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OPTIMAL DESIGNS FOR A CLASS OF POLYNOMIALS OF ODD OR EVEN DEGREE

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In the class of polynomials of odd (or even) degree up to the order $2r-1$ $(2r)$ optimal designs are determined which minimize a product of the variances of the estimates for the highest coefficients weighted with a prior $\gamma = (\gamma_1, \dots, \gamma_r)$, where the numbers γ_j correspond to the models of degree $2j-1$ $(2j)$ for $j = 1, \dots, r$. For a special class of priors, optimal designs of a very simple structure are calculated generalizing the D_1-optimal design for polynomial regression of degree $2r-1$ $(2r)$. The support of these designs splits up in three sets and the masses of the optimal design at the support points of every set are all equal.

The results are derived in a general context using the theory of canonical moments and continued fractions. Some applications are given to the D-optimal design problem for polynomial regression with vanishing coefficients of odd (or even) powers.

1. Introduction. Consider a polynomial regression model of degree $n \in \mathbb{N}$

$$g_n(x) = \sum_{i=0}^{n} \alpha_{n,i} x^i.$$

For each $x \in [-1, 1]$, a random variable $Y(x)$ with mean $g_n(x)$ and variance $\sigma^2 > 0$ can be observed. A design ξ is a probability measure on $[-1, 1]$. ξ is called an exact design consisting of N observations if ξ puts only masses $\xi(\{x_i\})$ at the points x_i, $i = 1, \dots, r$, subject to the restriction that $n_i = N\xi(\{x_i\})$ is an integer for all $i = 1, \dots, r$. In this case the experimenter takes N uncorrelated observations, n_i at each x_i, $i = 1, \dots, r$, and the covariance matrix of the least squares estimates for the unknown parameter vector $\alpha^{(n)} = (\alpha_{n,0}, \dots, \alpha_{n,n})$ is given by $(\sigma^2/N)M_n^{-1}(\xi)$, where

$$M_n(\xi) = \int_{-1}^{1} (1, \dots, x^n)^T (1, \dots, x^n)\, d\xi(x) \tag{1.1}$$

denotes the information matrix of the design ξ.

Almost all optimality criteria which can be used to discriminate between competing designs depend on the information matrix $M_n(\xi)$. In this paper we consider some generalizations of the famous D- and D_1-optimality criteria which depend on the determinants $\det M_l(\xi)$, $l = 1, \dots, n$, and are given below. The determinants $\det M_l(\xi)$ can be expressed in terms of the canonical

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moments of the design ξ and the optimal designs can be identified by its canonical moments [see Studden (1980, 1982a, b, 1989), Lau (1983, 1988), Lau and Studden (1985), Lim and Studden (1988) for more details]. In Section 2 we give a short review of this theory and determine explicit representations of designs corresponding to some special sequences of canonical moments.

In many practical experiments the form of the regression model (namely g_n) is not known by the experimenter. Classical optimal design theory is not applicable because it is generally based on the assumption of a given model. Läuter (1974) proposed a generalized D-optimality criterion under the assumption that the (unknown) model belongs to a given set of regression models and proved a Kiefer–Wolfowitz-type equivalence theorem. The optimal design with respect to Läuter's criterion allows good estimates in every model of the given set. A similar generalization of the integrated variance criterion was considered by Cook and Nachtsheim (1982). It is the purpose of this paper to determine explicit solutions of the design problem proposed by Läuter (1974) in the case of polynomial regression which generalize some results obtained by Dette (1990, 1991). To this end let

$$\mathscr{F}_n = \{g_l | l = 1, \dots, n\}$$

denote the set of all polynomial regression models up to degree $n \in \mathbb{N}$. A vector $\beta = (\beta_1, \dots, \beta_n)$ of positive numbers with $\sum_{l=1}^{n} \beta_l = 1$ is called prior for $\mathscr{F}_n$. The quantity β_l can be interpreted as a measure for the experimenter's belief about the adequacy of the model g_l. For a given prior β we call a design ξ_β optimal for the class $\mathscr{F}_n$ with respect to the prior β if ξ_β maximizes the function

$$\Psi_\beta(\xi) = \sum_{l=1}^{n} \frac{\beta_l}{l+1} \log[\det M_l(\xi)]. \tag{1.2}$$

Dette (1990) determined the optimal design for $\mathscr{F}_n$ with respect to the prior β in terms of canonical moments and identified a class of priors depending on a real parameter $z \in \{0\} \cup [1, \infty)$ which yields to optimal designs with a similar structure as the classical $D - (z = 1)$ and $D_1 - (z = 0)$ optimal design for polynomial regression of degree $n \in \mathbb{N}$. The support of the optimal design for the class $\mathscr{F}_n$ with respect to a prior $\beta(z)$ is given by the zeros of an orthogonal polynomial and all interior support points attain equal masses [see Hoel (1958), Kiefer and Wolfowitz (1959) and Studden (1982b)].

Sometimes an experimenter has more information about the adequacy of the models of $\mathscr{F}_n$. For example, it could be clear (from physical considerations) that the degree of the polynomial model which has to be fitted is even (or odd) and an upper bound say $n = 2r$ (or $n = 2r - 1$) is given by the experimenter. To get information about the exact degree, one could be interested in most precise estimates of the highest coefficients $\alpha_{2l,2l}$ (or $\alpha_{2l+1,2l+1}$) in the models g_{2l} (or g_{2l+1}). Because for a given design ξ, the variance of the estimate $\hat{\alpha}_{l,l}$ for $\alpha_{l,l}$ in the model g_l is proportional to $\det M_{l-1}(\xi)/\det M_l(\xi)$, a reasonable criterion to choose an experimental design is the maximization of

$$(1.3)\qquad \sum_{l=1}^{r} \gamma_l \log\left[\frac{\det M_{2l}(\xi)}{\det M_{2l-1}(\xi)}\right]$$

in the case of polynomial models of even degree and

$$(1.4)\qquad \sum_{l=1}^{r} \gamma_l \log\left[\frac{\det M_{2l-1}(\xi)}{\det M_{2l-2}(\xi)}\right]$$

in the case of polynomial models of odd degree. We call a design ξ_γ D_1-optimal for the class of polynomials of even (or odd) degree with respect to the prior $\gamma = (\gamma_1, \dots, \gamma_r)$ if ξ_γ maximizes the function defined in (1.3) [or (1.4)]. It is easy to see that (1.3) and (1.4) are obtained from the function $\Psi_\beta(\xi)$ for the priors

$$(1.5)\qquad \beta = (-2\gamma_1, 3\gamma_1, \dots, -2r\gamma_r, (2r+1)\gamma_r)$$

and

$$(1.6)\qquad \beta = (2\gamma_1, -3\gamma_2, \dots, -(2r-1)\gamma_r, 2r\gamma_r),$$

respectively. In order to determine D_1-optimal designs for the class of polynomials of even (or odd) degree, we also allow negative weights β_l in the optimality criterion (1.2) subject to the restriction

$$(1.7)\qquad \sigma_i := \sum_{l=i}^{n} \frac{l+1-i}{l+1}\beta_l > 0, \qquad i = 1, \dots, n,$$

which guarantees the existence of an optimal design for the class $\mathscr{F}_n$ with respect to the prior β supported by $n+1$ points (see Proposition 2.2.).

