The Annals of Statistics
1990, Vol. 18, No. 4, 1784–1804

A GENERALIZATION OF D- AND D_1-OPTIMAL DESIGNS IN POLYNOMIAL REGRESSION[1]

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In the class of polynomial regression models up to degree n we determine the design on $[-1, 1]$ that maximizes a product of $n+1$ determinants of information matrices weighted with a prior β, where the l-th information matrix corresponds to a polynomial regression model of degree l, for $l = 0, 1, \dots, n$. The designs are calculated using canonical moments. We identify a special class of priors $\beta(z)$ depending on one real parameter z so that analogous results are obtained as in the classical D- and D_1-optimal design problems. The interior support of the optimal design with respect to the prior $\beta(z)$ is given by the zeros of a Jacobi polynomial and all the interior support points have the same masses. The masses at the boundary points -1 and 1 are $(z+1)/2$ times bigger than the masses of the interior points.

The results found in one dimension are generalized to the problem of determining optimal product designs in the case of multivariate polynomial regression on the q-cube $[-1, 1]^q$. Explicit solutions are obtained for the D- and D_1-optimal product designs in the polynomial model of degree n for all $n \in \mathbb{N}$ and $q \in \mathbb{N}$.

1. Introduction. Consider a class of polynomial regression models

$$\mathscr{F}_n = \left\{ g_l \,\middle|\, g_l(x) = \sum_{i=0}^{l} \alpha_{l,i} x^i,\ l = 0, \dots, n \right\}.$$

For each $x \in [-1, 1]$ a random variable $Y(x)$ with mean $g_l(x)$ for some (unknown) $l \in \{0, 1, \dots, n\}$ and variance $\sigma^2/\lambda(x)$ can be observed. The function λ is called the efficiency function [see Fedorov (1972), page 66] and we assume that $\lambda(x)$ is of the special form $\lambda(x) = (1+x)^u(1-x)^v$, $u, v \in \{0, 1\}$. A design ξ is a probability measure on $[-1, 1]$. If N observations are taken and ξ concentrates mass ξ_i at the point x_i, where $N\xi_i = n_i$ are integers, the experimenter takes N uncorrelated observations n_i at each x_i. In this case the covariance matrix of the least squares estimate $\hat{\alpha}^{(l)}$ of $\alpha^{(l)} = (\alpha_{l,0}, \dots, \alpha_{l,l})^{\mathsf{T}}$ in the model g_l is given by $\sigma^2/NM_l^{-1}(\xi)$, where

$$M_l(\xi) = \int_{\mathscr{X}} (1, x, \dots, x^l)^{\mathsf{T}} (1, x, \dots, x^l) \lambda(x)\, d\xi(x)$$

denotes the information matrix of the design ξ. The variance of the esti-

Received May 1989; revised January 1990.
[1]Research partially supported by the Deutsche Forschungsgemeinschaft.
AMS 1980 *subject classifications*. 62K05, 62J05.
Key words and phrases. D-optimal design, D_s-optimal design, polynomial regression, model robust design, Läuter type design, product designs, canonical moments.

mate $\hat{g}_l(x) = \sum_{i=0}^{l} \hat{a}_{l,i} x^i$ of $g_l(x)$ at the point $x \in [-1, 1]$ is proportional to $d_l(x, \xi) = (1, x, \dots, x^l) M_l^{-1}(\xi)(1, x, \dots, x^l)^{\mathrm{T}}$. One of the more commonly used criteria for choosing a design ξ (for the model g_l) is the D-optimality criterion which maximizes the determinant of $M_l(\xi)$. The determinant of the information matrix can be expressed in terms of canonical moments and the D-optimal designs can easily be calculated by the maximization of det $M_l(\xi)$ in terms of canonical moments [see Studden (1980, 1982a, b), Lau and Studden (1985) and Lim and Studden (1988) for more details]. The theory of canonical moments is briefly stated in Section 2.

The theory of optimal design described so far is based on the assumption that the form of the regression model is known by the experimenter (namely, g_n). In many practical applications the experimenter has very little information about the model before the experiment is carried out. For the application of optimal design theory in this situation we only assume that the unknown model belongs to the class $\mathscr{F}_n$ and determine designs which allow a good estimate of the parameters [in the sense of Läuter (1974)] in any model of $\mathscr{F}_n$. For this task we use an optimality criterion proposed by Läuter (1974) depending on all the information matrices $M_l(\xi)$, $l = 0, 1, \dots, n$. A vector $\beta = (\beta_0, \beta_1, \dots, \beta_n)$ of real numbers is called a prior for $\mathscr{F}_n$ if β is a probability measure on $\{0, \dots, n\}$ or is, for $s \in \{1, \dots, n-1\}$, of the form

$$
\begin{aligned}
&\beta_0 = \cdots = \beta_{n-s-1} = 0, \qquad \beta_{n-s} = -\frac{n-s+1}{s}, \\
&\beta_{n-s+1} = \cdots = \beta_{n-1} = 0, \qquad \beta_n = \frac{n+1}{s}.
\end{aligned} \tag{1.1}
$$

For a given prior β on $\{0, \dots, n\}$ we call a design ξ_β optimal for $\mathscr{F}_n$ with respect to the prior β, if ξ_β maximizes the function

$$
\Psi_\beta(\xi) = \sum_{l=0}^{n} \frac{\beta_l}{l+1} \log(\det M_l(\xi)).
$$

For more details and for other optimality criteria in this connection, see Läuter (1974, 1976) and Cook and Nachtsheim (1982). Note that Ψ_β does not depend on β_0 when λ is the identical one-function and that the D-optimality criterion is obtained by the prior $\beta_D = (0, \dots, 0, 1)$. For the prior given in (1.1), which will be denoted β_{D_s}, $s \in \{1, \dots, n-1\}$, $\Psi_\beta(\xi)$ gives the D_s-optimality criterion [see Kiefer (1961)] which minimizes the determinant of the covariance matrix of the least squares estimate of the highest s parameters $\alpha_{n,n-s+1}, \dots, \alpha_{n,n}$ in the model g_n. In the case of D-optimality the equivalence theorem of Kiefer and Wolfowitz (1960) is a very useful tool for the determination of D-optimal designs. This result can be generalized to the optimality criterion defined previously [see Läuter (1974) for nonnegative priors and Kiefer (1961) for priors of the form (1.1)].

THEOREM 1.1. *For a given prior* $\beta = (\beta_0, \dots, \beta_n)$ *on* $\{0, 1, \dots, n\}$ *the following three conditions are equivalent*:

(i) *The design* ξ_β *is optimal for the class* $\mathscr{F}_n$ *with respect to the prior* β.
(ii) *The design* ξ_β *minimizes*

$$\Phi_\beta(\xi) = \max_{x \in [-1,1]} \lambda(x) \sum_{l=0}^{n} \frac{\beta_l}{l+1} d_l(x, \xi).$$

(iii) $$\Phi_\beta(\xi_\beta) = \max_{x \in [-1,1]} \lambda(x) \sum_{l=0}^{n} \frac{\beta_l}{l+1} d_l(x, \xi_\beta) = 1.$$

In Section 3 we derive some formulas for the computation of optimal designs for $\mathscr{F}_n$ by the application of this theory. The D- and D_1-optimal designs are of a very simple structure. It was shown by Hoel (1958) that in the case $\lambda(x) \equiv 1$ the D-optimal design [corresponding to the prior $\beta_D = (0, \dots, 0, 1)$ for $\mathscr{F}_n$] puts equal mass at the zeros of $(1 - x^2)P_n'(x)$, where P_n denotes the n-th Legendre polynomial and P_n' its derivative. The D_1-optimal design [corresponding to $\beta_{D_1} = (0, \dots, 0, -n, n+1)$] concentrates mass $1/(2n)$ on the boundary points -1 and 1, and mass $1/n$ on the zeros of $T_n'(x)$, where T_n is the Chebyshev polynomial of the first kind [see Kiefer and Wolfowitz (1959)].

