the Chebyshev polynomial of the first kind on the given interval. In the most cases the minimax optimal design can be found explicitly.

Key words and phrases: Approximate design theory, scalar optimality, minimax criterion, polynomial regression.

1. Introduction

Consider the polynomial regression model of degree d ($d \ge 1$)

$$y(x) = \sum_{i=0}^d artheta_i x^i, \quad x \in [a,b]$$

where $\vartheta = (\vartheta_0, \ldots, \vartheta_d)'$ is the vector of unknown parameters and the controlled variable x varies between a and b (a < b). In order to estimate the unknown parameters $\vartheta_i n$ uncorrelated observations Y_1, \ldots, Y_n are taken at points $x_1, \ldots, x_n \in$ [a, b] with expectation $y(x_i)$ $(i = 1, \ldots, n)$ and variance $\sigma^2 > 0$. An approximate

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design ξ is a probability measure on [a, b]. If ξ has finite support $\{x_1, \ldots, x_k\}$ with corresponding weights ξ_1, \ldots, ξ_k , then ξ_i represents the proportion of all n observations that have to be taken at x_i . The information matrix of ξ is defined by

$$M(\xi) = \int_a^b f(x) f'(x) d\xi(x)$$

where $f(x) = (1, x, ..., x^d)'$ denotes the vector of monomials up to the degree d. For a design ξ with finite support and masses $\xi_i = n_i/n$ (i = 1, ..., k) the inverse of the information matrix $M^{-1}(\xi)$ is proportional to the covariance matrix of the least squares estimator for ϑ . For a more detailed discussion of the statistical context of this setup we refer the reader to the textbooks of Fedorov (1972), Silvey (1980), Pazman (1986) and Pukelsheim (1993).

An optimal design maxi- or minimizes an appropriate functional depending on the information matrix or its inverse. In this paper we are interested in optimal designs with respect to Elfving's partial minimax criterion (Elfving (1959)). More precisely, let $I = \{i_1, \ldots, i_k\}$ denote a fixed subset of $\{0, \ldots, d\}$ corresponding to the parameters of interest and define $e_i = (0, \ldots, 0, 1, 0, \ldots, 0)' \in \mathbb{R}^{d+1}$ as the (i + 1)-th unit vector $(i = 0, \ldots, d)$. Following the work of Elfving (1959) we will call a design ξ minimax optimal for the parameters $\{\vartheta_i\}_{i\in I}$ if ξ^* allows the estimability of ϑ_i for all $i \in I$ (that is, $e_i \in \operatorname{range}(M(\xi))$) and ξ^* minimizes the function

$$\Phi_I(\xi) = \max_{i \in I} \{e'_i M^-(\xi) e_i\}$$

(here $M^-(\xi)$ denotes an arbitrary generalized inverse of $M(\xi)$). In contrary to the commonly used optimality criteria (e.g. D-, A- and E-optimality) the criterion Φ_I allows a very easy interpretation for the experimenter who is using minimax designs in practice. The variance of the least squares estimate for the individual parameter ϑ_i is proportional to $e'_i M^-(\xi) e_i$. Thus the minimax design minimizes the worst variance of the estimates for the parameters $\{\vartheta_i\}_{i\in I}$ and guarantees precise estimates for all parameters of interest. Unfortunately, the determination of minimax designs is a very hard problem. The criterion function is not necessarily differentiable and therefore even numerical procedures are difficult to implement in practice. A general discussion of minimax designs (including the above criterion) can be found in Wong (1992) and Dette and Studden (1992). Some numerical results for polynomial regression of lower degree and the full parameter subset $I = \{0, \ldots, d\}$ are given in Murty (1971).

In the present paper we show that the minimax problem for the parameters $\{\vartheta_i\}_{i\in I}$ is intimitately related to the problem of constructing optimal designs for the individual parameters ϑ_i $(i \in I)$. More precisely, in Section 3 sufficient conditions are stated guaranteeing that an optimal design for the individual parameter ϑ_{i^*} (i.e. the design ξ that minimizes $e'_{i^*}M^-(\xi)e_{i^*}$) is also minimax optimal. The results are used in Sections 4 and 5 to determine optimal minimax designs on symmetric intervals [-b,b] $(b \leq 1)$ and on nonnegative or nonpositive intervals. A motivating example is given in Section 2 which also shows that a conjecture (concerning minimax design on the interval [-1,1]) stated by Murty (1971) is not true in general.

2. A conjecture for the interval [-1, 1]

For the full parameter system $\{\vartheta_i\}_{i=0}^d$ and the interval [-1, 1] minimax optimal designs for polynomial regression were calculated numerically by Murty (1971) for degree $d \leq 12$ excluding 4 and 11. Based on these calculations Murty (1971) stated the following conjecture.

Let

(2.1)
$$T_d(x) := \sum_{j=0}^{\lfloor d/2 \rfloor} t_{d-2j} x^{d-2j} = \cos(d \arccos x)$$

denote the Chebyshev polynomial of the first kind on the interval [-1, 1] and ξ_j^* the optimal design for the individual coefficient ϑ_j . If there exists a unique maximum in the set $\{|t_{d-2j}| \mid j = 0, \ldots, \lfloor d/2 \rfloor\}$, say $|t_{d-2k}|$, then the optimal design for the individual coefficient ϑ_{d-2k} , namely ξ_{d-2k}^* , is also minimax optimal. In the case that the maximum is not unique and attained for two indices, say $|t_{d-2k}|$ and $|t_{d-2k+2}|$, a convex combination of ξ_{d-2k}^* and ξ_{d-2k+2}^* is minimax optimal.