In Section 3 we will identify a class of priors which yield to D_1-optimal designs for the class of polynomials of even (or odd) degree with a very simple structure. For example, in the case of equal weights $\gamma_l = 1/r$ the D_1-optimal design for the class of polynomials of odd degree [i.e., the design maximizing (1.4)] puts equal masses at the zeros of the polynomial

$$(1 - x^2)\left[C_{r-1}^{(3/2)}(T_2(x)) + C_{r-2}^{(3/2)}(T_2(x))\right].$$

Here $C_l^{(\alpha)}(x)$, $\alpha > -1/2$, denotes the lth ultraspherical polynomial which is the lth orthogonal polynomial with respect to the measure $(1-x^2)^{\alpha-1/2}\,dx$ and $T_l(x)$ denotes the lth Chebyshev polynomial of the first kind orthogonal with respect to the measure $(1-x^2)^{-1/2}\,dx$ [see Szegö (1959), page 81 or Abramowitz and Stegun (1964) for more details concerning these polynomials]. In Section 4 similar results are obtained for polynomials with vanishing coefficients of the odd (or even) powers. Among other things it is shown that the D-optimal design for the model $h_{2r}(x) = \sum_{l=0}^{r} \alpha_{l,l} x^{2l}$ on the interval $[-1,1]$ puts equal masses $1/(2(r+1))$ at the zeros of the polynomial $(1 - x^2)C_{r-1}^{(3/2)}(T_2(x))$ and mass $1/(r+1)$ at the point 0.

2. Canonical moments. In order to determine designs maximizing the function Ψ_β in (1.2), a short description of the theory of canonical moments is needed. More details and applications (in optimal design theory) can be found in the papers of Skibinsky (1967, 1968, 1969, 1986), Studden (1980, 1982a, 1982b, 1989) and Lau (1983, 1988). For an arbitrary design ξ on $[-1,1]$ let $c_k = \int_{-1}^{1} x^k \, d\xi(x)$ denotes the kth moment ($k = 0, 1, \dots$). The canonical moments are defined as follows. For a given set of moments $c_0, c_1, \dots, c_{i-1}$, let c_i^+ denote the maximum value of the ith moment over the set of measures having the given set of moments $c_0, \dots, c_{i-1}$ and let c_i^- denote the corresponding minimum value. The canonical moments are defined by

$$p_i = \frac{c_i - c_i^-}{c_i^+ - c_i^-}, \qquad i = 1, 2, \dots .$$

Note that $0 \le p_i \le 1$ and that the canonical moments are left undefined whenever $c_i^+ = c_i^-$. If i is the first index for which equality holds, then $0 < p_k < 1$, $k = 1, \dots, i-2$, and p_{i-1} must have the value 0 or 1 [see Skibinsky (1986)]. The determinants of the information matrices $M_l(\xi)$ can easily be expressed in terms of canonical moments [see Skibinsky (1968), Studden (1982b, 1988)].

PROPOSITION 2.1. *Let $q_j := 1 - p_j$ ($j \ge 1$), $\zeta_1 = p_1$ and $\zeta_j = q_{j-1}p_j$ ($j \ge 2$), then we have for the determinant of $M_l(\xi)$ defined by* (1.1),

$$\det M_l(\xi) = 2^{l(l+1)} \prod_{j=1}^{l} (\zeta_{2j-1}\zeta_{2j})^{l+1-j}, \qquad l = 0, 1, \dots, n.$$

The maximization of Ψ_β can now be carried out in terms of canonical moments. Straightforward algebra yields the following [see Dette (1990)].

PROPOSITION 2.2. *The optimal design ξ_β for the class $\mathscr{F}_n$ with respect to the prior β is uniquely determined by the canonical moments*

$$(2.1) \qquad \begin{aligned} p_{2i-1}(\xi_\beta) &= \frac{1}{2}, && i = 1, \dots, n, \\ p_{2i}(\xi_\beta) &= \frac{\sigma_i}{\sigma_i + \sigma_{i+1}}, && i = 1, \dots, n-1, \\ p_{2n}(\xi_\beta) &= 1, \end{aligned}$$

where the numbers σ_i are defined in (1.7).

The support of the design ξ_β corresponding to the canonical moments (2.1) is given by the zeros of the polynomial $(1 - x^2)Q_{n-1}(x, \xi_\beta)$, where $Q_k(x, \xi_\beta)$, $k = 0, 1, \dots$, are the polynomials of degree k orthogonal with respect to the measure $(1 - x^2)\, d\xi_\beta(x)$ [see Studden (1982b)]. A recursive relation of the polynomials $Q_k(x, \xi_\beta)$ and a representation of the weights at the support points using an equivalence theorem of Kiefer–Wolfowitz-type are given in

Dette (1990). It seems to be intractable to give analytic expressions of the weights and the polynomials $Q_k(x, \xi_\beta)$ for arbitrary sequences of canonical moments defined by (2.1). Nevertheless, Dette (1990) showed that the design corresponding to the sequence

$$
\begin{aligned}
p_{2i-1} &= \frac{1}{2}, \qquad i = 1, \dots, n,\\
p_{2i} &= \frac{z+n-i}{z+2(n-i)}, \qquad i = 1, \dots, n-1, \qquad (2.2)\\
p_{2n} &= 1
\end{aligned}
$$

for $z \in \{0\} \cup [1, \infty)$, is supported by the zeros of the polynomial $(1 - x^2)C_{n-1}^{((z+2)/2)}(x)$ and the masses at all interior support points are equal $1/(n + z)$ while the masses at the points -1 and 1 are given by $(z+1)/(2(n+z))$. Here $C_l^{(\alpha)}(x)$, $\alpha > -1/2$, denotes the lth ultraspherical polynomial which is the lth orthogonal polynomial with respect to the measure $(1 - x^2)^{\alpha - 1/2}\,dx$. The canonical moments of (2.2) correspond to optimal designs for $\mathscr{F}_n$ with respect to special priors $\beta(z)$, where $z \in \{0\} \cup [1, \infty)$. The cases $z = 0$ and $z = 1$ give the canonical moments of the D_1- and D-optimal design and were solved earlier by Studden (1982b). In the case $z = 2$ the sequence (2.2) corresponds to the optimal design for the class $\mathscr{F}_n$ with respect to a prior which puts equal weight on all the models of $\mathscr{F}_n$ [see Dette (1990)]. For $z = q \in \mathbb{N}$ the sequence (2.2) also appears in the determination of D-optimal product designs for multivariate polynomial regression on the q-cube [see Lim and Studden (1988)].

In the following we will give some generalizations of these results which can be used to solve the design problems described in the introduction. To this end let $T_l(x)$ denote the lth Chebyshev polynomial of the first kind and $U_l(x)$ the lth Chebyshev polynomial of the second kind which are the orthogonal polynomials with respect to the measures $(1 - x^2)^{-1/2}\,dx$ and $(1 - x^2)^{1/2}\,dx$, respectively [see Szegö (1959) or Abramowitz and Stegun (1964)]. For $k \in \mathbb{N}$, $r \in \mathbb{N}$, $m \in \mathbb{N}_0 = \mathbb{N} \cup \{0\}$, $m < 2k$ and $z > -1$, define the following sequences of canonical moments:

$$
\begin{aligned}
p_{2kj-m} &= \frac{r-j+z}{2(r-j)+z}, \qquad j = 1, \dots, r-1,\\
p_{2kr-m} &= 1, \qquad (2.3)\\
p_i &= \frac{1}{2}, \qquad \text{otherwise } (i < 2kr - m),
\end{aligned}
$$

$$
\begin{aligned}
p_{2kj-m} &= \frac{r-j}{2(r-j)+z}, \qquad j = 1, \dots, r-1,\\
p_{2kr-m} &= 0, \qquad (2.4)\\
p_i &= \frac{1}{2}, \qquad \text{otherwise } (i < 2kr - m).
\end{aligned}
$$

The following theorem gives the support of designs corresponding to sequences of the form (2.3) or (2.4).

THEOREM 2.3. *Let $k \in \mathbb{N}$, $r \in \mathbb{N}$, $m \in \mathbb{N}_0$, $m < 2k$ and $z > -1$.*

(a) *The design corresponding to the sequence of canonical moments given in* (2.3) *is supported by the zeros of the polynomial*

$$(1 - x^2)\left[U_{k-1-p}(x)C_{r-1}^{((z+2)/2)}(T_k(x)) + U_{p-1}(x)C_{r-2}^{((z+2)/2)}(T_k(x))\right]$$

if $m = 2p$ ($p \in \mathbb{N}_0$, $p < k$) is an even number and supported by the zeros of the polynomial

$$(1 - x)\Big[\{U_{k-p}(x) + U_{k-p-1}(x)\}C_{r-1}^{((z+2)/2)}(T_k(x)) + \{U_{p-1}(x) + U_{p-2}(x)\}C_{r-2}^{((z+2)/2)}(T_k(x))\Big]$$

if $m = 2p - 1$ ($p \in \mathbb{N}, 2p - 1 < 2k$) is odd.