In Section 4 we will consider a one-parameter family of priors $\beta(z)$ on $\{0, 1, \dots, n\}$ depending on a real parameter $z \in \{0\} \cup [1, \infty)$ [see (4.1) for definition]. Optimal designs for $\mathscr{F}_n$ with respect to the prior $\beta(z)$ are of the same simple structure as the D- and D_1-optimal designs. The supports of these designs are given by the zeros of the polynomials

$$(1+x)^{1-u}(1-x)^{1-v} P_{n-1+u+v}^{((z+1)/2-v,(z+1)/2-u)}(x),$$

where $P_n^{(\gamma,\delta)}(x)$ denotes the n-th Jacobi polynomial which is the n-th orthogonal polynomial with respect to the measure $(1-x)^\gamma(1+x)^\delta\,dx$ [see Szegö (1959), pages 58–60, or Abramowitz and Stegun (1964)]. The optimal design puts equal masses on all interior support points. If the support contains the points -1 or 1, their masses are $(z+1)/2$ times bigger than the masses of the interior support points (see Theorem 4.3). It is also shown that the D- and D_1-optimality criteria are obtained as the special cases $z = 1$ and $z = 0$, respectively, and that for $z = 2$ the prior $\beta(2)$ puts equal weight to all models of $\mathscr{F}_n$ [i.e., $\beta_l(2)/(l+1) = \text{const}$ for all $l = 0, \dots, n$].

In the last section of this paper we will generalize these results to the case of multivariate polynomial regression on the q-cube, $q \in \mathbb{N}$, and determine the optimal product designs [in the sense of Lim and Studden (1988)] for the class of polynomial models in q variables up to degree n. As special cases we obtain explicit representations of the D- and D_1-optimal product designs in the multivariate polynomial model of degree n for all $n \in \mathbb{N}$ and $q \in \mathbb{N}$.

2. Canonical moments. In this section we mention some results concerning canonical moments of a probability measure on [0, 1]. More details and applications of this theory can be found in the papers of Skibinsky (1967, 1968, 1969, 1986) and Studden (1980, 1982a, b). Let $c_k = \int_0^1 x^k \, d\xi(x)$, $k = 0, 1, \dots,$ denote the k-th moment of a probability measure on $[0, 1]$. For a given set of moments $c_0, c_1, \dots, c_{i-1}$, let c_i^+ denote the maximum value of the i-th 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 this 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), Section 1]. The determinants of the information matrices $M_l(\xi)$ (for probability measures on $[0, 1]$) can easily be expressed in terms of canonical moments [see Skibinsky (1968) and Studden (1982b)]. The formulas are given in the following theorem.

THEOREM 2.1. *Let* $M_l(\xi) = \int_0^1 (1, \dots, x^l)^T (1, \dots, x^l) \tilde{\lambda}(x) \, d\xi(x)$, $l = 0, 1, \dots, n$, *where* $\tilde{\lambda}(x) = x^u (1-x)^v$, $u, v \in \{0, 1\}$. *Then the following representations hold, where* $q_j = 1 - p_j$ $(j \ge 1)$ *and* $\zeta_0 = 1$, $\gamma_0 = 1$, $\zeta_1 = p_1$, $\gamma_1 = q_1$, $\zeta_j = q_{j-1} p_j$ *and* $\gamma_j = p_{j-1} q_j$ $(j \ge 2)$:

$$\det M_l(\xi) = \prod_{i=1}^{l} (\zeta_{2i-1}\zeta_{2i})^{l+1-i} \quad \textit{if } (u, v) = (0, 0);$$

$$\det M_l(\xi) = \prod_{i=0}^{l} (\gamma_{2i}\gamma_{2i+1})^{l+1-i} \quad \textit{if } (u, v) = (0, 1);$$

$$\det M_l(\xi) = \prod_{i=0}^{l} (\zeta_{2i}\zeta_{2i+1})^{l+1-i} \quad \textit{if } (u, v) = (1, 0);$$

$$\det M_l(\xi) = \prod_{i=1}^{l+1} (\gamma_{2i-1}\gamma_{2i})^{l+2-i} \quad \textit{if } (u, v) = (1, 1).$$

The next theorems are very useful in finding the support and the weights of designs having a terminating sequence of canonical moments [see Studden (1982b)].

THEOREM 2.2. *The design* ξ *corresponding to the sequence of canonical moments* $(p_1, \dots, p_{2k-1}, 0)$ *is supported by the zeros of* $P_k(x, \xi)$.

The design ξ *corresponding to the sequence of canonical moments* $(p_1, \dots, p_{2k-1}, 1)$ *is supported by the zeros of* $x(1-x)Q_{k-1}(x, \xi)$.

The design ξ *corresponding to the sequence of canonical moments* $(p_1, \dots, p_{2k}, 0)$ *is supported by the zeros of* $xR_k(x, \xi)$.

The design ξ *corresponding to the sequence of canonical moments* $(p_1, \dots, p_{2k}, 1)$ *is supported by the zeros of* $(1-x)S_k(x, \xi)$.

The polynomials $\{P_k\}$, $\{Q_k\}$, $\{R_k\}$ *and* $\{S_k\}$ *satisfy the following recursive relations*:

$$P_{j+1}(x,\xi) = (x - \zeta_{2j} - \zeta_{2j+1})P_j(x,\xi) - \zeta_{2j-1}\zeta_{2j}P_{j-1}(x,\xi), \qquad j \geq 1;$$

$$Q_{j+1}(x,\xi) = (x - \gamma_{2j+2} - \gamma_{2j+3})Q_j(x,\xi) - \gamma_{2j+1}\gamma_{2j+2}Q_{j-1}(x,\xi), \quad j \geq 0;$$

$$R_{j+1}(x,\xi) = (x - \zeta_{2j+1} - \zeta_{2j+2})R_j(x,\xi) - \zeta_{2j}\zeta_{2j+1}R_{j-1}(x,\xi), \qquad j \geq 0;$$

$$S_{j+1}(x,\xi) = (x - \gamma_{2j+1} - \gamma_{2j+2})S_j(x,\xi) - \gamma_{2j}\gamma_{2j+1}S_{j-1}(x,\xi), \qquad j \geq 1;$$

where

$$\begin{aligned} Q_{-1}(x,\xi) &= R_{-1}(x,\xi) = 0, \\ P_0(x,\xi) &= Q_0(x,\xi) = R_0(x,\xi) = S_0(x,\xi) = 1, \\ S_1(x,\xi) &= x - \gamma_2, \\ P_1(x,\xi) &= x - \zeta_1. \end{aligned}$$

The polynomials $\{P_j\}$, $\{Q_j\}$, $\{R_j\}$ *and* $\{S_j\}$ *are orthogonal to* $d\xi$, $x(1-x)\,d\xi$, $x\,d\xi$ *and* $(1-x)\,d\xi$, *respectively.*

Note that the four designs described in Theorem 2.2 are, respectively, the lower and upper principal representations of the sequences $(p_1,\dots,p_{2n-1})$ and $(p_1,\dots,p_{2n})$ which are described in the book of Karlin and Studden [(1966), pages 45–47] and in the paper of Skibinsky [(1986), Section 1]. In the last-named work one can also find other recursion formulae for the preceding polynomials.

THEOREM 2.3. (i) *The supports of the measures corresponding to the sequences* $(p_1,\dots,p_k,0)$ *and* $(p_k,\dots,p_1,0)$ *are the same.*

(ii) *The supports of the measures corresponding to the sequences* $(p_1,\dots,p_k,1)$ *and* $(q_k,\dots,q_1,1)$ *are the same.*

3. Optimal designs for $\mathscr{F}_n$. In this section we determine the optimal design ξ_β for $\mathscr{F}_n$ with respect to a given prior β (in the sense of Section 1) on $\{0,1,\dots,n\}$. For the direct application of the theorems given in Section 2 (which also can be formulated for other intervals), we consider the interval $[0,1]$ and only the four efficiency functions $\tilde{\lambda}(x) = x^u(1-x)^v$ for which $u, v \in \{0,1\}$. Optimal designs on $[-1,1]$ for the given efficiency function $\lambda(x) = (1+x)^u(1-x)^v$ are obtained by a simple linear transformation [see Fedorov (1972), pages 80–82].