The optimal designs for the individual coefficients are well known and were determined by Studden (1968). In that paper it was shown that the support points of ξ_{d-2j}^* are the so called Chebyshev points $s_{\nu} = \cos(((d-\nu)/d)\pi)$ ($\nu = 0, \ldots, d$) which are the points where the polynomial $|T_d(x)|^2$ attains its maximum in [-1, 1]. The masses of ξ_{d-2j}^* at the support points s_{ν} are given by $|\ell_{\nu,d-2j}|/|t_{d-2j}|$ where $\ell_{\nu,j}$ are the coefficients of the Lagrange interpolation polynomials $L_{\nu}(x)$ at the knots s_0, \ldots, s_d , defined by

$$L_{
u}(x) = \sum_{j=0}^{d} \ell_{
u,j} x^{j}$$
 and $L_{
u}(s_{\mu}) = \delta_{
u,\mu}$ $(
u, \mu = 0, \dots, d)$

The second part of the conjecture applies for polynomial regression of degree 4 where the Chebyshev polynomial is given by $T_4(x) = 8x^4 - 8x^2 + 1$. Averaging the designs ξ_4^* and ξ_2^* Murty (1971) claims that the design $\tilde{\xi} = (\xi_4^* + \xi_2^*)/2$ which puts masses 3/32, 8/32, 10/32, 8/32, 3/32 at the points -1, $-1/\sqrt{2}$, 0, $1/\sqrt{2}$, 1 is minimax optimal for the full parameter set $\{\vartheta_i\}_{i=0}^4$ with $\Phi_I(\tilde{\xi}) = 992/15 \approx$ 66.1333. We applied a numerical procedure of Remez type (see Studden and Tsay (1976)) in order to determine the optimal minimax design for polynomial regression of degree 4. Our calculations showed that the minimax optimal design ξ^* is supported at the points -1, -0.7086, 0, 0.7086, 1 with masses 0.0958, 0.246, 0.3164, 0.246, 0.0958, respectively. The value of the criterion Φ_I at the point ξ^* is given by $\Phi_I(\xi^*) \approx 66.1137 < \Phi_I(\tilde{\xi})$ which shows that the design $\tilde{\xi} = (\xi_4^* + \xi_2^*)/2$ cannot be the minimax optimal design. Moreover, we see that the minimax optimal design ξ^* can never be represented as a convex combination of ξ_4^* and ξ_2^* because all these designs must have support $\{-1, -1/\sqrt{2}, 0, 1/\sqrt{2}, 1\}$ (in fact ξ is minimax optimal among all designs supported at these points). This disproves the second part of Murty's conjecture (even the numerical calculations which led Murty to his conjecture seem to be incorrect). Although we cannot present a counterexample to the first part of the conjecture stated in Murty (1971) it fails to carry over to arbitrary intervals [-b, b] with $b \leq 1$ if the maximum coefficient of $T_d(x)$ is unique. This is indicated by the following example.

Consider a polynomial regression model of degree 4 on the interval [-b, b]where b < 1. The Chebyshev polynomials on this interval are easily obtained from (2.1)

(2.2)
$$T_d^b(x) = \sum_{j=0}^d t_{d-2j}^b x^{d-2j} = T_d\left(\frac{x}{b}\right) = \sum_{j=0}^d \frac{t_{d-2j}}{b^{d-2j}} x^{d-2j}$$

and the maximum coefficient of $T_4^b(x)$ is unique and given by $t_4^b = t_4/b^4 = 8/b^4$. By Murty's conjecture the optimal design for the highest coefficient ξ_4^* which puts masses proportional to 1:2:2:2:1 at the points $-b, -b/\sqrt{2}, 0, b/\sqrt{2}, b$ should be optimal, at least when b is very close to 1 (note that the design for the highest coefficient is the D_1 -optimal design which can easily be transferred from the interval [-1, 1] to arbitrary intervals (see e.g. Studden (1982))). Straightforward but tedious calculations show that the inverse of the information matrix of ξ_4^* is given by

$$M^{-1}(\xi_4^*) = b^{-8} \begin{pmatrix} 4b^6 & 0 & -12b^6 & 0 & 8b^4 \\ 0 & 20b^6 & 0 & -24b^4 & 0 \\ -12b^6 & 0 & 72b^4 & 0 & -64b^2 \\ 0 & -24b^4 & 0 & 32b^2 & 0 \\ 8b^4 & 0 & -64b^2 & 0 & 64 \end{pmatrix}.$$

If $\sqrt[4]{8/9} < b < 1$, then the maximum of the diagonal elements m^{ii} of $M^{-1}(\xi_4^*)$ is unique and attained for $m^{33} = 72b^{-4}$. To check if ξ_4^* is minimax optimal for $\{\vartheta_i\}_{i=0}^4$ we apply the equivalence theorem for minimax optimality (see e.g. Wong (1992) or Dette and Studden (1992)). In the case of optimality ξ_4^* has to satisfy

$$(e_3'M^{-1}(\xi_4^*)f(x))^2 = b^{-16}(64b^2x^4 - 72b^4x^2 + 12b^6)^2 \le 72b^{-4} = e_3'M^{-1}(\xi_4^*)e_3$$

for all $x \in [-b, b]$ $(\sqrt[4]{8/9} < b < 1)$, which is obviously not fulfilled for x = 0. Therefore ξ_4^* cannot be minimax optimal whenever $\sqrt[4]{8/9} < b < 1$ (note that ξ_4^* is in fact minimax optimal if $b < \sqrt[4]{8/9}$ because in this case the maximum of the diagonal elements of $M^{-1}(\xi_4^*)$ is m^{55}). Thus, Murty's mathematical description of the optimal minimax design seems to be not appropriate. Nevertheless, the results of the following sections show that in many cases the optimal designs for the individual coefficients play a particular role in the determination of the minimax optimal design.