(b) *The design corresponding to the sequence of canonical moments given in* (2.4) *is supported by the zeros of the polynomial*

$$T_{k-p}(x)C_{r-1}^{((z+2)/2)}(T_k(x)) - T_p(x)C_{r-2}^{((z+2)/2)}(T_k(x))$$

if $m = 2p$ ($p \in \mathbb{N}_0, p < k$) is even and supported by the zeros of the polynomial

$$(1 + x)\Big[\{U_{k-p}(x) - U_{k-p-1}(x)\}C_{r-1}^{((z+2)/2)}(T_k(x)) - \{U_{p-1}(x) - U_{p-2}(x)\}C_{r-2}^{((z+2)/2)}(T_k(x))\Big]$$

if $m = 2p - 1$ ($p \in \mathbb{N}, 2p - 1 < 2k$) is odd.

To prove Theorem 2.3, we need some results concerning the theory of continued fractions [see Perron (1954) or Wall (1948)]. To this end let

$$b_0 + \frac{a_1|}{|b_1} + \frac{a_2|}{|b_2} + \frac{a_3|}{|b_3} + \cdots$$

denote a continued fraction and its nth convergent by ($A_{-1} = B_{-1} = 0$, $A_0 = b_0$, $B_0 = 1$)

$$b_0 + \frac{a_1|}{|b_1} + \frac{a_2|}{|b_2} + \cdots + \frac{a_n|}{|b_n} =: \frac{A_n}{B_n}.$$

It is known [see Perron (1952), page 4] that the numerator A_n and denominator B_n of the nth convergent are given by the determinants

$$A_n = K\begin{pmatrix} & a_1 & \cdots & a_n & \\ b_0 & & \cdots & & b_n \end{pmatrix} := \det\begin{pmatrix} b_0 & -1 & & & \\ a_1 & b_1 & -1 & & \\ & & \ddots & & \\ & & & & -1 \\ & & & a_n & b_n \end{pmatrix},$$

$$B_n = K\begin{pmatrix} & a_2 & \cdots & a_n & \\ b_1 & & \cdots & & b_n \end{pmatrix} = \det\begin{pmatrix} b_1 & -1 & & & \\ a_2 & b_2 & -1 & & \\ & & \ddots & & \\ & & & & -1 \\ & & & a_n & b_n \end{pmatrix}.$$

In the proof of Theorem 2.3, continued fractions are involved which are of the following form:

$$
\begin{aligned}
L_l(x) := {} & \frac{f_0|}{|x} + \underbrace{\frac{a|}{|x} + \cdots + \frac{a|}{|x}}_{l-2} + \frac{f_1|}{|x} + \frac{f_2|}{|x} + \underbrace{\frac{a|}{|x} \cdots + \frac{a|}{|x}}_{k-2} \\
& + \frac{f_3|}{|x} + \cdots + \frac{f_{2r-2}|}{|x} + \underbrace{\frac{a|}{|x} + \cdots + \frac{a|}{|x}}_{k-2},
\end{aligned} \tag{2.5}
$$

and we have to find a suitable representation of the denominator of (2.5). By a contraction of (2.5) in the way that the convergents of the transformed continued fraction attain the values

$$\frac{A_{l-1}}{B_{l-1}}, \frac{A_{k+l-1}}{B_{k+l-1}}, \frac{A_{2k+l-1}}{B_{2k+l-1}}, \dots$$

successively [see Perron (1954), pages 11–12], the following result can be obtained by straightforward algebra.

Lemma 2.4. *Let* $D_{-1}(x) := 0$, $D_0(x) := 1$ *and*

$$D_l(x) = K\begin{pmatrix} & \overbrace{a \cdots a}^{l-1} & \\ x & \cdots & x \end{pmatrix}.$$

For the continued fraction in (2.5) *the representation* $L_l(x) = M_l(x)/N_l(x)$ *holds, where*

$$
\begin{aligned}
N_l(x) = K\Bigg(& \begin{matrix} (-1)^{k-1} f_2 f_3 a^{k-2} D_{l-1}(x) \\ D_{l-1}(x)[xD_{k-1}(x) + f_2 D_{k-2}(x)] + f_1 D_{l-2}(x) D_{k-1}(x) \end{matrix} \\
& \begin{matrix} (-1)^{k-1} f_4 f_5 a^{k-2} & \cdots & (-1)^{k-1} f_{2r-4} f_{2r-3} a^{k-2} \\ xD_{k-1}(x) + (f_3 + f_4) D_{k-2}(x) & \cdots & xD_{k-1}(x) + (f_{2r-2} + f_{2r-2}) D_{k-2}(x) \end{matrix} \Bigg)
\end{aligned} \tag{2.6}
$$

and

$$
\begin{aligned}
M_l(x) = {} & f_0 \frac{D_{l-2}(x)}{D_{l-1}(x)} N_l(x) + (-1)^{l-1} a^{l-2} f_0 f_1 \frac{D_{k-1}(x)}{D_{l-1}(x)} \\
& \times K\begin{pmatrix} (-1)^{k-1} f_4 f_5 a^{k-2} & \cdots & (-1)^{k-1} f_{2r-4} f_{2r-3} a^{k-2} \\ xD_{k-1}(x) + (f_3 + f_4) D_{k-2}(x) & \cdots & xD_{k-1}(x) + (f_{2r-3} + f_{2r-2}) D_{k-2}(x) \end{pmatrix}.
\end{aligned} \tag{2.7}
$$

We are now able to give the proof of Theorem 2.3.

Proof of Theorem 2.3. Consider the case (b) and even $m = 2p$. The other cases are treated similarly. Let $G(x)$ denote the Stieltjes transform of the measure corresponding to the canonical moments in (2.4). It is known [see

Wall (1948) or Perron (1954)] that $G(x)$ has a continued fraction expansion of the form

$$
\begin{aligned}
G(x) = \int_{-1}^{1} \frac{d\xi(t)}{x-t} &= \frac{1|}{|x+1-2\zeta_1} - \frac{4\zeta_1\zeta_2|}{|x+1-2(\zeta_2+\zeta_3)} \\
&\quad - \cdots - \frac{4\zeta_{2kr-2p-3}\zeta_{2kr-2p-2}|}{|x+1-2(\zeta_{2kr-2p-2}+\zeta_{2kr-2p-1})},
\end{aligned} \tag{2.8}
$$

where the number ζ_j are defined in Proposition 2.1. Assume $p < k-1$ and $k > 1$ (the case $p = k-1$ and $k = 1$ are treated similarly), from (2.4) we have

$$
\begin{aligned}
4\zeta_1\zeta_2 &= \frac{1}{2}, \qquad \zeta_{2j}+\zeta_{2j+1} = \frac{1}{2}, \qquad j = 1,\dots,kr-p-1, \\
4\zeta_{2kj-2p-1}\zeta_{2kj-2p} &= \frac{1}{2}\frac{r-j}{2(r-j)+z} =: -f_{2j-1}, \qquad j = 1,\dots,r-1, \\
4\zeta_{2kj-2p+1}\zeta_{2kj-2p+2} &= \frac{1}{2}\frac{r-j+z}{2(r-j)+z} =: -f_{2j}, \qquad j = 1,\dots,r-1, \\
4\zeta_{2i-1}\zeta_{2i} &= \frac{1}{4}, \qquad \text{otherwise } (i < kr-p).
\end{aligned} \tag{2.9}
$$