THEOREM 3.1. *Let* $\tilde{\lambda}(x) \equiv 1$ *and* $n \geq 1$. *The optimal design for the class* $\mathscr{F}_n$ *with respect to the prior* $\beta = (0,\beta_1,\dots,\beta_n)$ *is the distribution* ξ_β *on* $[0,1]$

which is uniquely determined by the canonical moment sequence

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

where the numbers σ_i *are defined by*

$$\sigma_i = \sum_{l=i}^{n} \frac{l+1-i}{l+1}\beta_l, \qquad i = 1,\dots,n.$$

The support of ξ_β *is given by the* $n+1$ *zeros of the polynomial* $x(1-x)\times Q_{n-1}(x,\xi_\beta)$ *(defined in Theorem 2.2). For the masses of* ξ_β *at the support points* $0 = x_1 < x_2 < \cdots < x_n < x_{n+1} = 1$ *we have*

$$(3.2)\qquad \xi_\beta(\{x_j\}) = \frac{\beta_n}{n+1}\left[1 - \sum_{i=0}^{n-1} \tau_i k_i(\xi_\beta) P_i^2(x_j,\xi_\beta)\right]^{-1}, \qquad j = 1,\dots,n+1.$$

The polynomials $\{P_j(x,\xi_\beta)\}$ *are also defined in Theorem 2.2 and the numbers* τ_i *and* $k_i(\xi)$ *are given by* $[k_0(\xi) = 1]$

$$\tau_i = \sum_{l=i}^{n-1} \frac{\beta_l}{l+1}, \qquad k_i(\xi) = \frac{\det M_{i-1}(\xi)}{\det M_i(\xi)}, \qquad i = 1,\dots,n-1.$$

PROOF. Applying Theorem 2.1, we obtain for the function Ψ_β,

$$
\begin{aligned}
\Psi_\beta(\xi) &= \sum_{l=0}^{n} \frac{\beta_l}{l+1} \log(\det M_l(\xi))\\
&= \sum_{i=1}^{n} \sigma_i \log(\zeta_{2i-1}\zeta_{2i})\\
&= \sum_{i=1}^{n} \sigma_i \log(p_{2i-1}q_{2i-1}) + \sum_{i=1}^{n-1} \log(p_{2i}^{\sigma_i} q_{2i}^{\sigma_{i+1}}) + \sigma_n \log p_{2n}.
\end{aligned}
$$

Simple algebra shows that Ψ_β is maximized by the canonical moments given in (3.1). By Theorem 2.2 we conclude that the support of ξ_β is given by the zeros of the polynomial $x(1-x)Q_{n-1}(x,\xi_\beta)$. This theorem also shows that the polynomials $\{P_j(x,\xi)\}$ are orthogonal with respect to the measure $d\xi(x)$. A standard argument in the theory of orthogonal polynomials [see Szegö (1959), page 28] gives

$$\int_0^1 P_l^2(x,\xi)\,d\xi(x) = \frac{\det M_l(\xi)}{\det M_{l-1}(\xi)} = \frac{1}{k_l(\xi)}, \qquad l \ge 1.$$

Therefore, the polynomials $\{\sqrt{k_j(\xi)}\, P_j(x,\xi)\}$ form an orthonormal system with respect to the measure $d\xi$ and it follows

$$(3.3) \qquad d_l(x,\xi) = \sum_{i=0}^{l} k_i(\xi) P_i^2(x,\xi), \qquad l = 0,1,\dots,n,$$

for every design ξ on $[0,1]$ with $0 < p_k < 1$ for $k = 0,1,\dots,2n-1$ and $p_{2n} = 1$. Because the support of ξ_β consists of $n+1$ points, we have for $l = n$ [see Fedorov (1972), page 147],

$$(3.4) \qquad d_n(x,\xi_\beta) = \sum_{i=1}^{n+1} \frac{L_i^2(x)}{\xi_\beta(\{x_i\})},$$

where $L_i(x)$ denotes the Lagrange interpolation polynomial at the support points $x_1,\dots,x_{n+1}$ of ξ_β. It is a simple consequence of Theorem 1.1 that the function $\Theta_\beta(x,\xi_\beta) = \sum_{l=0}^{n}[\beta_l/(l+1)]\, d_l(x,\xi_\beta)$ attains its maximum value in $[0,1]$ at the support points of the optimal design ξ_β. This together with Theorem 1.1, (3.3) and (3.4) implies, for $j = 1,2,\dots,n+1$,

$$\begin{aligned} 1 = \Phi_\beta(\xi_\beta) &= \max_{x\in[0,1]} \Theta_\beta(x,\xi_\beta) = \Theta_\beta(x_j,\xi_\beta) \\ &= \sum_{l=0}^{n-1} \frac{\beta_l}{l+1} \sum_{i=0}^{l} k_i(\xi_\beta) P_i^2(x_j,\xi_\beta) + \frac{\beta_n}{n+1}\frac{1}{\xi_\beta(\{x_j\})} \\ &= \sum_{i=0}^{n-1} \tau_i k_i(\xi_\beta) P_i^2(x_j,\xi_\beta) + \frac{\beta_n}{n+1}\frac{1}{\xi_\beta(\{x_j\})}. \end{aligned}$$

Solving the last equation we obtain (3.2), and Theorem 3.1 is proved. □

The following auxiliary result, which also holds for every symmetric design, is a simple consequence of Theorem 2.2 and describes the connection between the polynomials $\{P_j(x,\xi_\beta)\}$ and $\{Q_j(x,\xi_\beta)\}$.

LEMMA 3.2. *For the polynomials* $\{Q_j(x,\xi_\beta)\}$ *and* $\{P_j(x,\xi_\beta)\}$ *defined by Theorem* 2.2, *we have, for* $j \ge 2$,

$$P_j(x,\xi_\beta) - Q_j(x,\xi_\beta) = -\tfrac{1}{4} p_{2(j-1)}(\xi_\beta) p_{2j}(\xi_\beta) Q_{j-2}(x,\xi_\beta).$$

In the cases $\tilde\lambda(x) = x$, $\tilde\lambda(x) = 1-x$ and $\tilde\lambda(x) = x(1-x)$ the optimal designs for $\mathscr{F}_n$ with respect to the prior β are obtained in the same way. The corresponding formulas will not be given here. We only state the solutions in terms of canonical moments.

THEOREM 3.3. *The canonical moments of the optimal design for $\mathscr{F}_n$ with respect to the prior β are given by the following*:

$$
\text{(i)} \quad \begin{aligned} p_{2i-1}(\xi_\beta) &= \frac{1}{2}, && i = 1, \dots, n+1,\\ p_{2i}(\xi_\beta) &= \frac{\sigma_i}{\sigma_{i-1} + \sigma_i}, && i = 1, \dots, n,\\ p_{2n+2}(\xi_\beta) &= 0, && \textit{in the case } \tilde{\lambda}(x) = x(1-x); \end{aligned}
$$

$$
\text{(ii)} \quad \begin{aligned} p_{2i}(\xi_\beta) &= \frac{1}{2}, && i = 1, \dots, n,\\ p_{2i-1}(\xi_\beta) &= \frac{\sigma_i}{\sigma_{i-1} + \sigma_i}, && i = 1, \dots, n,\\ p_{2n+1}(\xi_\beta) &= 0, && \textit{in the case } \tilde{\lambda}(x) = 1-x; \end{aligned}
$$

$$
\text{(iii)} \quad \begin{aligned} p_{2i}(\xi_\beta) &= \frac{1}{2}, && i = 1, \dots, n,\\ p_{2i-1}(\xi_\beta) &= \frac{\sigma_{i-1}}{\sigma_{i-1} + \sigma_i}, && i = 1, \dots, n,\\ p_{2n+1}(\xi_\beta) &= 1, && \textit{in the case } \tilde{\lambda}(x) = x. \end{aligned}
$$