3. Preliminary results

Intuitively, one of the optimal designs ξ_i for estimating the individual parameters ϑ_i $(i \in I)$ should be a good candidate for the minimax optimal design for the parameter system $\{\vartheta_i\}_{i\in I}$. In this section we will discuss some general aspects of the relationship between these two optimality criteria. Throughout this paper it is assumed that there exists an index $k \in I$ such that the optimal design ξ_k^* for estimating the individual coefficient ϑ_k (i.e. the designs that minimizes $e'_k M^-(\xi)e_k$) has a nonsingular information matrix $M(\xi^*_k)$. In this case it follows by standard results of optimal design theory (see e.g. Kiefer (1959)) that there exists an optimal design ξ^*_k for estimating ϑ_k supported at exactly d + 1 points, say $s_0 < s_1 < \cdots < s_d$. This property will usually depend on the index set $I \subseteq \{0, \ldots, d\}$ and on the underlying interval [a, b]. It is obviously fulfilled for the full index set $I = \{0, \ldots, d\}$ and arbitrary intervals [a, b]. In the following sections two other cases which guarantee the existence of an index $k \in I$ such that $M(\xi^*_k)$ is nonsingular are discussed in more detail: In the first case assume that [a, b] is a nonnegative or nonpositive interval and that $I \neq \{0\}$ or $0 \notin [a, b]$. In this case there exists an index $k \in I \setminus \{0\}$ such that ξ^*_k is supported at exactly d + 1 points (see Heiligers (1992)). Secondly, if [a, b] is symmetric (i.e. a = -b, b > 0) and $I \neq \{0\}$ contains at least one of the integers d - 2i ($i \in \{0, \ldots, \lfloor d/2 \rfloor\}$), then there exists an index $k = d - 2j \in I$, such that ξ^*_k is symmetric and supported at exactly d + 1 points (see Studden (1968) and Heiligers (1992)).

In the following we want to state a condition guaranteeing that the design ξ_k^* is also minimax optimal for estimating the parameter system $\{\vartheta_i\}_{i\in I}$. To this end we introduce the two $(d+1) \times (d+1)$ matrices $F = [f(s_0), \ldots, f(s_d)]$ and $L = (\ell_{\nu,j})_{\nu,j=0}^d = F^{-1}$. Let

$$F\binom{j}{\nu} := F\binom{0 \cdots j-1 \quad j+1 \cdots d}{0 \cdots \nu-1 \quad \nu+1 \cdots d}$$

denote the determinant of the matrix which is obtained from F by deleting the j-th row and the ν -th column, then the elements of L can be represented as

(3.1)
$$\ell_{\nu,j} = (-1)^{\nu+j} \cdot F\binom{j}{\nu} / |F|$$

(here |F| denotes the determinant of F). Moreover the elements of L are the coefficients of the Lagrange interpolation polynomials $L_{\nu}(x) = \sum_{j=0}^{d} \ell_{\nu,j} x^{j}$ (defined by $L_{\nu}(s_{\mu}) = \delta_{\nu\mu}$).

THEOREM 3.1. Let ξ_k^* $(k \in I)$ denote an optimal design for estimating the individual coefficient ϑ_k supported at d+1 points $a = s_0 < s_1 < \cdots < s_{d-1} < s_d = b$. If the coefficients of the Lagrange interpolation polynomials $L_{\nu}(x) = \sum_{j=0}^{d} \ell_{\nu,j} x^j$ at these points satisfy for all $i \in I$

(3.2)
$$\sum_{\nu=0}^{d} \frac{|\ell_{\nu,i}|^2}{|\ell_{\nu,k}|} \le \sum_{\nu=0}^{d} |\ell_{\nu,k}|,$$

then the design ξ_k^* is also minimax optimal for the parameter system $\{\vartheta_i\}_{i\in I}$.

PROOF. By an application of Elfving's theorem (Elfving (1952)) we obtain for the weights of ξ_k^* at the support points $s_0 < \cdots < s_d$

(3.3)
$$p_{\nu} := \xi_k^*(\{s_{\nu}\}) = \frac{|\ell_{\nu,k}|}{\sum_{\mu=0}^d |\ell_{\mu,k}|} \quad \nu = 0, \dots, d.$$

Let $P = \text{diag}(p_0, \ldots, p_d)$, then the inverse of the information matrix of ξ_k^* can be written as $M^{-1}(\xi_k^*) = L'P^{-1}L$ and the diagonal elements are given by

$$(M^{-1}(\xi_k^*))_{ii} = e_i'L'P^{-1}Le_i = \sum_{\nu=0}^d \frac{|\ell_{\nu,i}|^2}{|\ell_{\nu,k}|} \cdot \sum_{\nu=0}^d |\ell_{\nu,k}|.$$

From the assumption (3.2) we have $\Phi_I(\xi_k^*) = (M^{-1}(\xi_k^*))_{kk}$ and the optimality of ξ_k^* now implies its minimax optimality. \Box

Theorem 3.1 directs our interests to the coefficients $|\ell_{\nu,j}|$ of the Lagrange interpolation polynomials corresponding to the support points $s_0 < s_1 < \cdots < s_d$ of the optimal design ξ_k^* for estimating the individual coefficient ϑ_k . In general these coefficients can only be calculated by numerical methods. Nevertheless, we can show some monotonicity properties of the ratios of these coefficients, which turn out to be extremely useful for the determination of minimax designs in the following sections. The proof of the following result is deferred to the Appendix, the proof of Lemma 3.2 is similar and therefore omitted.

LEMMA 3.1. Let $\{s_0, \ldots, s_d\} = \{-s_0, \ldots, -s_d\}$, then the ratio $|\ell_{\nu,d-2i-2}|/|\ell_{\nu,d-2i}|$ is an increasing function in $\nu \in \{0, \ldots, \lfloor d/2 \rfloor\}$ (for every fixed $i \in \{0, \ldots, \lfloor d/2 \rfloor - 1\}$).

LEMMA 3.2. a) Let $0 \leq s_0 < \cdots < s_d$, then the ratio $|\ell_{\nu,i}|/|\ell_{\nu,i+1}|$ is a decreasing function in $\nu \in \{0, \ldots, d\}$ (for every fixed $i \in \{0, \ldots, d-1\}$).

b) Let $s_0 < \cdots < s_d \leq 0$, then the ratio $|\ell_{\nu,i+1}|/|\ell_{\nu,i}|$ is a decreasing function in $\nu \in \{0, \ldots, d\}$ (for every fixed $i \in \{0, \ldots, d-1\}$).