From (2.8) it follows that the design ξ corresponding to the canonical moments in (2.4) is supported by the zeros of the denominator of $G(x)$ which is given by the polynomial ($a = -1/4$):

$$
\begin{aligned}
Q(x,\xi) &= xK\begin{pmatrix} \overbrace{a\ \cdots\ a}^{k-p-2} f_1 f_2 \overbrace{a\ \cdots\ a}^{k-2} f_3 f_4 a \ \cdots\ a f_{2r-3} f_{2r-2} \overbrace{a\ \cdots\ a}^{k-2} \\ x \qquad\qquad\qquad \cdots \qquad\qquad\qquad x \end{pmatrix} \\
&\quad - \frac{1}{2}K\begin{pmatrix} \overbrace{a\ \cdots\ a}^{k-p-2} f_1 f_2 \overbrace{a\ \cdots\ a}^{k-2} f_3 f_4 a \ \cdots\ a f_{2r-3} f_{2r-2} \overbrace{a\ \cdots\ a}^{k-2} \\ x \qquad\qquad\qquad \cdots \qquad\qquad\qquad x \end{pmatrix} \\
&=: xQ_{k-p}(x) - \frac{1}{2}Q_{k-p-1}(x).
\end{aligned}
$$

The polynomials $Q_l(x)$ are the polynomials in the denominator of the continued fraction given in (2.5) and we can apply Lemma 2.4. To this end, let $F_0^{((z+2)/2)}(x) := 1$, $F_1^{((z+2)/2)}(x) = x$ and

$$
F_l^{((z+2)/2)}(x) := K\begin{pmatrix} & -\dfrac{(l-1)(l+z)}{(z+2l-2)(z+2l)} & -\dfrac{(l-2)(l+z-1)}{(z+2l-4)(z+2l-2)} & \cdots & -\dfrac{1}{z+4} & \\ x & & \cdots & & & x \end{pmatrix}. \tag{2.10}
$$

It can be shown that the polynomials $F_l^{((z+2)/2)}(x)$ are proportional to the ultraspherical polynomials $C_l^{((z+2)/2)}(x)$ [see Abramowitz and Stegun (1964)], that is,

$$F_l^{((z+2)/2)}(x) = \left[\frac{2^l\Gamma(l+(z+2)/2)}{\Gamma(l+1)\Gamma((z+2)/2)}\right]^{-1} C_l^{((z+2)/2)}(x). \tag{2.11}$$

Moreover we have from (2.9) for the polynomials $D_l(x)$ defined by Lemma 2.4 [see Abramowitz and Stegun (1964), formula 22.5.7]

$$D_l(x) = K\begin{pmatrix} & -\frac{1}{4} & \cdots & -\frac{1}{4} & \\ x & & \cdots & & x \end{pmatrix} = \frac{1}{2^l}U_l(x), \tag{2.12}$$

$$\begin{aligned} xD_{k-1}(x) - \frac{1}{2}D_{k-2}(x) &= \left(\frac{1}{2}\right)^{k-1}[xU_{k-1}(x) - U_{k-2}(x)] \\ &= \left(\frac{1}{2}\right)^{k-1} T_k(x). \end{aligned} \tag{2.13}$$

Observing (2.9), (2.10), (2.12) and (2.13), the polynomials $N_l(x)$ in Lemma 2.4 can be calculated as follows ($l = k-p, l = k-p-1$):

$$\begin{aligned} N_l(x) &= \left(\frac{1}{2}\right)^{(r-1)(k-1)+(l-1)} \\ &\quad\times\Bigg[-\frac{r-1+z}{z+2r-2}\,\frac{r-2}{z+2r-4}U_{l-1}(x)F_{r-3}^{((z+2)/2)}(T_k(x)) \\ &\qquad+\Bigg\{U_{l-1}(x)\left\{xU_{k-1}(x) - \frac{r-1+z}{z+2r-2}U_{k-2}(x)\right\} \\ &\qquad\qquad-\frac{r-1}{z+2r-2}U_{l-2}(x)U_{k-1}(x)\Bigg\}F_{r-2}^{((z+2)/2)}(T_k(x))\Bigg] \\ &= \left(\frac{1}{2}\right)^{(r-1)(k-1)+(l-1)}\Bigg[U_{l-1}(x)F_{r-1}^{((z+2)/2)}(T_k(x)) \\ &\qquad+\frac{r-1}{z+2r-2}U_{k-l-1}(x)F_{r-2}^{((z+2)/2)}(T_k(x))\Bigg], \end{aligned}$$

where the last row results from (2.13), a recursive relation of the polynomials $F_l^{((z+2)/2)}(x)$ and the fact

$$U_{l-1}(x)U_{k-2}(x) - U_{l-2}(x)U_{k-1}(x) = U_{k-l-1}(x) \tag{2.14}$$

[see Abramowitz and Stegun (1964), page 782]. Using similar arguments (2.9), (2.10), (2.12), (2.13), (2.14) and the representation of $N_l(x)$ it can be shown that the function $M_l(x)$ defined by (2.7) is a polynomial, that is, ($f_0 = 1$)

$$\begin{aligned} M_l(x) = \left(\frac{1}{2}\right)^{(r-1)(k-1)+(l-2)}\Bigg[&U_{l-2}(x)F_{r-1}^{((z+2)/2)}(T_k(x)) \\ &+\frac{r-1}{z+2r-2}U_{k-l}(x)F_{r-2}^{((z+2)/2)}(T_k(x))\Bigg]. \end{aligned} \tag{2.15}$$

Because the polynomial $Q_l(x)$ is the denominator of the continued fraction (2.5), we obtain from Lemma 2.4, (2.14) and (2.15) that the design ξ corresponding to the canonical moments in (2.4) is supported by zeros of the polynomial

$$Q(x,\xi) = xQ_{k-p}(x) - \frac{1}{2}Q_{k-p-1}(x) = xN_{k-p}(x) - \frac{1}{2}N_{k-p-1}(x)$$
$$= \left(\frac{1}{2}\right)^{(k-1)r-p}\Bigg[\{xU_{k-p-1}(x) - U_{k-p-2}(x)\}F_{r-1}^{((z+2)/2)}(T_k(x)) + \frac{r-1}{z+2r-2}\{xU_{p-1}(x) - U_{p-2}(x)\}F_{r-2}^{((z+2)/2)}(T_k(x))\Bigg].$$

From (2.11) and (2.13), we have

$$Q(x,\xi) = \frac{\Gamma(r)\Gamma((z+2)/2)}{\Gamma(r+(z/2))}\left(\frac{1}{2}\right)^{rk-p-1} \times\{T_{k-p}(x)C_{r-1}^{((z+2)/2)}(T_k(x)) - T_p(x)C_{r-2}^{((z+2)/2)}(T_k(x))\}$$

which proves the assertion of the theorem. □

The weights at the support points x_j of the design corresponding to the sequences of canonical moments (2.3) and (2.4) can be calculated using a partial fraction expansion of the Stieltjes transform $G(x)$. For the sequence (2.4), the denominator of the Stieltjes transform (2.8) is given by the polynomial $N_{k-p}(x)$ and this yields

$$\xi(\{x_j\}) = G(x)(x-x_j)\big|_{x=x_j} = \frac{N_{k-p}(x_j)}{(d/dx)Q(x,\xi)|_{x=x_j}}$$
$$(2.16)\qquad = \frac{U_{k-p-1}(x_j)C_{r-1}^{((z+2)/2)}(T_k(x_j)) + U_{p-1}(x_j)C_{r-2}^{((z+2)/2)}(T_k(x_j))}{(d/dx)\left[T_{k-p}(x)C_{r-1}^{((z+2)/2)}(T_k(x)) - T_p(x)C_{r-2}^{((z+2)/2)}(T_k(x))\right]\Big|_{x=x_j}}.$$