EXAMPLE. Let $n = 3$, $\tilde{\lambda}(x) \equiv 1$ and $\beta = (0, \beta_1, \beta_2, \beta_3)$ [we put $\beta_0 = 0$ because in the case $\tilde{\lambda}(x) \equiv 1$ we have $M_0(\xi) = 1$ for all designs ξ]. By Theorem 3.1, the support of the optimal design ξ_β for $\mathscr{F}_n$ is given by $\operatorname{supp}(\xi_\beta) = \{0, (1-x)/2, (1+x)/2, 1\}$, where, for $\beta_3 = 1 - \beta_1 - \beta_2$,

$$
x = \sqrt{p_2(\xi_\beta) q_4(\xi_\beta)} = \sqrt{\frac{(1-\beta_1-\beta_2)(9-3\beta_1-\beta_2)}{(5-3\beta_1-\beta_2)(9-9\beta_1-5\beta_2)}}.
$$

To calculate the weights of ξ_β at the point 0 we remark that (3.3) and Theorem 2.1 give here

$$
d_1(0, \xi_\beta) = 1 + \frac{1}{p_2(\xi_\beta)}, \qquad d_2(0, \xi_\beta) = 1 + \frac{1}{p_2(\xi_\beta)} + \frac{q_2(\xi_\beta)}{p_2(\xi_\beta) p_4(\xi_\beta)}.
$$

Thus, we obtain by (3.2) and (3.1),

$$
\begin{aligned} \xi_\beta(\{0\}) &= \frac{\beta_3}{4}\left[1 - \left(\frac{\beta_1}{2} + \frac{\beta_2}{3}\right)\left(1 + \frac{1}{p_2(\xi_\beta)}\right) - \frac{\beta_2}{3}\frac{q_2(\xi_\beta)}{p_2(\xi_\beta)p_4(\xi_\beta)}\right]^{-1}\\ &= \frac{1}{12}\,\frac{9-3\beta_1-\beta_2}{3-2\beta_1-\beta_2}. \end{aligned}
$$

The other weights are obtained by the symmetry of the optimal design ξ_β at the point $\frac{1}{2}$,

$$\xi_\beta(\{0\}) = \xi_\beta(\{1\}),$$

$$\xi_\beta\left(\left\{\frac{1-x}{2}\right\}\right) = \xi_\beta\left(\left\{\frac{1+x}{2}\right\}\right) = \frac{1}{2} - \xi_\beta(\{0\}) = \frac{1}{12}\frac{9-9\beta_1-5\beta_2}{3-2\beta_1-\beta_2}.$$

4. A special class of priors. The D- and D_1-optimality criteria are special cases [$\beta = (0,\dots,0,1)$ and $\beta = (0,\dots,0,-n,n+1)$] within the general class of the priors defined in Section 1. The optimal designs connected to these criteria are of a very simple structure (see Section 1). In this section we will show that many priors yield optimal designs for $\mathscr{F}_n$ with the same simple structure as in the cases just mentioned. In what follows, $\Gamma(z)$ denotes the gamma function defined for $z \in \mathbb{R} \setminus \{0, -1, -2, \dots\}$. We begin our investigations with the following result, which is used to define a special class of priors depending on a real parameter z.

LEMMA 4.1. *Let $n \in \mathbb{N}$, $q \in \mathbb{N}_0$ and $z \in \mathbb{R} \setminus \{0, -1, -2, \dots\}$. Then we have for all $i = 0, 1, \dots, n$,*

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

PROOF. For $q \in \mathbb{N}_0$ and $i \in \{0, \dots, n\}$, let

$$f_{q,i}(z) = \sum_{l=i}^{n} \frac{\Gamma(q+l+1-i)}{\Gamma(l+1-i)} \frac{\Gamma(n+z-l-1)}{\Gamma(n+1-l)}.$$

Then we obtain, observing the functional equation of the gamma function, for $q \geq 1$, $i \geq 1$,

$$f_{q,i-1}(z) = f_{q,i}(z) + q f_{q-1,i-1}(z).$$

Note that $f_{q,n}(z) = \Gamma(q+1)\Gamma(z-1)$ and $f_{q,n+1}(z) = 0$ for all $q \in \mathbb{N}_0$ and $n \in \mathbb{N}$ and the assertion of Lemma 4.1 now follows by some induction arguments. □

Let us now define a prior $\beta(z) = (\beta_0(z), \dots, \beta_n(z))$ for $\mathscr{F}_n$, $n \in \mathbb{N}$, depending on the real number $z \in \mathbb{R} \setminus \{0, -1, -2, \dots\}$, by

$$\beta_l(z) = (l+1)\frac{\Gamma(n+z-l-1)}{\Gamma(n+1-l)} \frac{\Gamma(z+1)}{\Gamma(z-1)} \frac{\Gamma(n+1)}{\Gamma(n+z+1)}, \qquad l = 0, 1, \dots, n. \tag{4.1}$$

Lemma 4.1 ($q = 1$) shows that $\sum_{l=0}^{n} \beta_l(z) = 1$ and we obtain the D- and D_1-optimality criteria from the following proposition, which is a simple consequence from elementary properties of the gamma function.

PROPOSITION 4.2. *Let $n \in \mathbb{N}_0$ and $\beta(z) = (\beta_0(z), \dots, \beta_n(z))$, defined by (4.1). Then we have*

(i) $$\lim_{z \to 1} \beta(z) = (0, \dots, 0, 1),$$

(ii) $$\lim_{z \to 0} \beta(z) = (0, \dots, 0, -n, n+1).$$

To guarantee that the numbers defined in (4.1) form a prior for the class $\mathscr{F}_n$ in the sense explained in Section 1, we have to make a suitable restriction on the domain of the parameter z. To this end, we collect all *priors* defined by (4.1) in the set

$$B_n = \{\beta(z) = (\beta_0(z), \dots, \beta_n(z)) | z \geq 1 \text{ or } z = 0\},$$

where the interpretation of $\beta(0)$ and $\beta(1)$ is in the sense of Proposition 4.2.

In what follows, let $P_n^{(\gamma, \delta)}(x)$, for $\gamma, \delta > -1$, and $G_n^{(p,q)}(x)$, for $p - q > -1$, $q > 0$, denote the Jacobi polynomials on $[-1, 1]$ and $[0, 1]$, respectively. $\{P_n^{(\gamma, \delta)}(x)\}$ and $\{G_n^{(p,q)}(x)\}$ are orthogonal with respect to the measures $(1 - x)^{\gamma}(1 + x)^{\delta}\,dx$ and $x^{q-1}(1 - x)^{p-q}\,dx$ on the corresponding intervals [see Szegö (1959), pages 58–77, or Abramowitz and Stegun (1964), pages 774–777, for more details] and are related by the formula

$$P_n^{(\gamma, \delta)}(x) = \frac{\Gamma(2n + \gamma + \delta + 1)}{n!\,\Gamma(n + \gamma + \delta + 1)} G_n^{(\gamma + \delta + 1, \delta + 1)}\left(\frac{x + 1}{2}\right). \tag{4.2}$$

THEOREM 4.3. *Let $\lambda(x) = (1 + x)^u(1 - x)^v$, $u, v \in \{0, 1\}$, $\beta(z) \in B_n$ and $n \in \mathbb{N}$. The optimal design $\xi_{\beta(z)}$ for $\mathscr{F}_n$ with respect to the prior $\beta(z)$ is supported by the zeros of the polynomial*

$$(1 + x)^{1-u}(1 - x)^{1-v} P_{n-1+u+v}^{((z+1)/2 - v, (z+1)/2 - u)}(x).$$

The optimal design $\xi_{\beta(z)}$ concentrates equal mass on all support points which are in the interior of $[-1, 1]$. If there are any support points at -1 or 1 (this depends on u, v), their masses are $(z + 1)/2$ times bigger than the masses of the interior support points.