Minimax designs on symmetric intervals

Throughout this section we assume a symmetric interval [-b, b] for the controlled variable x where $0 < b \leq 1$. For the index set I we require the assumption

$$(4.1) d-2i-1 \in I \Rightarrow d-2i \in I$$

which will become essential in the proof of the following theorem. Note that (4.1) was also assumed by Heiligers (1992) and Pukelsheim and Studden (1993) who determined the *E*-optimal design for parameter subsystems. If $I \neq \{0\}$ then there exists an index $d - 2k \in I$ and the results of Studden (1968) show, that the optimal design ξ_{d-2k}^* for estimating the individual coefficient is supported at the transformed Chebyshev points $s_{\nu} = b \cdot \cos(((d - \nu)/d)\pi) \ (\nu = 0, \ldots, d)$ with masses $\xi_{d-2k}^*(s_{\nu}) = |\ell_{\nu,d-2k}| / \sum_{\nu=0}^d |\ell_{\nu,d-2k}|$ where $\ell_{\nu,d-2k}$ denotes the coefficient of x^{d-2k} in the ν -th Lagrange interpolation polynomial with knots s_0, \ldots, s_d . In the following t_{d-2j} denotes the coefficient of x^{d-2j} in the Chebyshev polynomial of the first kind on the interval [-1, 1] defined in (2, 1) (see e.g. Rivlin (1990)).

THEOREM 4.1. If the index set $I \neq \{0\}$ satisfies (4.1) and there exists an index $0 \neq d - 2k \in I$ such that

(4.2)
$$\frac{d-2i}{d-2k} \le \left|\frac{t_{d-2k}}{t_{d-2i}}\right|^2 b^{4(k-i)} \quad \text{for all } d-2i \in I \text{ with } i \le k$$

and

(4.3)
$$\frac{d(d+1)-2i}{d(d+1)-2k}\frac{d-2k+1}{d-2i+1} \le \left|\frac{t_{d-2k}}{t_{d-2i}}\right|^2 b^{4(k-i)}$$
for all $d-2i \in I$ with $i \ge k$

holds, then the optimal design ξ_{d-2k}^* for estimating the individual coefficient ϑ_{d-2k} of a polynomial regression on the interval [-b,b] $(0 < b \leq 1)$ is also minimax optimal for the parameter subset $\{\vartheta_i\}_{i\in I}$. Moreover, the only index $d-2k \in I$, where (4.2) and (4.3) could be satisfied, is the index where the maximum in the set $\{|t_{d-2i}|/b^{d-2i} | d-2i \in I\}$ is attained.

PROOF. We will show that the conditions (4.2) and (4.3) imply the assumption of Theorem 3.1. In a first step we note that it is sufficient to prove

(4.4)
$$\sum_{\nu=0}^{d} \frac{|\ell_{\nu,d-2i}|^2}{|\ell_{\nu,d-2k}|} \le \sum_{\nu=0}^{d} |\ell_{\nu,d-2k}| \quad \text{if } d-2i \in I.$$

To show that (4.4) implies condition (3.2) of Theorem 3.1 we have to prove that (3.2) holds also for the remaining indices $d - 2i - 1 \in I$ which differ from d by an odd number. To this end we use assumption (4.1) and the fact that $|\ell_{\nu,d-2i-1}| = |s_{\nu}||\ell_{\nu,d-2i}| \leq b|\ell_{\nu,d-2i}| \leq |\ell_{\nu,d-2i}|$ which is an immediate consequence of the definition of the Lagrange interpolation polynomials (see e.g. Cantor (1977)). Thus we obtain from (4.4) for all $d - 2i - 1 \in I$ that

$$\sum_{\nu=0}^{d} \frac{|\ell_{\nu,d-2i-1}|^2}{|\ell_{\nu,d-2k}|} \le \sum_{\nu=0}^{d} \frac{|\ell_{\nu,d-2i}|^2}{|\ell_{\nu,d-2k}|} \le \sum_{\nu=0}^{d} |\ell_{\nu,d-2k}|.$$

In a second step we will now prove that (4.4) (and therefore (3.2)) follows from the assertions stated in the theorem. To this end we note that every polynomial of degree $d P_d(x) = \sum_{j=0}^d a_{d-j} x^{d-j}$ can be written as $P_d(x) = \sum_{\nu=0}^d L_{\nu}(x) P_d(s_{\nu})$ which yields for the coefficients a_{d-2j-1}

$$a_{d-2j-1} = \sum_{\nu=0}^{d} P_d(s_{\nu})\ell_{\nu,d-2j-1} = \sum_{\nu=0}^{d} P_d(s_{\nu})s_{\nu}\ell_{\nu,d-2j} \qquad \left(j=0,\ldots,\left\lfloor\frac{d}{2}\right\rfloor\right).$$

Inserting for $P_d(x)$ the Chebyshev polynomial of the second kind (of degree d-1)

$$U_{d-1}\left(\frac{x}{b}\right) = \sum_{j=0}^{d-1} u_{d-1-2j}\left(\frac{x}{b}\right)^{d-2j-1} = \frac{\sin(d\arccos(x/b))}{\sin(\arccos(x/b))} \quad (x \in [-b,b])$$

(see Szegö (1976)) we obtain

$$\frac{u_{d-2j-1}}{b^{d-2j-1}} = \sum_{\nu=0}^{d} U_{d-1}(s_{\nu}) s_{\nu} \ell_{\nu,d-2j} = bd \cdot \{(-1)^{d} \ell_{0,d-2j} + \ell_{d,d-2j}\}$$
$$= 2bd \cdot (-1)^{d} \cdot \ell_{0,d-2j}$$

where we have used in the last equality that

$$U_{d-1}(s_{\nu}) = 0 \quad (\nu = 1, \dots, d-1),$$

$$U_{d-1}(s_d) = (-1)^{d-1} U_{d-1}(s_0) = d,$$

$$\ell_{0,d-2j} = (-1)^d \ell_{d,d-2j}.$$

An application of the well known relationship $T'_d(x) = d \cdot U_{d-1}(x)$ yields $u_{d-2j-1} = ((d-2j)/d)t_{d-2j}$ and for the coefficients of the Lagrange interpolation polynomial $L_0(x)$

(4.5)
$$|\ell_{0,d-2j}| = |t_{d-2j}| \cdot \frac{d-2j}{2d^2} b^{-(d-2j)} \qquad \left(j = 0, \dots, \left\lfloor \frac{d}{2} \right\rfloor\right).$$