The expression (2.16) can be reduced essentially in the cases $m=0$ and $m=k$. For example, in the case $k=2p=m$, the denominator of (2.16) is given by [note $(d/dx)C_n^{(\alpha)}(x) = 2\alpha C_{n-1}^{(\alpha+1)}(x)$]

$$\frac{d}{dx}Q(x,\xi) = \frac{d}{dx}\left[T_p(x)\{C_{r-1}^{((z+2)/2)}(T_{2p}(x)) - C_{r-2}^{((z+2)/2)}(T_{2p}(x))\}\right]$$
$$(2.17)\qquad = pU_{p-1}(x)\{C_{r-1}^{((z+2)/2)}(T_{2p}(x)) - C_{r-2}^{((z+2)/2)}(T_{2p}(x))\} + 2p(z+2)T_p(x)U_{2p-1}(x) \times\{C_{r-2}^{((z+4)/2)}(T_{2p}(x)) - C_{r-3}^{((z+4)/2)}(T_{2p}(x))\}.$$

From Theorem 2.3, the support points x_j are given by the zeros of the polynomial $Q(x,\xi) = T_p(x)\{C_{r-1}^{((z+2)/2)}(T_{2p}(x)) - C_{r-2}^{((z+2)/2)}(T_{2p}(x))\}$. If $T_p(x_j) =$

0, it follows that $T_{2p}(x_j) = -1$ and we obtain from (2.16) and $C_n^{((z+2)/2)}(-1) = (-1)^n\Gamma(n+z+2)/(\Gamma(n+1)\Gamma(z+2))$ [see Abramowitz and Stegun (1964), page 777] by straightforward algebra that

$$\xi(\{x_j\}) = \frac{z+1}{p(z+2r-1)} \quad \text{if } T_p(x_j) = 0.$$

Now consider the case $C_{r-1}^{((z+2)/2)}(T_{2p}(x_j)) = C_{r-2}^{((z+2)/2)}(T_{2p}(x_j))$. Observing formula 22.7.21 in Abramowitz and Stegun (1964), the recurrence relation of the ultraspherical polynomials and the equation $T_p(x)U_{2p-1}(x) - U_{p-1}(x)T_{2p}(x) = U_{p-1}(x)$ it follows from (2.17) and straightforward calculations that

$$\begin{aligned}
&\frac{d}{dx}Q(x_j,\xi)\\
&\quad= \frac{2pT_p(x_j)U_{2p-1}(x_j)}{1-T_{2p}^2(x_j)}\\
&\qquad\times\Big[(z+r)C_{r-2}^{((z+2)/2)}\big(T_{2p}(x_j)\big) - (r-1)T_{2p}(x_j)C_{r-1}^{((z+2)/2)}\big(T_{2p}(x_j)\big)\\
&\qquad -(z+r-1)C_{r-3}^{((z+2)/2)}\big(T_{2p}(x_j)\big) + (r-2)T_{2p}(x_j)C_{r-2}^{((z+2)/2)}\big(T_{2p}(x_j)\big)\Big]\\
&\quad= 2pU_{p-1}(x_j)\Big[(r-1)C_{r-1}^{((z+2)/2)}\big(T_{2p}(x_j)\big) + (z+r)C_{r-2}^{((z+2)/2)}\big(T_{2p}(x_j)\big)\Big]\\
&\quad= 2pU_{p-1}(x_j)C_{r-2}^{((z+2)/2)}\big(T_{2p}(x_j)\big)[z+2r-1].
\end{aligned}$$

From (2.16), we have ($k = 2p$):

$$\xi(\{x_j\}) = \frac{1}{p(z+2r-1)} \quad \text{if } C_{r-1}^{((z+2)/2)}\big(T_{2p}(x_j)\big) - C_{r-2}^{((z+2)/2)}\big(T_{2p}(x_j)\big) = 0.$$

In other cases a similar reasoning holds. The results are stated in the following theorems [we have proved Theorem 2.6(b1) here].

THEOREM 2.5. *Let $m = 0$ and $k, r \in \mathbb{N}$.*

(a) *The design ξ corresponding to the canonical moments given in* (2.3) *is supported by the zeros of the polynomial*

$$(1-x^2)U_{k-1}(x)C_{r-1}^{((z+2)/2)}(T_k(x))$$

and the weights at the support points are given by

$$\xi(\{x_j\}) = \begin{cases} \dfrac{1}{k(z+r)}, & \text{if } C_{r-1}^{((z+2)/2)}\big(T_k(x_j)\big) = 0,\\[2ex] \dfrac{z+1}{2}\dfrac{1}{k(z+r)}, & \text{if } x_j = \mp 1,\\[2ex] (z+1)\dfrac{1}{k(z+r)}, & \text{if } U_{k-1}(x_j) = 0. \end{cases}$$

(b) *The design ξ corresponding to the canonical moments given in* (2.4) *is supported by the zeros of the polynomial*

$$T_k(x)C_{r-1}^{((z+2)/2)}(T_k(x)) - C_{r-2}^{((z+2)/2)}(T_k(x)) = \frac{r}{z}C_r^{(z/2)}(T_k(x))$$

and puts equal masses at all support points.

THEOREM 2.6. *Let $m = k$ and $k, r \in \mathbb{N}$.*

(a1) *In the case of even $k = 2p$, the design corresponding to the canonical moments given in* (2.3) *is supported by the zeros of the polynomial*

$$(1 - x^2)U_{p-1}(x)\{C_{r-1}^{((z+2)/2)}(T_{2p}(x)) + C_{r-2}^{((z+2)/2)}(T_{2p}(x))\}$$

and the weights at the support points are

$$\xi(\{x_j\}) = \begin{cases} \dfrac{1}{p(z+2r-1)}, & \text{if } C_{r-1}^{((z+2)/2)}(T_{2p}(x_j)) \\ & \quad + C_{r-2}^{((z+2)/2)}(T_{2p}(x)) = 0, \\ \dfrac{z+1}{2}\dfrac{1}{p(z+2r-1)}, & \text{if } x_j = \mp 1, \\ (z+1)\dfrac{1}{p(z+2r-1)}, & \text{if } U_{p-1}(x_j) = 0. \end{cases}$$

(a2) *In the case of odd $k = 2p - 1$, the design corresponding to the canonical moments given in* (2.3) *is supported by the zeros of the polynomial*

$$(1 - x)[U_{p-1}(x) + U_{p-2}(x)][C_{r-1}^{((z+2)/2)}(T_{2p-1}(x)) + C_{r-2}^{((z+2)/2)}(T_{2p-1}(x))]$$

and the weights at the support points are

$$\xi(\{x_j\}) = \begin{cases} \dfrac{2}{(z+2r-1)(2p-1)}, & \text{if } C_{r-1}^{((z+2)/2)}(T_{2p-1}(x_j)) \\ & \quad + C_{r-2}^{((z+2)/2)}(T_{2p-1}(x_j)) = 0, \\ \dfrac{z+1}{(z+2r-1)(2p-1)}, & \text{if } x_j = 1, \\ \dfrac{2(z+1)}{(z+2r-1)(2p-1)}, & \text{if } U_{p-1}(x_j) + U_{p-2}(x_j) = 0. \end{cases}$$

(b1) *In the case of even $k = 2p$, the design corresponding to the canonical moments given in* (2.4) *is supported by the zeros of the polynomial*

$$T_p(x)[C_{r-1}^{((z+2)/2)}(T_{2p}(x)) - C_{r-2}^{((z+2)/2)}(T_{2p}(x))]$$

and the weights at the support points are

$$\xi(\{x_j\}) = \begin{cases} \dfrac{z+1}{p(z+2r-1)}, & \text{if } T_p(x_j) = 0, \\ \dfrac{1}{p(z+2r-1)}, & \text{if } C_{r-1}^{((z+2)/2)}(T_{2p}(x_j)) - C_{r-2}^{((z+2)/2)}(T_{2p}(x_j)) = 0. \end{cases}$$