PROOF. The proof of Theorem 4.3 has to be given separately in all four cases of the efficiency function λ. For brevity, only the case $(u, v) = (0, 0)$ will be considered. For $z = 1$, Theorem 4.3 gives the classical D-optimal designs in polynomial regression [see Fedorov (1972), page 88, and Studden (1982b)]. In what follows we therefore assume $z \neq 1$ and show by Theorem 3.1 that the support of an optimal design $\xi_{\beta(z)}$ for $\mathscr{F}_n$ with respect to the prior $\beta(z) \in B_n$ on the interval [0, 1] is given by the $n+1$ zeros $0 = x_1 < x_2 < \cdots < x_n < x_{n+1} = 1$ of the polynomial

$$x(1-x)G_{n-1}^{(z+2,(z+3)/2)}(x), \tag{4.3}$$

and that the weights at the support points are

$$\begin{aligned} \xi_{\beta(z)}(\{0\}) &= \xi_{\beta(z)}(\{1\}) = \frac{1}{n+z}\frac{z+1}{2}, \\ \xi_{\beta(z)}(\{x_j\}) &= \frac{1}{n+z}, \qquad j = 2,\dots,n. \end{aligned} \tag{4.4}$$

The statement of Theorem 4.3 [in the case $(u,v) = (0,0)$] then follows by a linear transformation and (4.2). Lemma 4.1 (in the case $q = 1$) gives for the numbers σ_i defined in Theorem 3.1,

$$\sigma_i = \sum_{l=i}^{n} \frac{l+1-i}{l+1}\beta_l(z) = \frac{\Gamma(n+1)}{\Gamma(n+z+1)}\frac{\Gamma(n+1+z-i)}{\Gamma(n+1-i)}, \tag{4.5}$$

and thus we have, using (3.1) for the even-order canonical moments of the optimal design $\xi_{\beta(z)}$,

$$\begin{aligned} p_{2i}(\xi_{\beta(z)}) &= \frac{z+n-i}{z+2(n-i)}, \\ q_{2i}(\xi_{\beta(z)}) &= \frac{n-i}{z+2(n-i)}, \\ \frac{p_{2i}(\xi_{\beta(z)})}{q_{2i}(\xi_{\beta(z)})} &= \frac{z+n-i}{n-i}. \end{aligned} \tag{4.6}$$

[Note that, by (3.1), all odd-order moments are $\frac{1}{2}$.] In what follows we will suppress the dependence of the canonical moments $p_i(\xi_{\beta(z)})$ and the numbers $k_i(\xi_{\beta(z)})$ from the optimal design $\xi_{\beta(z)}$ and write for simplicity p_i and k_i. By another application of Lemma 4.1, we can now express the numbers τ_i of Theorem 3.1 in terms of the canonical moments of $\xi_{\beta(z)}$,

$$\tau_i = \sum_{l=i}^{n-1} \frac{\beta_l(z)}{l+1} = \frac{\Gamma(z+1)\Gamma(n+1)}{\Gamma(n+z+1)}\left[\frac{z}{(n+z-i)}\prod_{j=i}^{n-1}\frac{p_{2j}}{q_{2j}} - 1\right], \tag{4.7}$$

and obtain by Theorem 2.1 for the constants k_i,

$$k_{n-j} = \frac{4}{p_{2(n-j)}q_{2(n-j-1)}}k_{n-j-1}, \qquad j = 1,2,\dots,n-2. \tag{4.8}$$

The following two identities are shown by the application of Theorem 2.2 and

Lemma 3.2:

$$P_{l-1}(x,\xi_{\beta(z)})Q_{l-1}(x,\xi_{\beta(z)}) = P_{l-1}^2(x,\xi_{\beta(z)}) + \tfrac{1}{4}p_{2(l-2)}p_{2(l-1)}P_{l-1}(x,\xi_{\beta(z)})Q_{l-3}(x,\xi_{\beta(z)}), \tag{4.9}$$

$$\begin{aligned} P_{l}(x,\xi_{\beta(z)})Q_{l-2}(x,\xi_{\beta(z)}) &= P_{l-1}^2(x,\xi_{\beta(z)}) + \tfrac{1}{4}p_{2(l-2)}P_{l-1}(x,\xi_{\beta(z)})Q_{l-3}(x,\xi_{\beta(z)}) \\ &\quad - \tfrac{1}{4}p_{2(l-1)}q_{2(l-2)}P_{l-2}(x,\xi_{\beta(z)})Q_{l-2}(x,\xi_{\beta(z)}). \end{aligned} \tag{4.10}$$

Note that the equations (4.8), (4.9) and (4.10) hold for every symmetric design ξ. They are used to prove the following lemma, which is the essential part in the proof of Theorem 4.3.

LEMMA 4.4. *Let $z \in \mathbb{R}_0^+ \setminus \{1\}$ and define, for $l = 0, 1, \dots, n-2$,*

$$c(l,z) = \frac{1}{z-1}\left[\prod_{j=1}^{l+1}\frac{p_{2(n-j)}}{q_{2(n-j)}} - (z+l+1)\right].$$

Then we have, for $l = 1, 2, \dots, n-2$,

$$\begin{aligned} \sum_{i=n-l}^{n-1} k_i\tau_i P_i^2(x,\xi_{\beta(z)}) &= k_{n-1}\tau_{n-1}P_{n-1}(x,\xi_{\beta(z)})Q_{n-1}(x,\xi_{\beta(z)}) \\ &\quad - k_{n-l-1}\tau_{n-1}\big[c(l,z)P_{n-l}(x,\xi_{\beta(z)})Q_{n-l-2}(x,\xi_{\beta(z)}) \\ &\qquad - c(l-1,z)P_{n-l-1}(x,\xi_{\beta(z)})Q_{n-l-1}(x,\xi_{\beta(z)})\big]. \end{aligned}$$

PROOF. Observing (4.7) and (4.8), straightforward algebra gives

$$\frac{1}{4}k_{n-l-1}p_{2(n-l-2)}\big[c(l,z) - c(l-1,z)p_{2(n-l-1)}\big] = k_{n-l-2}c(l+1,z), \tag{4.11}$$

$$c(l,z) - c(l-1,z) = \frac{\tau_{n-l-1}}{\tau_{n-1}}. \tag{4.12}$$

For $l = 1$ the statement is easily verified, noting (4.8), (4.9) and $c(0,z) = 0$. To show that l implies $l+1$, $l \le n-3$, we use (4.9) and (4.10) and obtain

$$\begin{aligned} &k_{n-1}\tau_{n-1}Q_{n-1}(x,\xi_{\beta(z)})P_{n-1}(x,\xi_{\beta(z)}) \\ &\quad = k_{n-l-1}\tau_{n-1}\Big\{\big[c(l,z) - c(l-1,z)\big]P_{n-l-1}^2(x,\xi_{\beta(z)}) \\ &\qquad + P_{n-l-1}(x,\xi_{\beta(z)})Q_{n-l-3}(x,\xi_{\beta(z)})\tfrac{1}{4}p_{2(n-l-2)} \\ &\qquad \times\big[c(l,z) - c(l-1,z)p_{2(n-l-1)}\big] \\ &\qquad - c(l,z)\tfrac{1}{4}p_{2(n-l-1)}q_{2(n-l-2)}P_{n-2-l}(x,\xi_{\beta(z)})Q_{n-l-2}(x,\xi_{\beta(z)})\Big\} \\ &\qquad + \sum_{i=n-l}^{n-1} k_i\tau_i P_i^2(x,\xi_{\beta(z)}). \end{aligned}$$