Assume now that $i \leq k$ then Lemma 3.1 and (4.5) yield that

(4.6)
$$\frac{|\ell_{\nu,d-2i}|}{|\ell_{\nu,d-2k}|} = \prod_{j=i+1}^{k} \frac{|\ell_{\nu,d-2j+2}|}{|\ell_{\nu,d-2j}|} \le \prod_{j=i+1}^{k} \frac{|\ell_{0,d-2j+2}|}{|\ell_{0,d-2j}|} = \frac{|\ell_{0,d-2i}|}{|\ell_{0,d-2k}|}$$
$$= \frac{d-2i}{d-2k} \cdot \frac{|t_{d-2i}|}{|t_{d-2k}|} \cdot b^{2(i-k)}$$

for all $\nu \in \{0, \ldots, \lfloor d/2 \rfloor\}$ and $i \leq k$. Applying this inequality, the assumption (4.2) and the "symmetry" $|\ell_{\nu,d-2j}| = |\ell_{d-\nu,d-2j}|$ (see e.g. Cantor (1977)) we obtain (for $i \leq k, d-2i \in I$)

$$\begin{split} \sum_{\nu=0}^{d} \frac{|\ell_{\nu,d-2i}|^2}{|\ell_{\nu,d-2k}|} &\leq \frac{d-2i}{d-2k} \cdot \left| \frac{t_{d-2i}}{t_{d-2k}} \right| \cdot b^{2(i-k)} \cdot \sum_{\nu=0}^{d} |\ell_{\nu,d-2i}| \\ &\leq \left| \frac{t_{d-2k}}{t_{d-2i}} \right| b^{2(k-i)} \cdot \sum_{\nu=0}^{d} |\ell_{\nu,d-2i}| = \sum_{\nu=0}^{d} |\ell_{\nu,d-2k}| \end{split}$$

where we have used the identity $\sum_{\nu=0}^{d} |\ell_{\nu,d-2j}| = |t_{d-2j}| \cdot b^{-(d-2j)}$ (for j = i, k) which follows by similar arguments as given in Pukelsheim and Studden (1993) for the case b = 1. This shows that (4.2) implies (4.4) if $i \leq k$ and $d - 2i \in I$. Using similar arguments it can be proved that in the case $i \geq k$ the inequality (4.4) follows from the assumption (4.3), which completes the proof of the first part of the theorem. For the remaining part observe that the left hand sides of (4.2) and (4.3) are always greater or equal than 1 while this is only possible for all terms appearing

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on the right hand sides if the maximum in the set $\{|t_{d-2i}|/b^{d-2i} \mid d-2i \in I\}$ is attained for the index d-2k. \Box

COROLLARY 4.1. If $I = \{0, ..., d\}$ and there exists an index $d - 2k \in I$ such that

(4.7)
$$\frac{16(d-k)^2k^2}{(d-2k)(d-2k+2)(d-2k+1)^2} \le b^4$$

and

(4.8)
$$\frac{16(k+1)^2(d-k-1)^2}{(d-2k-1)(d-2k+1)(d-2k)^2} \cdot \frac{d(d+1)-2k}{d(d+1)-2k-2} \ge b^4$$

then the optimal design ξ_{d-2k}^* for estimating the individual coefficient ϑ_{d-2k} of a polynomial regression on the interval [-b,b] is also minimax optimal for the full parameter set $\{\vartheta_i\}_{i=0}^d$. Moreover, the only index d-2k, where (4.7) and (4.8) could be satisfied, is the index where the maximum in the set $\{|t_{d-2i}|/b^{d-2i} | i \in \{0,\ldots,\lfloor d/2 \rfloor\}$ is attained.

PROOF. Using a similar argument as given in (4.6) it can be seen that (4.2) and (4.3) in Theorem 4.1 follow from

(4.9)
$$\frac{d-2i+2}{d-2i} \le b^4 \left| \frac{t_{d-2i}}{t_{d-2i+2}} \right|^2 = b^4 \cdot \left[\frac{(d-2i+1)(d-2i+2)}{4i(d-i)} \right]^2$$

if $i \leq k$, and

$$(4.10) \qquad \frac{d(d+1)-2i-2}{d(d+1)-2i} \frac{d-2i+1}{d-2i-1} \le b^{-4} \left| \frac{t_{d-2i}}{t_{d-2i-2}} \right|^2 \\ = b^{-4} \left[\frac{4(i+1)(d-i-1)}{(d-2i-1)(d-2i)} \right]^2,$$

if $i \geq k$. Here we used the well known representation

(4.11)
$$|t_{d-2i}| = d \cdot 2^{d-1-2i} \frac{(d-i-1)!}{i!(d-2i)!}$$

for the coefficients of the Chebyshev polynomial of the first kind (see e.g. Rivlin (1990)). Observing that the left hand sides of (4.7) and (4.8) are increasing functions in k we obtain that (4.9) and (4.10) are implied by (4.7) and (4.8) and the assertion of the Corollary follows by an application of Theorem 4.1. \Box

Remark 4.1. Note that a similar argument as given in the proof of Theorem 4.1 shows that the conditions (4.2) and (4.3) will never be fulfilled if the maximum of the absolute values of the coefficients $|t_{d-2j}|/b^{d-2j}$ is obtained for two indices $d-2k_1, d-2k_2 \in I$. It is also worthwhile to mention that the index d-2k where the maximum is attained will depend heavily on the size of the interval [-b, b].

Finally, if the index set I consists only of indices that differ from d by an even number, then a detailed investigation of the proof of Theorem 4.1 shows that the assertion of this theorem holds for all b > 0.