(b2) *In the case of odd $k = 2p - 1$, the design corresponding to the canonical moments given in* (2.4) *is supported by the zeros of the polynomial*

$$(1+x)\left[U_{p-1}(x) - U_{p-2}(x)\right]\left[C_{r-1}^{((z+2)/2)}(T_{2p-1}(x)) - C_{r-2}^{((z+2)/2)}(T_{2p-1}(x))\right]$$

and the weights at the support points are

$$\xi(\{x_j\}) = \begin{cases} \dfrac{2}{(z+2r-1)(2p-1)}, & \text{if } C_{r-1}^{((z+2)/2)}(T_{2p-1}(x_j)) \\ & \quad - C_{r-2}^{((z+2)/2)}(T_{2p-1}(x_j)) = 0, \\ \dfrac{z+1}{(z+2r-1)(2p-1)}, & \text{if } x_j = -1, \\ \dfrac{2(z+1)}{(z+2r-1)(2p-1)}, & \text{if } U_{p-1}(x_j) - U_{p-2}(x_j) = 0. \end{cases}$$

Theorem 2.5 and 2.6 can roughly be summarized in the following way. The support of a design ξ corresponding to the sequences (2.3) and (2.4) in the case $m = 0$ and $m = k$ splits up in three different sets A_1, A_2, A_3. The first set A_1 is the set of the zeros of a polynomial in $T_k(x)$. A_2 is the set of the zeros of a linear combination of Chebyshev polynomials of the first or second kind (note that A_2 can be empty) and A_3 is a subset of the boundary $\{-1, 1\}$ (A_3 can be empty). The design ξ puts equal masses at all support points of A_1. If there are any support points in A_2 and A_3, their masses are $z + 1$ times and $(z + 1)/2$ times bigger than the masses of the points in A_1.

3. Optimal designs for the class of polynomials of odd or even degree. Using the results of Section 2, it is possible to identify the optimal design for the class $\mathscr{F}_{kr}$ with respect to special priors [i.e., the design which maximizes $\Psi_\beta(\xi)$]. To this end, let $z > -1$, $k \in \mathbb{N}$, $r \in \mathbb{N}$ and define $\beta = (\beta_1, \dots, \beta_{kr})$ by

$$\begin{aligned} \beta_{kj-1}(z) &:= -kjz\frac{\Gamma(r)\Gamma(z+r-j)}{\Gamma(r-j+1)\Gamma(z+r)}, && j = 1,\dots,r, \\ \beta_{kj}(z) &:= (kj+1)z\frac{\Gamma(r)\Gamma(z+r-j)}{\Gamma(r-j+1)\Gamma(z+r)}, && j = 1,\dots,r, \\ \beta_i(z) &:= 0 \quad \text{if } i \notin \{kj-1, kj \mid j = 1,\dots,r\}, && 1 \le i \le kr, \end{aligned} \tag{3.1}$$

if $k \geq 2$ and let

$$\beta_j(z) := (j+1)z(z-1)\frac{\Gamma(r)\Gamma(z+r-j-1)}{\Gamma(r-j+1)\Gamma(z+r-1)(r+2z-1)}, \quad j = 1,\dots,r, \tag{3.2}$$

in the case $k = 1$. Straightforward calculations show $\Sigma_{j=1}^{kr}\beta_j(z) = 1$ [see Dette (1990), Lemma 4.1]. The canonical moments of the optimal design for the class $\mathscr{F}_{kr}$ with respect to an arbitrary prior β are given in Proposition 2.2. Observing the equation

$$\sum_{l=i}^{r} \frac{\Gamma(q+l+1-i)}{\Gamma(l+1-i)} \frac{\Gamma(r+z-l-1)}{\Gamma(r+1-l)} = \frac{\Gamma(q+1)}{\Gamma(z+q)} \frac{\Gamma(z-1)}{\Gamma(r+1-i)} \times \Gamma(r+z+q-i)$$

[see Dette (1990), Lemma 4.1], it is easy to show that the canonical moments of the optimal design for the class $\mathscr{F}_{kr}$ with respect to the prior $\beta(z)$ are given in (2.3). By an application of Theorem 2.5(a), we have proved:

THEOREM 3.1. *The optimal design $\xi_{\beta(z)}$ for the class $\mathscr{F}_{kr}$ with respect to the prior $\beta(z)$ given in* (3.1) *and* (3.2) *is supported by the zeros of the polynomial*

$$(1-x^2)U_{k-1}(x)C_{r-1}^{((z+2)/2)}(T_k(x)).$$

The weights of the support points are given by

$$\xi_\beta(\{x\}) = \begin{cases} \dfrac{1}{k(z+r)}, & \text{if } C_{r-1}^{((z+2)/2)}(T_k(x)) = 0, \\ \dfrac{z+1}{2}\dfrac{1}{k(z+r)}, & \text{if } x = \mp 1, \\ (z+1)\dfrac{1}{k(z+r)}, & \text{if } U_{k-1}(x) = 0. \end{cases}$$

Note that the case $k = 1$, $z \in \{0\} \cup [1, \infty)$ was already considered by Dette (1990). We have now proved that his results hold for all $z > -1$. Theorem 3.1 has only practical interest in the case $k = 1$ because the priors β_l should reflect the experimenters belief about the adequacy of the models $g_l \in \mathscr{F}_{kr}$. Nevertheless it is an important tool to determine D_1-optimal designs for the class of polynomials of even degree with respect to special priors $\gamma_j(z)$,

$j = 1, \ldots, r$. Observing (1.3) and (1.5), we obtain immediately from Theorem 3.1 ($k = 2$):

THEOREM 3.2. *Let $z > -1$ and*

$$\gamma_j(z) = z\frac{\Gamma(r)\Gamma(r-j+z)}{\Gamma(r-j+1)\Gamma(z+r)}, \qquad j = 1, \ldots, r.$$

The D_1-optimal design for the class of polynomials of even degree (up to the order $2r$) with respect to the prior $\gamma(z) := (\gamma_1(z), \ldots, \gamma_r(z))$ [i.e., the design which maximizes (1.3)] is supported by the zeros of the polynomial

$$(1 - x^2)xC_{r-1}^{((z+2)/2)}(2x^2 - 1)$$

and the masses at the support points are given by

$$\xi_{\gamma(z)}(\{x\}) = \begin{cases} \dfrac{1}{2(z+r)}, & \text{if } C_{r-1}^{((z+2)/2)}(2x^2 - 1) = 0, \\ \dfrac{z+1}{4(z+r)}, & \text{if } x = \mp 1, \\ \dfrac{z+1}{2(z+r)}, & \text{if } x = 0. \end{cases}$$

If $z = 0$, it can be shown by simple calculations that the corresponding prior is given by $\gamma(0) = (0, \ldots, 0, 1)$. Thus Theorem 3.2 gives the solution of the usual D_1-optimality criterion for polynomial regression of degree $2r$ [see Kiefer and Wolfowitz (1959)]. For $z = 1$ the prior $\gamma(1)$ puts equal weight $1/r$ on all the polynomial models of even degree lower than $2r$. This design could be used if it is assumed that the unknown regression model is a polynomial of even degree up to the order $2r$. For $z = 2$, the corresponding prior is given by

$$\gamma(2) = \frac{2}{r(r+1)}(r, r-1, \ldots, 2, 1),$$

while for $z = 3$ it is

$$\gamma(3) = \frac{3}{r(r+1)(r+2)}(r(r+1), (r-1)r, \ldots, 6, 2).$$

If z is increasing the prior $\gamma(z)$ puts less weight at the models of higher degree [note that $\lim_{z \to \infty} \gamma(z) = (1, 0, \ldots, 0)$]. Therefore the experimenter could use priors $\gamma(z)$ for increasing z if he wants to fit a quadratic polynomial with some protection against polynomials of higher (even) degree. Note that a similar reasoning holds also for the priors considered in Theorem 3.1. Especially the case $z = 0$ gives the D_1-optimal design for polynomial regression of kr while the prior $\beta(1)$ could be used if polynomials of degree $k, 2k, \ldots, rk$ are considered and no model is preferred. Examples for the applications of the theorems are given in Section 5.

The following theorem states an analogous result for polynomials of odd degree up to the order $2r - 1$. The proof follows directly from Proposition 2.2 and Theorem 2.6 and is omitted.