An application of (4.8), (4.11) and (4.12) yields

$$k_{n-1}\tau_{n-1}P_{n-1}(x,\xi_{\beta(z)})Q_{n-1}(x,\xi_{\beta(z)}) - \sum_{i=n-l-1}^{n-1}\tau_i k_i P_i^2(x,\xi_{\beta(z)})$$
$$= k_{n-l-2}\tau_{n-1}\big[c(l+1,z)P_{n-l-1}(x,\xi_{\beta(z)})Q_{n-l-3}(x,\xi_{\beta(z)})$$
$$-c(l,z)P_{n-l-2}(x,\xi_{\beta(z)})Q_{n-l-2}(x,\xi_{\beta(z)})\big],$$

which completes the proof of Lemma 4.4. □

We now continue the proof of Theorem 4.2. Noting (4.7) and (4.12), we have by Lemma 4.4, for $l = n-2$,

$$\sum_{i=1}^{n-1} k_i\tau_i P_i^2(x,\xi_{\beta(z)}) - k_{n-1}\tau_{n-1}P_{n-1}(x,\xi_{\beta(z)})Q_{n-1}(x,\xi_{\beta(z)})$$
$$= k_1\tau_1 P_1^2(x,\xi_{\beta(z)}) - c(n-2,z)k_1\tau_{n-1}P_2(x,\xi_{\beta(z)})$$
$$+ c(n-3,z)k_1\tau_{n-1}P_1(x,\xi_{\beta(z)})Q_1(x,\xi_{\beta(z)})$$
$$= \frac{n}{z+n} - (n+z-1)\frac{\Gamma(z+1)\Gamma(n+1)}{\Gamma(n+1+z)}.$$

The weights at the support points of $\xi_{\beta(z)}$ are given by (3.2) in Theorem 3.1. Noting the definition of $\beta_n(z)$, we obtain

$$\xi_{\beta(z)}(\{x_j\}) = \frac{\beta_n(z)}{n+1}\Bigg[1 - \tau_0 - k_{n-1}\tau_{n-1}P_{n-1}(x_j,\xi_\beta)Q_{n-1}(x_j,\xi_\beta)$$
$$-\frac{n}{z+n} + (z+n-1)\frac{\Gamma(z+1)\Gamma(n+1)}{\Gamma(n+z+1)}\Bigg]^{-1}$$
$$= \big[n+z-(z-1)k_{n-1}Q_{n-1}(x_j,\xi_\beta)P_{n-1}(x_j,\xi_\beta)\big]^{-1}.$$

Theorem 3.1 gives $Q_{n-1}(x_j,\xi_\beta) = 0$, $j = 2,\dots,n$. This yields

$$\xi_{\beta(z)}(\{x_j\}) = \frac{1}{n+z}, \qquad j = 2,\dots,n,$$

and assertion (4.4) follows from the symmetry of the optimal design at the point $x = \frac{1}{2}$. To prove (4.3), we apply Theorem 2.3, which shows that the supports of $\xi_{\beta(z)}$ and ξ^* are the same, where ξ^* is given by the canonical moments

$$p_{2i-1}(\xi^*) = \frac{1}{2}, \qquad i = 1,2,\dots,n,$$
$$p_{2i}(\xi^*) = \frac{\sigma_{n-i+1}}{\sigma_{n-i}+\sigma_{n-i+1}} = \frac{i}{z+2i}, \qquad i = 1,\dots,n-1,$$
$$p_{2n}(\xi^*) = 1.$$

By Theorem 2.2 we have $\operatorname{supp}(\xi_{\beta(z)}) = \{x \in [0,1] | x(1-x)Q_{n-1}(x,\xi^*) = 0\}$, where $Q_{n-1}(x,\xi^*)$ is defined by the recursive relation, with $Q_0(x,\xi^*) = 1$ and $Q_1(x,\xi^*) = x - \frac{1}{2}$,

$$Q_{j+1}(x,\xi^*) = \left(x - \frac{1}{2}\right)Q_j(x,\xi^*) - \frac{1}{4}\frac{j(z+j+1)}{(z+2j)(z+2j+2)}Q_{j-1}(x,\xi^*), \qquad j \geq 1. \tag{4.13}$$

The recursion coefficients in (4.13) can be identified with those of the Jacobi polynomials $G_n^{(z+2,(z+3)/2)}(x)$ on the interval $[0,1]$ [see Abramowitz and Stegun (1964), page 782]. Thus we obtain (4.3), which completes the proof of Theorem 4.3 [in the case $(u,v) = (0,0)$]. □

EXAMPLES. (i) Let $z = 0$ or $z = 1$. Noting $P_n'(x) = [(n+1)/2]P_{n-1}^{(1,1)}(x)$ and $T_n'(x) = \text{const}\ P_{n-1}^{(1/2,1/2)}(x)$ [see Abramowitz and Stegun (1964)], and noting Proposition 4.2, we obtain the D- and D_1-optimal designs given by Hoel (1958), Kiefer and Wolfowitz (1959) and Studden (1982b).

(ii) Let $(u,v) = (1,1)$ and $\beta(z) \in \beta_n$. The weights of the optimal design $\xi_{\beta(z)}$ for $\mathscr{F}_n$ with respect to the prior $\beta(z)$ do not depend on z and are all equal. $\xi_{\beta(z)}$ is supported by the zeros of the Jacobi polynomial $P_{n+1}^{((z-1)/2,(z-1)/2)}(x)$. This design is also the classical D-optimal design in the polynomial regression model $g_n(x)$ for the given efficiency function $\lambda(x) = (1-x^2)^{(z+1)/2}$ [see Fedorov (1972), page 88].

(iii) Let $(u,v) = (0,0)$, $n \geq 1$ and $z = 2$. By (4.1) we have

$$\frac{\beta_l(z)}{l+1} = \frac{2}{(n+1)(n+2)}, \qquad l = 0,1,\ldots,n.$$

Thus, the design maximizing the product $\prod_{l=0}^{n} \det M_l(\xi)$ (all models have the same weight) is given by the zeros of the polynomial $(1-x^2)U_n'(x)$, where $U_n(x)$ is the Chebyshev polynomial of the second kind. The masses of $\xi_{\beta(z)}$ are $1/(n+2)$ at the interior support points and $\frac{3}{2}[1/(n+2)]$ at the points -1 and 1. This design could be used if the experimenter has no knowledge which of the models of $\mathscr{F}_n$ is a proper model.

THEOREM 4.4. *Let $\lambda(x) = (1+x)^u(1-x)^v$, $u, v \in \{0,1\}$. The optimal design $\xi_{\beta(z)}$ for $\mathscr{F}_n$ with respect to the prior $\beta(z) \in B_n$ converges to the* arcsin-*distribution when $n \to \infty$.*

PROOF. We prove the assertion for $(u,v) = (0,0)$. The other cases are treated similarly. Because the canonical moments of the optimal design $\xi_{\beta(z)}$ are given by (3.4) and (4.6), we have $\lim_{n\to\infty} p_i(\xi_{\beta(z)}) = \frac{1}{2}$. The arcsin-distribution is the only distribution having $p_i = \frac{1}{2}$ for all $i \in \mathbb{N}$, which proves Theorem 4.4. □

5. Optimal product designs for multivariate polynomial regression. The results given so far can be generalized to multivariate polynomial regression on the q-cube $[-1,1]^q$. For simplicity, we use the same notations as in the previous sections although the meaning is sometimes different. For $x = (x_1, \dots, x_q)^{\mathrm{T}} \in [-1,1]^q$, let

$$g_l(x) = \sum_{i=1}^{N_{q,l}} f_i^{(l)}(x)\theta_i^{(l)} = f^{(l)\mathrm{T}}(x)\theta^{(l)}$$

denote a polynomial regression model of degree $l \in \mathbb{N}_0$. Thus the regression functions $f_i^{(l)}$ are the $N_{q,l} := \binom{l+q}{q}$ different functions of the form $\prod_{i=1}^q x_i^{m_i}$, where m_i are nonnegative integers with sum less than or equal to l. The models up to degree n are collected in the set

$$\mathscr{F}_n = \{g_l | g_l(x) = f^{(l)\mathrm{T}}(x)\theta^{(l)}, l = 0, \dots, n\}, \quad \text{where } \theta^{(l)} = \left(\theta_1^{(l)}, \dots, \theta_{N_{q,l}}^{(l)}\right)^{\mathrm{T}}.$$