Example 4.1. Let [a, b] = [-1, 1], $I = \{0, \ldots, d\}$ and $1 \le d \le 15$. Straightforward calculations show that the conditions of Corollary 4.1 are satisfied except in the cases d = 4, 5, 11 (note that for d = 4 and 11 the maximum of the absolute values of the coefficients of $T_d(x)$ occurs at two positions (see e.g. Davis (1963)). Corollary 4.1 yields that for d = 1, 2, 3 the design ξ_{d-4}^* for d = 6, 7, 8, 9, 10 the design ξ_{d-2}^* and for d = 12, 13, 14, 15 the design ξ_{d-4}^* is minimax optimal for the full parameter set $\{\vartheta_i\}_{i=0}^d$. By the results of Studden (1968) all these designs are supported at the Chebyshev points $s_{\nu} = \cos(((d - \nu)/d)\pi) \ (\nu = 0, \ldots, d)$ and the masses are given by (3.3). Finally in the case d = 5 we obtain by direct calculations that ξ_3^* is minimax optimal which shows that the conditions in Theorem 4.1 and Corollary 4.1 are only sufficient but not necessary.

To give an example for the application of Theorem 4.1 consider the case d = 6and the interval [-1, 1]. Here $T_6(x) = 32x^6 - 48x^4 + 18x^2 - 1$ and we obtain that for the index sets $\{0, 4\}$, $\{2, 4\}$ $\{4, 6\}$, $\{0, 2, 4\}$, $\{0, 4, 6\}$, $\{2, 4, 6\}$, $\{0, 2, 4, 6\}$ the minimax optimal design for the parameter subsystem $\{\vartheta_i\}_{i \in I}$ is given by ξ_4^* while for the index sets $\{0, 6\}$ and $\{2, 6\}$, $\{0, 2, 6\}$ the optimal design for the highest coefficient ξ_6^* is minimax optimal. Finally, for the parameter $\{\vartheta_0, \vartheta_2\}$ the minimax optimal designs is given by ξ_2^* . All minimax optimal designs for these subsets are supported at the Chebyshev points -1, $-\sqrt{3/4}$, -0.5, 0, 0.5, $\sqrt{3/4}$ and 1 while the masses will depend on the particular index set I and are given by (3.3). The results still hold if the index sets I contain also indices d - 2i - 1 according to condition (4.1).

Minimax designs on nonnegative or nonpositive intervals

Throughout this section we will assume that $0 \le a < b$. The case $a < b \le 0$ can be treated in exactly the same way and is omitted for the sake of brevity. The arguments are essentially the same as in Section 4 (involving more complicated algebra) and we will only sketch the main steps. In what follows let

$$T_d^*(x) = T_d(2x-1) = \sum_{j=0}^d t_{d-j}^* x^{d-j}, \quad x \in [0,1]$$

denote the Chebyshev polynomial of the first kind on the interval [0, 1] (orthogonal with respect to the measure $dx/\sqrt{x(1-x)}$ with $T_d^*(1) = 1$) and let

$$s_{\nu}^{*} = \frac{(b-a)\cos(((d-\nu)/d)\pi) + (b+a)}{2} \qquad (\nu = 0, \dots, m)$$

be the transformed Chebyshev points on the interval [a, b]. It is well known (see e.g. Abramowitz and Stegun (1964), p. 775, 22.3.3) that

(5.1)
$$t_{d-j}^* = (-1)^j \frac{\sqrt{\pi} d\Gamma(2d-j)}{\Gamma(j+1)\Gamma(d-j+1)\Gamma(d-j+1/2)} \quad (j=0,\dots,d)$$

(e.g. $T_2^*(x) = 8x^2 - 8x + 1$). If $L_{\nu}(x) = \sum_{j=0}^d \ell_{\nu,j}^* x^j$ denotes the Lagrange interpolation polynomial corresponding to $a = s_0^* < s_1^* < \cdots < s_{d-1}^* < s_d^* = b$, then we obtain in the same way as in Section 4 for every polynomial $P_d(x) = \sum_{j=0}^d a_j x^j$ of degree d that

(5.2)
$$a_j = \sum_{\nu=0}^d P_d(s_{\nu}^*) \ell_{\nu,j}^* \quad (j = 0, \dots, d).$$

Consider the interval [0, 1] and insert in (5.2) the two polynomials $(1-x)U_{d-1}^*(x)$ and $xU_{d-1}^*(x)$, where

$$U_{d-1}^*(x) = U_{d-1}(2x-1)$$

= $\sum_{j=0}^{d-1} u_j^* x^j = \sum_{j=0}^{d-1} (-1)^{d-1-j} \frac{\Gamma(3/2)\Gamma(d+1+j)}{\Gamma(j+3/2)\Gamma(j+1)\Gamma(d-j)} x^j$

is the Chebyshev polynomial of the second kind transformed to the interval [0, 1]. Thus a straighforward calculation yields that the Lagrange interpolation polynomials $L_0^{[0,1]}(x)$ and $L_d^{[0,1]}(x)$ with knots $s_{\nu}^* = (\cos(((d-\nu)/d)\pi) + 1)/2$ on the interval [0, 1] have coefficients $(u_{-1}^* = u_d^* = 0)$

$$\begin{split} \ell_{0,j}^{[0,1]} &= \frac{(-1)^j}{d} (u_j^* - u_{j-1}^*) = \frac{(-1)^j}{d} \frac{\Gamma(3/2)\Gamma(d+j)}{\Gamma(j+3/2)\Gamma(d-j+1)\Gamma(j+1)} \left\{ d^2 + \frac{j}{2} \right\}, \\ \ell_{d,j}^{[0,1]} &= \frac{(-1)^{d-j}}{d} u_{j-1}^* = \frac{(-1)^{d-j}}{d} \frac{\Gamma(3/2)\Gamma(d+j)}{\Gamma(j+1/2)\Gamma(j)\Gamma(d-j+1)}. \end{split}$$

The coefficients of the Lagrange interpolation polynomials $L_0(x)$ and $L_d(x)$ with knots $s_0^* < \cdots < s_d^*$ for an arbitrary interval [a, b] can now easily be obtained by a linear transformation

(5.3)
$$\ell_{0,i}^{*} = \frac{(-1)^{i}}{d} \sum_{j=i}^{d} \frac{a^{j-i}}{(b-a)^{j}} {j \choose i} \frac{\Gamma(3/2)\Gamma(d+j)}{\Gamma(j+3/2)\Gamma(d-j+1)\Gamma(j+1)} \left\{ d^{2} + \frac{j}{2} \right\},$$
$$\ell_{d,i}^{*} = \frac{(-1)^{d+i}}{d} \sum_{j=i}^{d} \frac{a^{j-i}}{(b-a)^{j}} {j \choose i} \frac{\Gamma(3/2)\Gamma(d+j)}{\Gamma(j)\Gamma(j+1/2)\Gamma(d-j+1)}$$

and for the coefficients of the Chebyshev polynomial $T_d(x-a)/(b-a) = \sum_{j=0}^d t_j^{[a,b]} \cdot x^j$ we have

(5.4)
$$t_k^{[a,b]} = \sum_{j=k}^d \binom{j}{k} \frac{a^{j-k}}{(b-a)^j} |t_j^*| \quad (k \in I).$$

We are now in a position to state a result analogous to Theorem 4.1. The proof uses the same arguments as the proof of the corresponding result in Section 4 (where Lemma 3.1 has to be replaced by Lemma 3.2) and is therefore omitted.