THEOREM 3.3. *Let $z > -1$ and*

$$\gamma_j(z) = z\frac{\Gamma(r)\Gamma(r-j+z)}{\Gamma(r-j+1)\Gamma(z+r)}, \qquad j = 1, \dots, r.$$

The D_1-optimal design for the class of polynomials of odd degree (up to the order $2r - 1$) with respect to the prior $\gamma(z) = (\gamma_1(z), \dots, \gamma_r(z))$ [i.e., the design which maximizes (1.4)] is supported by the zeros of the polynomial

$$(1 - x^2)\left[C_{r-1}^{((z+2)/2)}(2x^2 - 1) + C_{r-2}^{((z+2)/2)}(2x^2 - 1)\right]$$

and the masses at the support points are given by

$$\xi_{\gamma(z)}(\{x\}) = \begin{cases} \dfrac{1}{z + 2r - 1}, & \text{if } C_{r-1}^{((z+2)/2)}(2x^2 - 1) \\ & \quad + C_{r-2}^{((z+2)/2)}(2x^2 - 1) = 0, \\ \dfrac{z+1}{2}\dfrac{1}{z + 2r - 1}, & \text{if } x = \mp 1. \end{cases}$$

EXAMPLES. (i) Suppose $r = 3$ and $z = 1$. The D_1-optimal design for the linear, cubic and polynomial of fifth degree with respect to the prior $\gamma(1) = (1/3, 1/3, 1/3)$ is supported by the points

$$-1, -\sqrt{\frac{4+\sqrt{6}}{10}}, -\sqrt{\frac{4-\sqrt{6}}{10}}, \sqrt{\frac{4-\sqrt{6}}{10}}, \sqrt{\frac{4+\sqrt{6}}{10}}, 1$$

and the weights at all support points are equal.

(ii) Let $r = 3$ and $z = 6$, the corresponding prior is given by $\gamma(6) = (3/4, 3/14, 1/28)$ and puts the most weight on the linear model. The D_1-optimal design for the polynomial of odd degree up to the order 5 is supported by the points

$$-1, -\sqrt{\frac{9+\sqrt{11}}{20}}, -\sqrt{\frac{9-\sqrt{11}}{20}}, \sqrt{\frac{9-\sqrt{11}}{20}}, \sqrt{\frac{9+\sqrt{11}}{20}}, 1$$

and the masses at the support points are proportional 7 : 2 : 2 : 2 : 2 : 7.

4. Optimal design for polynomials with vanishing coefficients. Let $h_{2l}(x) = \sum_{i=0}^{l} \alpha_{l,i} x^{2i}$ and $h_{2l-1}(x) = \sum_{i=1}^{l} \delta_{l,i} x^{2i-1}$ denote a polynomial with vanishing coefficients of the odd and even powers, respectively. All models up to degree $2r$ or $2r - 1$ are collected in the sets

$$\mathscr{F}_r^E = \{h_{2l}(x) | l = 1, \dots, r\},$$

$$\mathscr{F}_r^U = \{h_{2l-1}(x) | l = 1, \dots, r\}.$$

The information matrices of a design ξ for the models $h_{2l}(x)$ and $h_{2l-1}(x)$ are given by

$$M_{2l}^E(\xi) = \begin{pmatrix} c_0 & c_2 & \cdots & c_{2l} \\ c_2 & c_4 & \cdots & c_{2l+2} \\ \vdots & \vdots & \ddots & \vdots \\ c_{2l} & c_{2l+2} & \cdots & c_{4l} \end{pmatrix},$$

$$M_{2l-1}^U(\xi) = \begin{pmatrix} c_2 & c_4 & \cdots & c_{2l} \\ c_4 & c_6 & \cdots & c_{2l+2} \\ \vdots & \vdots & \ddots & \vdots \\ c_{2l} & c_{2l+2} & \cdots & c_{4l-2} \end{pmatrix},$$

where $c_j = \int_{-1}^{1} x^j \, d\xi(x)$ are the ordinary moments of ξ. In order to find optimal designs for the class $\mathscr{F}_r^E$ (and $\mathscr{F}_r^U$) [i.e., designs which maximize $\sum_{l=1}^{r} \gamma_l/(l+1) \det M_{2l}^E(\xi)$ for a given prior $\gamma = (\gamma_1, \dots, \gamma_r)$], we have to find representations of the determinants $M_{2l}^E(\xi)$ [and $M_{2l-1}^U(\xi)$] in terms of the canonical moments of ξ. A result similar to that given in Proposition 2.1 can be obtained for symmetric designs on $[-1, 1]$.

LEMMA 4.1. *Let ξ denote a symmetric design on $[-1,1]$ with canonical moments $p_1, p_2 \dots$ and $\zeta_i = q_{i-1} p_i$ ($q_0 := 1$), then the following representations hold*:

$$\det M_{2l}^E(\xi) = 2^{2l(l+1)} \prod_{j=1}^{l} (\zeta_{4j-3}\zeta_{4j-2}\zeta_{4j-1}\zeta_{4j})^{l+1-j},$$

$$\det M_{2l-1}^U(\xi) = 2^{2l^2} (\zeta_1\zeta_2)^l \prod_{j=1}^{l-1} (\zeta_{4j-1}\zeta_{4j}\zeta_{4j+1}\zeta_{4j+2})^{l-j}.$$

PROOF. The polynomials orthogonal with respect to the measure $d\xi(x)$ satisfy the recursive relation [see Studden (1982b)] $P_0(x) = 1$, $P_1(x) = x$,

$$\begin{aligned} P_{l+1}(x) &= (x + 1 - 2(\zeta_{2l} + \zeta_{2l+1}))P_l(x) + 4\zeta_{2l-1}\zeta_{2l}P_{l-1}(x) \\ &= xP_l(x) - q_{2l-2}p_{2l}P_{l-1}(x), \end{aligned}$$

where the last equation follows from the symmetry of ξ which implies that all canonical moments of odd order are 1/2. The L_2-norm of $P_l(x)$ with respect to $d\xi(x)$ is given by [see Lau (1983) or Studden (1989)]

$$\int_{-1}^{1} P_l^2(x) \, d\xi(x) = 2^{2l} \zeta_1\zeta_2 \cdots \zeta_{2l-1}\zeta_{2l}. \tag{4.1}$$

Because of the symmetry of ξ $P_{2l}(x)$ is a polynomial in x^2. This yields $(1, x^2, \dots, x^{2l})^T = A(P_0(x), P_2(x), \dots, P_{2l}(x))^T$, where A is an upper triangular matrix with elements in the diagonal equal 1. From (4.1) it follows that

$$\det M_{2l}^E(\xi) = \prod_{j=0}^{l} \int_{-1}^{1} P_{2j}^2(x)\, d\xi(x) = 2^{2l(l+1)} \prod_{j=1}^{l} \left(\zeta_{4j-3}\zeta_{4j-2}\zeta_{4j-1}\zeta_{4j}\right)^{l+1-j}.$$

The representation of the determinant $M_{2l-1}^U(\xi)$ is derived in the same way.