For each $x \in [-1,1]^q$, a random variable $Y(x)$ with mean $g_l(x)$ for some (unknown) $l \in \{0, \dots, n\}$ and with variance $\sigma^2/\lambda(x)$ can be observed where the efficiency function λ is of the special form

$$\lambda(x) = \prod_{i=1}^{q} (1+x_i)^{u_i}(1-x_i)^{v_i} \quad \text{with } u_i, v_i \in \{0,1\}, i = 1, \dots, q. \tag{5.1}$$

A design η is a probability measure on $[-1,1]^q$. The information matrix in the model g_l is given by

$$M_l(\eta) = \int_{[-1,1]^q} f^{(l)}(x) f^{(l)\mathrm{T}}(x)\lambda(x)\,d\eta(x).$$

The generalization of the function Ψ_β defined in Section 1 to the situation stated in this section is given by

$$\Psi_\beta(\eta) = \sum_{l=0}^{n} \frac{\beta_l}{N_{q,l}} \log(\det[M_l(\eta)]),$$

where $\beta = (\beta_0, \dots, \beta_n)$ is a prior on $\{0, 1, \dots, n\}$. The notion prior is again used for probability measures on $\{0, 1, \dots, n\}$ or for vectors of the form ($s \in \{0, 1, \dots, n-1\}$)

$$\begin{aligned} &\beta_0 = \cdots = \beta_{n-s-1} = 0, \qquad \beta_{n-s} = -\frac{N_{q,n-s}}{N_{q,n} - N_{q,n-s}}, \\ &\beta_{n-s+1} = \cdots = \beta_{n-1} = 0, \qquad \beta_n = \frac{N_{q,n}}{N_{q,n} - N_{q,n-s}}, \end{aligned} \tag{5.2}$$

which yields the D_s-optimality criterion used if only the s highest order terms are of interest [note that (5.2) gives (1.1) in the case $q = 1$]. We call a design η optimal for the class $\mathscr{F}_n$ with respect to the prior β if η maximizes Ψ_β.

D-Optimal designs for the model g_n [which correspond to the prior $\beta_D = (0, \dots, 0, 1)$] are only obtained numerically for small n or q [see Kôno (1962), Farrell, Kiefer and Walbran (1967) and Lim and Studden (1988) for more details]. If n increases ($n \geq 5$), there are many numerical problems in the determination of the optimal design. To avoid such difficulties, Lim and Studden (1988) suggested maximizing $\det[M_n(\eta)]$ only over the class of product measures

$$\Xi := \{\eta = \xi_1 \times \xi_2 \times \cdots \times \xi_q \,|\, \xi_i \text{ is probability measure on } [-1,1],\ i = 1,\dots,q\}$$

on $[-1,1]^q$ and determined the D- and D_s-optimal product designs for all $q \in \mathbb{N}$ and $n \in \mathbb{N}$ in terms of canonical moments. They also give some efficiency calculations which indicate that there is not much loss using an optimal product design instead of an optimal design. In this section we calculate the optimal product designs (in Ξ) for the class $\mathscr{F}_n$ with respect to priors of similar structure as in (4.1). For brevity, the results are only stated for the constant efficiency function apart from Theorem 5.5.

THEOREM 5.1. *For the efficiency $\lambda(x) \equiv 1$, the optimal product design for $\mathscr{F}_n$ with respect to the prior β over the class of product designs Ξ is given by $\eta_\beta = \xi_\beta \times \cdots \times \xi_\beta$. For the canonical moments of ξ_β we have*

$$(5.3)\qquad \begin{aligned} p_{2i-1}(\xi_\beta) &= \frac{1}{2}, && i = 1,\dots,n,\\ p_{2i}(\xi_\beta) &= \frac{\sigma_i}{\sigma_i + \sigma_{i+1}}, && i = 1,\dots,n-1,\\ p_{2n}(\xi_\beta) &= 1, \end{aligned}$$

where the numbers σ_i are defined by

$$(5.4)\qquad \sigma_i = \sum_{l=i}^{n} \frac{N_{q,l-i}}{N_{q,l}} \beta_l \quad \text{for } i = 0,1,\dots,n.$$

PROOF. Let $\eta = \xi_1 \times \cdots \times \xi_q \in \Xi$ denote a product measure on $[-1,1]^q$ and let $\{p_i^{(j)}\}_{i \geq 1}$ denote the sequence of canonical moments which corresponds to the measure ξ_j, $j = 1,\dots,q$. We define the quantities (see also Theorem 2.2)

$$\zeta_1^{(j)} = p_1^{(j)}, \qquad \zeta_i^{(j)} = (1 - p_{i-1}^{(j)})p_i^{(j)} \quad \text{for } i \geq 2,\ j = 1,\dots,q$$

and obtain for the determinants $M_l(\eta)$ [see Lim and Studden (1988) for a proof],

$$\det[M_l(\eta)] = C_{l,q} \prod_{j=1}^{q} \prod_{i=1}^{l} \left[\prod_{k=1}^{i} \left(\zeta_{2k-1}^{(j)} \zeta_{2k}^{(j)} \right) \right]^{N_{q-1,l-i}},$$

where the constant $C_{l,q}$ depends only on l and q. Thus, we have [note that

$M_1(\eta) = 1$ if $\lambda(x) \equiv 1$ and $\Sigma_{i=k}^{l} N_{q-1,l-i} = N_{q,l-k}$, by Lemma 4.1]

$$\begin{aligned}\exp(\Psi_\beta(\eta)) &= \prod_{l=1}^{n} (\det[M_l(\eta)])^{\beta_l/N_{q,l}} \\ &= C_n \prod_{l=1}^{n} \left[\prod_{j=1}^{q} \prod_{i=1}^{l} \prod_{k=1}^{i} \left(\zeta_{2k-1}^{(j)}\zeta_{2k}^{(j)}\right)^{N_{q-1,l-i}} \right]^{\beta_l/N_{q,l}} \\ &= C_n \prod_{j=1}^{q} \prod_{l=1}^{n} \prod_{k=1}^{l} \left(\zeta_{2k-1}^{(j)}\zeta_{2k}^{(j)}\right)^{(\beta_l/N_{q,l})\Sigma_{i=k}^{l} N_{q-1,l-i}} \\ &= C_n \prod_{j=1}^{q} \prod_{k=1}^{n} \left(\zeta_{2k-1}^{(j)}\zeta_{2k}^{(j)}\right)^{\sigma_k},\end{aligned}$$

where the constant C_n depends only on n. The maximization of Ψ_β over the class of product measures Ξ can now be carried out determining the design ξ_β which maximizes $\prod_{k=1}^{n}(\zeta_{2k-1}^{(1)}\zeta_{2k}^{(1)})^{\sigma_k}$ and forming the product measure $\eta_\beta = \xi_\beta \times \cdots \times \xi_\beta$. Simple algebra shows that the canonical moments of the design ξ_β are given by (5.3), which completes the proof of Theorem 5.1. □

EXAMPLE. Let $n = 2$, $q \in \mathbb{N}$, $\lambda(x) \equiv 1$, $\beta_0 = 0$ and $\beta_1 = 1 - \beta_2$. Straightforward algebra yields

$$p_1(\xi_\beta) = \frac{1}{2}, \qquad p_2(\xi_\beta) = \frac{1 + [q/(q+2)]\beta_2}{1 + \beta_2},$$

$$p_3(\xi_\beta) = \frac{1}{2}, \qquad p_4(\xi_\beta) = 1,$$

and we obtain using Theorem 4.3, for $z = [(1 + \beta_2)/\beta_2](q + 2)/2 - 2$ and $n = 2$,

$$\operatorname{supp}(\xi_\beta) = \{-1, 0, 1\},$$

$$\xi_\beta(\{-1\}) = \xi_\beta(\{1\}) = \frac{1 + [q/(q+2)]\beta_2}{2(1 + \beta_2)},$$

$$\xi_\beta(\{0\}) = \frac{2}{q+2}\,\frac{\beta_2}{1 + \beta_2}.$$

Theorem 5.1 shows that $\eta_\beta = \xi_\beta \times \cdots \times \xi_\beta$ is the optimal product design for $\mathscr{F}_2$ with respect to the prior $\beta = (0, 1 - \beta_2, \beta_2)$. The D- and D_1-optimal product design for the quadratic model g_2 are obtained for $\beta_D = (0, 0, 1)$ and $\beta_{D_1} = (0, -2/q, (q + 2)/q)$, respectively.