THEOREM 5.1. If $I \neq \{0\}$ and there exists an index $k \in I$ such that

(5.5)
$$\left|\frac{\ell_{0,i}^*}{\ell_{0,k}^*}\right| \le \left|\frac{t_k^{[a,b]}}{t_i^{[a,b]}}\right| \quad \text{for all } i \le k \text{ with } i \in I$$

and

(5.6)
$$\left|\frac{\ell_{d,i}^*}{\ell_{d,k}^*}\right| \le \left|\frac{t_k^{[a,b]}}{t_i^{[a,b]}}\right| \quad \text{for all } i \ge k \text{ with } i \in I$$

hold, where the quantities $\ell_{0,i}^*$, $\ell_{d,i}^*$ and $t_j^{[a,b]}$ are defined in (5.3) and (5.4), then the optimal design ξ_k^* for estimating the individual coefficient ϑ_k is also minimax optimal for the parameter system $\{\vartheta_i\}_{i \in I}$.

Remark 5.1. As in Section 4, the only appropriate candidate k in Theorem 5.1 is the index $k \in I$ where the absolute value of the coefficients of the Chebyshev polynomial $T_d(x-a)/(b-a) = \sum_{j=0}^d t_j^{[a,b]} x^j$ is maximal. The conditions (5.5) and (5.6) are easy to verify on a computer using the representation for the $l_{\nu,j}^*$ and $t_j^{[a,b]}$ given in (5.3) and (5.4), respectively.

Example 5.1. Consider the interval [a,b] = [1,2], $I = \{0,\ldots,d\}$ and polynomial regression models of degree $1 \leq d \leq 20$. Then it can easily be shown that the conditions (5.5) and (5.6) are satisfied except for d = 1 and d = 4. In these cases a direct calculation shows that the minimax optimal designs are given by ξ_1^* and ξ_2^* , respectively. All other cases are covered by Theorem 5.1, and we obtain the following minimax optimal designs for the full parameter set $\{\vartheta_i\}_{i=0}^d$; for d = 2, 3 the design ξ_{d-1}^* , for d = 4, 5, 6 the design ξ_{d-2}^* , for d = 7, 8 the design ξ_{d-3}^* , for d = 9, 10, 11 the design ξ_{d-4}^* , for d = 12, 13 the design ξ_{d-5}^* , for d = 14, 15, 16 the design ξ_{d-6}^* , for d = 17, 18 the design ξ_{d-7} and for d = 19, 20 the design ξ_{d-8}^* . All these designs are supported at the Chebyshev points on [1, 2], $s_{\nu}^* = (\cos(((d-\nu)/d)\pi)+3)/2$ ($\nu = 0, \ldots, d$) and the masses of ξ_{d-j}^* at the support points s_{ν} are proportional to $|\ell_{\nu,d-j}^*|$ (see Studden (1968)).

The situation in Theorem 5.1 becomes more transparent in the case a = 0, where $\sum_{j=\ell}^{d} {j \choose \ell} (a^{j-\ell}/(b-a)^{j}) |t_{j}^{*}| \ (\ell = i, k)$ reduces to the term $|t_{\ell}^{*}| \cdot b^{-\ell}$ and the conditions (5.5) and (5.6) have the same form as the corresponding conditions in Theorem 4.1. For the full parameter set $I = \{0, \ldots, d\}$ we obtain in this case an analogue of Corollary 4.1 which is stated here for the sake of completeness.

COROLLARY 5.1. If $I = \{0, ..., d\}$ and there exists an index k such that

(5.7)
$$\frac{(d-k)^2(d+k)^2}{k(k+1)(k+1/2)^2} \le b^2$$

and

(5.8)
$$\frac{(d+k-1)^2(d-k+1)^2}{k^2(k^2-1/4)} \cdot \frac{2d^2+k}{2d^2+k-1} \ge b^2$$

holds, then the optimal design ξ_k^* for estimating the individual coefficient of a polynomial regression on the interval [0,b] is also minimax optimal for the full parameter set $\{\vartheta_i\}_{i=0}^d$. Moreover, the only index k where (5.7) and (5.8) could be satisfied, is the index where the maximum in the set $\{|t_j^*|/b^j \mid j = 0, \ldots, d\}$ is attained.

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Appendix

PROOF OF LEMMA 3.1. Observing that the coefficients of the Lagrange interpolation polynomials have the sign pattern $\operatorname{sign}(\ell_{\nu,d-2i}) = (-1)^{d-\nu+i}$ (see e.g. Pukelsheim and Studden (1993)) we obtain that the assertion of the lemma is equivalent to

(A.1)
$$\left| \begin{pmatrix} \ell_{\nu,d-2i} & \ell_{\nu+1,d-2i} \\ \ell_{\nu,d-2i-2} & \ell_{\nu+1,d-2i-2} \end{pmatrix} \right| \ge 0$$

where $\nu \in \{0, \dots, \lfloor d/2 \rfloor - 1\}$ (here |A| denotes the determinant of the matrix A). Recalling the definition of $F\begin{pmatrix} j\\ \nu \end{pmatrix}$ in (3.1) we see that (A.1) is equivalent to