Note that the symmetry of the design ξ is an essential assumption of Lemma 4.1. For example, the determinant of $M_1^U(\eta)$ of an arbitrary design η on $[-1, 1]$ is given by

$$\det M_1^U(\eta) = c_2 = 4\zeta_1(\zeta_1 + \zeta_2) - 4\zeta_1 + 1$$

and this expression corresponds only for a symmetric design ($\zeta_1 = 1/2$) with the result of Lemma 4.1. Because the underlying interval is $[-1, 1]$ and the functions

$$\Phi_\gamma^E(\xi) := \sum_{l=1}^{r} \frac{\gamma_l}{l+1} \log\left[\det M_{2l}^E(\xi)\right]$$

and

$$\Phi_\gamma^U(\xi) := \sum_{l=1}^{r} \frac{\gamma_l}{l} \log\left[\det M_{2l-1}^U(\xi)\right]$$

are concave for nonnegative priors γ_l, we may assume that there exist symmetric optimal designs for the classes $\mathscr{F}_r^E$ and $\mathscr{F}_r^U$. By straightforward algebra we obtain from Lemma 4.1 and Theorem 2.5:

THEOREM 4.2. *The canonical moments of the optimal design on* $[-1, 1]$ *for the class* $\mathscr{F}_r^E$ *with respect to a nonnegative prior* $(\gamma_1, \dots, \gamma_r)$ [*i.e., the design which maximizes* $\Phi_\gamma^E(\xi)$] *are given by*

$$p_{4i} = \frac{\sigma_i^E}{\sigma_i^E + \sigma_{i+1}^E}, \qquad i = 1, \dots, r-1, \qquad p_{4r} = 1, \qquad p_j = \frac{1}{2} \text{ otherwise},$$

where the numbers σ_i^E *are defined by* $\sigma_i^E := \sum_{l=i}^{r}((l+1-i)/(l+1))\gamma_l$. *The canonical moments of the symmetric D-optimal design (on* $[-1, 1]$*) for the class* $\mathscr{F}_r^U$ *with respect to the nonnegative prior* $(\gamma_1, \dots, \gamma_r)$ [*i.e., the design which maximizes* $\Phi_\gamma^U(\xi)$] *are given by*

$$p_{4i-2} = \frac{\sigma_i^U}{\sigma_i^U + \sigma_{i+1}^U}, \qquad i = 1, \dots, r-1, \qquad p_{4r-2} = 1, \qquad p_j = \frac{1}{2} \text{ otherwise},$$

where the numbers σ_i^U *are defined by* $\sigma_i^U := \sum_{l=i}^{r}((l+1-i)/l)\gamma_l$.

THEOREM 4.3. *The D-optimal design (on $[-1, 1]$) for the polynomial $h_{2r}(x) = \sum_{j=0}^{r} \alpha_l x^{2l}$ is supported by the zeros of the polynomial*

$$x(1 - x^2)C_{r-1}^{(3/2)}(2x^2 - 1)$$

and the masses at the support points are proportional $1 : \cdots : 1 : 2 : 1 : \cdots : 1$. The symmetric D-optimal design (on $[-1, 1]$) for the polynomial $h_{2r-1}(x) = \sum_{l=1}^{r} \delta_l x^{2l-1}$ is supported by the zeros of the polynomial

$$(1 - x^2)\left[C_{r-1}^{(3/2)}(2x^2 - 1) + C_{r-2}^{(3/2)}(2x^2 - 1)\right]$$

and puts equal masses at all support points.

The optimal designs for the classes $\mathscr{F}_r^E$ and $\mathscr{F}_r^U$ can be transformed to other intervals of the form $[-a, a]$ $(a > 0)$ [see Fedorov (1972), page 80]. A transformation to arbitrary intervals is not possible in general. Note that similar results can be obtained for priors $\gamma(z)$ defined in Theorem 3.2 which are not given here.

5. Applications of the results. In this section we will apply the results of Section 3 and 4 to derive optimal designs for certain situations in polynomial regression. The procedure is as follows. The experimenter has to fix a suitable class of models (e.g., polynomials of odd degree). A prior is put on every model and the optimality criterion (1.2), (1.3) or (1.4) is used to determine designs for the discrimination between the competing models. We will demonstrate this procedure in two examples.

EXAMPLE 1 (Polynomial regression of degree 3 or 6). Assume that an experimenter wants to fit a cubic polynomial having some protection against a polynomial of degree 6. In this case we can use Theorem 3.1 ($k = 3, r = 2$) with $z = 1$ and obtain that the optimal design for the cubic polynomial and the polynomial of degree 6 is supported at the points

$$-1, -\sqrt{\tfrac{3}{4}}, -\tfrac{1}{2}, 0, \tfrac{1}{2}, \sqrt{\tfrac{3}{4}}, 1$$

with masses proportional to $1 : 1 : 2 : 1 : 2 : 1 : 1$. It may be of some interest to calculate the efficiency of this design for the two models. The usual D-efficiency for the polynomial of degree k is defined by

$$E_k = \left(\frac{\det M_k(\xi)}{\sup_\eta \det M_k(\eta)} \right)^{1/(k+1)}.$$

(Note that the designs are constructed to select an adequate model in a given class of models but after the decision for one model all parameters of this model have to be estimated. For this reason we use the D-efficiency criterion.) From Proposition 2.1 we see that the above design has efficiency $E_3 = 0.8445$ for the cubic model and $E_6 = 0.7375$ for the model of degree 6. If the experimenter wants to increase the efficiency of the design for the cubic model, he has to chose larger values for the parameter z. For example, for $z = 7$ the optimal design is supported at the same points as in the case $z = 1$ with masses proportional to $4:1:1:8:1:1:4$. The efficiencies for this design are given by $E_3 = 0.9074$ and $E_6 = 0.6844$.

EXAMPLE 2 (Polynomials of even degree up to the order 6). Assume that an experimenter wants to fit one of the models

$$a_0 + a_1x + a_2x^2, \qquad a_0 + a_1x + a_2x^2 + a_3x^3 + a_4x^4,$$

$$a_0 + a_1x + \cdots + a_6x^6,$$

because he knows (for example, from physical considerations) that the degree of the (unknown) model must be even. If he has no preference for any of the models a suitable prior (to decide which of the models is adequate) would be $\gamma(1) = (1/3, 1/3, 1/3)$ which corresponds to $z = 1$. From Theorem 3.2, we now obtain that the D_1 optimal design for the three models is supported at the seven points

$$-1, -\sqrt{\frac{1 + 1/\sqrt{5}}{2}}, -\sqrt{\frac{1 - 1/\sqrt{5}}{2}}, 0, \sqrt{\frac{1 - 1/\sqrt{5}}{2}}, \sqrt{\frac{1 + 1/\sqrt{5}}{2}}, 1,$$

with masses proportional to $1:1:1:2:1:1:1$. The efficiencies of this design for the different models are given by $E_2 = 0.7969$, $E_4 = 0.8786$ and $E_6 = 0.9482$, respectively. If the experimenter prefers the quadratic model and wants to have some protection against the other models, a suitable choice would be $z = 3$ which corresponds to the prior $\gamma(3) = (3/5, 3/10, 1/10)$ and yields to a design supported at the points

$$-1, -\sqrt{\frac{1 + 1/\sqrt{7}}{2}}, -\sqrt{\frac{1 - 1/\sqrt{7}}{2}}, 0, \sqrt{\frac{1 - 1/\sqrt{7}}{2}}, \sqrt{\frac{1 + 1/\sqrt{7}}{2}}, 1,$$

with masses proportional to $2:1:1:4:1:1:2$. The efficiencies of this design are given by $E_2 = 0.8485$, $E_4 = 0.8843$ and $E_6 = 0.8280$.

Note that an important advantage of the above designs is the simple form of the weights which can easily be realized in practice (nearly without rounding procedures). The results of Section 4 allow the determination of D- (D_1-) optimal designs for polynomials with vanishing coefficients of the powers of odd (or even) order. These models are obtained from some symmetry assumption of the experimenter on the underlying model.

EXAMPLE 3 (Polynomials with vanishing coefficients). From Theorem 4.3 we have that the D-optimal design for the polynomial $h_2(x) = a_0 + a_1x^2$ ($x \in [-1, 1]$) is supported at the points $-1, 0, 1$ with masses proportional to $1:2:1$ [note that this design is also the D_1-optimal design for the polynomial

$g_2(x) = \alpha_0 + \alpha_1 x + \alpha_2 x^2$]. The D-optimal design for the model $h_4(x) = a_0 + a_1 x^2 + a_2 x^4$ puts masses proportional to $1:1:2:1:1$ at the points $-1, -1/\sqrt{2}, 0, 1/\sqrt{2}, 1$.

Theorem 4.3 also shows that the symmetric D-optimal design for the model $h_3(x) = \delta_1 x + \delta_2 x^3$ is supported at the points $-1, 1/\sqrt{3}, 1/\sqrt{3}, 1$ and all masses at the support points are equal.

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