(A.2)
$$(-1) \cdot \left| \begin{pmatrix} F\begin{pmatrix} d-2i \\ \nu \end{pmatrix} & F\begin{pmatrix} d-2i \\ \nu+1 \end{pmatrix} \\ F\begin{pmatrix} d-2i-2 \\ \nu \end{pmatrix} & F\begin{pmatrix} d-2i-2 \\ \nu+1 \end{pmatrix} \end{pmatrix} \right| \ge 0.$$

In the following we will make use of the fact that

(A.3)
$$F\begin{pmatrix} d-2i\\ \nu \end{pmatrix} = c_{2i}(s_0, \dots, s_{\nu-1}, s_{\nu+1}, \dots, s_d)F\begin{pmatrix} d\\ \nu \end{pmatrix}$$

where $c_j(s_0, \ldots, s_{\nu-1}, s_{\nu+1}, \ldots, s_d)$ is the *j*-th elementary symmetric function of $s_0, \ldots, s_{\nu-1}, s_{\nu+1}, \ldots, s_d$, that is the coefficient of $x^{d-j}(-1)^{d-j}$ in the polynomial $\prod_{j=0, j \neq \nu}^d (x-s_j)$. To prove (A.3) observe the identity

$$\begin{vmatrix} 1 & \cdots & 1 & 1 & \cdots & 1 & 1 \\ s_0 & s_{\nu-1} & s_{\nu+1} & s_d & x \\ \vdots & & \vdots & \vdots & \vdots \\ s_0^d & \cdots & s_{\nu-1}^d & s_{\nu+1}^d & \cdots & s_d^d & x^d \end{vmatrix} \end{vmatrix}$$
$$= \prod_{j=0, j \neq \nu}^d (x - s_j) \cdot F\begin{pmatrix} d \\ \nu \end{pmatrix}$$
$$= F\begin{pmatrix} d \\ \nu \end{pmatrix} \cdot \sum_{j=0}^d x^{d-j} (-1)^j c_j (s_0, \dots, s_{\nu-1}, s_{\nu+1}, \dots, s_d)$$

(both polynomials have the same zeros $s_0, \ldots, s_{\nu-1}, s_{\nu+1}, \ldots, s_d$ and the same leading coefficient) and equate the coefficients of x^{d-2i} . For any symmetric set $\alpha_1 < \cdots < \alpha_d$ we obtain for the corresponding symmetric functions

$$c_{2i+1}(\alpha_1, \dots, \alpha_d) = 0, \quad c_{2i}(\alpha_1, \dots, \alpha_d) = (-1)^i c_i(\alpha_1^2, \dots, \alpha_d^2)$$

if d is even and

$$c_i(\alpha_1,\ldots,\alpha_d) = c_i(\alpha_1,\ldots,\alpha_{(d-1)/2},0,\alpha_{(d+3)/2},\ldots,\alpha_d)$$
$$= c_i(\alpha_1,\ldots,\alpha_{(d-1)/2},\alpha_{(d+3)/2},\ldots,\alpha_d)$$

if d is odd (here we used that $\alpha_{(d+1)/2} = 0$). This shows that (note that $s_{\nu} = -s_{d-\nu}$ and that $\nu \in \{0, \ldots, \lfloor d/2 \rfloor\}$)

$$\begin{aligned} c_{2i}(s_0, \dots, s_{\nu-1}, s_{\nu+1}, \dots, s_d) \\ &= c_{2i}(s_0, \dots, s_{\nu-1}, s_{\nu+1}, \dots, s_{d-\nu-1}, s_{d-\nu+1}, \dots, s_d) \\ &+ s_{d-\nu}c_{2i-1}(s_0, \dots, s_{\nu-1}, s_{\nu+1}, \dots, s_{d-\nu-1}, s_{d-\nu+1}, \dots, s_d) \\ &= (-1)^i c_i(s_0^2, \dots, s_{\nu-1}^2, s_{\nu+1}^2, \dots, s_d^2). \end{aligned}$$

Observing the last identity, (A.3), (A.2) and (A.1) the assertion of the theorem can now be written as

(A.4)
$$\left| \begin{pmatrix} c_i(s_0^2, \dots, s_{\nu-1}^2, s_{\nu+1}^2, \dots, s_d^2) & c_i(s_0^2, \dots, s_{\nu}^2, s_{\nu+2}^2, \dots, s_d^2) \\ c_{i+1}(s_0^2, \dots, s_{\nu-1}^2, s_{\nu+1}^2, \dots, s_d^2) & c_{i+1}(s_0^2, \dots, s_{\nu}^2, s_{\nu+2}^2, \dots, s_d^2) \end{pmatrix} \right| \ge 0.$$

Finally, we remark that

$$c_i(s_0^2, \dots, s_{\nu-1}^2, s_{\nu+1}^2, \dots, s_d^2) = c_i(s_0^2, \dots, s_{\nu-1}^2, s_{\nu+2}^2, \dots, s_d^2) + s_{\nu+1}^2 c_{i-1}(s_0^2, \dots, s_{\nu-1}^2, s_{\nu+2}^2, \dots, s_d^2)$$

and straightforward algebra shows that (A.4) and (therefore the assertion of the lemma) is equivalent to

$$\begin{aligned} & (s_{\nu}^2 - s_{\nu+1}^2) \\ & \cdot \left| \begin{pmatrix} c_i(s_0^2, \dots, s_{\nu-1}^2, s_{\nu+2}^2, \dots, s_d^2) & c_{i-1}(s_0^2, \dots, s_{\nu-1}^2, s_{\nu+2}^2, \dots, s_d^2) \\ c_{i+1}(s_0^2, \dots, s_{\nu-1}^2, s_{\nu+2}^2, \dots, s_d^2) & c_i(s_0^2, \dots, s_{\nu-1}^2, s_{\nu+2}^2, \dots, s_d^2) \end{pmatrix} \right| \ge 0 \end{aligned}$$

We have $s_{\nu}^2 - s_{\nu+1}^2 \ge 0$ (because $\nu \in \{0, \ldots, \lfloor d/2 \rfloor - 1\}$ and the nonnegativity of the second factor is a well known result in the theory of symmetric functions (see e.g. Beckenbach and Bellman (1965), p. 11). This completes the proof of Lemma 3.1.

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