We will now define a class of priors depending on one real parameter [the generalization of (4.1)] by

$$B_n = \{\beta(z) = (\beta_0(z), \ldots, \beta_n(z)) \mid z \geq 1 \text{ or } z = 0\},$$

where

$$\beta_l(z) = N_{q,l}\frac{\Gamma(n+z-l-1)}{\Gamma(n+1-l)}\frac{\Gamma(z+q)}{\Gamma(z-1)}\frac{\Gamma(n+1)}{\Gamma(n+z+q)}, \qquad l = 0, 1, \dots, n. \tag{5.5}$$

Here the priors $\beta(1)$ and $\beta(0)$ have to be interpreted as the limits

$$\beta(1) := \lim_{z \to 1} \beta(z) = (0, \dots, 0, 1),$$

$$\beta(0) := \lim_{z \to 0} \beta(z) = \left(0, \dots, 0, -\frac{N_{q,n-1}}{N_{q-1,n}}, \frac{N_{q,n}}{N_{q-1,n}}\right) = \left(0, \dots, 0, -\frac{n}{q}, \frac{n+q}{q}\right). \tag{5.6}$$

Note that (5.5) gives (4.1) for $q = 1$. $\beta(1)$ and $\beta(0)$ correspond to the D- and D_1-optimal designs and we have $\sum_{l=0}^{n}\beta_l(z) = 1$ by Lemma 4.1. For priors defined by (5.5) we obtain the following theorem.

THEOREM 5.2. *Let $\lambda(x) \equiv 1$, $q \in \mathbb{N}$ and $n \in \mathbb{N}$. The optimal product design $\eta_{q,n,z}$ for $\mathscr{F}_n$ with respect to the prior $\beta(z) \in B_n$ over the class Ξ is given by $\eta_{q,n,z} = \xi_{q,n,z} \times \cdots \times \xi_{q,n,z}$. The design $\xi_{q,n,z}$ on $[-1,1]$ is supported by the zeros of the polynomial $(1-y^2)P_{n-1}^{((z+q)/2,(z+q)/2)}(y)$. For the masses of $\xi_{q,n,z}$ at the support points we have*

$$\xi_{q,n,z}(\{y\}) = \begin{cases} \dfrac{z+q}{2}\dfrac{1}{n+z+q-1} & \text{if } y \in \{-1,1\}, \\[2ex] \dfrac{1}{n+z+q-1} & \text{if } y \in (-1,1) \cap \operatorname{supp}(\xi_{q,n,z}). \end{cases}$$

PROOF. By Theorem 5.1, the optimal product design for $\mathscr{F}_n$ with respect to the prior $\beta(z)$ is given by $\eta_{q,n,z} = \xi_{q,n,z} \times \cdots \times \xi_{q,n,z}$, where $\xi_{q,n,z}$ is determined by the canonical moments in (5.3). Using Lemma 4.1, we obtain for the quantities σ_i defined by (5.4), $i = 0, 1, \dots, n$,

$$\sigma_i = \sum_{l=i}^{n}\frac{N_{q,l-i}}{N_{q,l}}\beta_l(z) = \frac{\Gamma(n+1)}{\Gamma(n+z+q)}\frac{\Gamma(n+z+q-i)}{\Gamma(n+1-i)}.$$

Note that Lemma 4.1 cannot be applied for $z = 0$ and $z = 1$. In these cases the representation of σ_i can be derived directly, observing (5.6). Thus, we have for the canonical moments of $\xi_{q,n,z}$

$$p_{2i-1}(\xi_{q,n,z}) = \frac{1}{2}, \qquad i = 1, \dots, n,$$

$$p_{2i}(\xi_{q,n,z}) = \frac{z+q-1+n-i}{z+q-1+2(n-i)}, \qquad i = 1, \dots, n-1,$$

$$p_{2n}(\xi_{q,n,z}) = 1,$$

which correspond to the canonical moments given in (4.6). Because the canonical moments are invariant under transformations of the interval we can apply Theorem 4.3, for $(u, v) = (0, 0)$, and obtain the assertion of the Theorem 5.2. □

Note that the design $\xi_{q,n,z}$ depends only on the sum of q and z, where q is the dimension of $[-1, 1]^q$ and z the weighting parameter for $\mathscr{F}_n$. Therefore, $\xi_{q,n,z}$ is also the optimal design for $\mathscr{F}_n$ with respect to the prior $\beta(q+z-1)$ in the case of one-dimensional polynomial regression, i.e., $\xi_{q,n,z} = \xi_{1,n,q+z-1}$. The next two corollaries, which are the special cases $z = 1$ and $z = 0$ of Theorem 5.2, give the D- and D_1-optimal product designs for all $q \in \mathbb{N}$ and $n \in \mathbb{N}$.

COROLLARY 5.3. *Let $\lambda(x) \equiv 1$, $q \in \mathbb{N}$ and $n \in \mathbb{N}$. The D-optimal product design $\eta_{q,n,1}$ over the class Ξ is given by $\eta_{q,n,1} = \xi_{q,n,1} \times \cdots \times \xi_{q,n,1}$. The design $\xi_{q,n,1}$ on $[-1,1]$ is supported by the zeros of the polynomial $(1-y^2)P_{n-1}^{((q+1)/2,(q+1)/2)}(y)$. For the masses of $\xi_{q,n,1}$ at the support points we have*

$$\xi_{q,n,1}(\{y\}) = \begin{cases} \dfrac{q+1}{2}\dfrac{1}{n+q} & \text{if } y \in \{-1, 1\}, \\[2ex] \dfrac{1}{n+q} & \text{if } y \in (-1,1) \cap \operatorname{supp}(\xi_{q,n,1}). \end{cases}$$

COROLLARY 5.4. *Let $\lambda(x) \equiv 1$, $q \in \mathbb{N}$ and $n \in \mathbb{N}$. The D_1-optimal product design $\eta_{q,n,0}$ over the class Ξ is given by $\eta_{q,n,0} = \xi_{q,n,0} \times \cdots \times \xi_{q,n,0}$. The design $\xi_{q,n,0}$ on $[-1,1]$ is supported by the zeros of the polynomial $(1-y^2)P_{n-1}^{(q/2,q/2)}(y)$. For the masses of $\xi_{q,n,0}$ at the support points we have*

$$\xi_{q,n,0}(\{y\}) = \begin{cases} \dfrac{q}{2}\dfrac{1}{n+q-1} & \text{if } y \in \{-1, 1\}, \\[2ex] \dfrac{1}{n+q-1} & \text{if } y \in (-1,1) \cap \operatorname{supp}(\xi_{q,n,0}). \end{cases}$$

The following theorem, which states the analogous result for efficiency functions of the form (5.1), can be proved by similar arguments, using the corresponding statements of Sections 2, 3 and 4.

THEOREM 5.5. *Let $q \in \mathbb{N}$, $n \in \mathbb{N}$ and $\lambda(x) = \prod_{i=1}^{q}(1 + x_i)^{u_i}(1 - x_i)^{v_i}$, where $u_i, v_i \in \{0, 1\}$ for $i = 1, \dots, q$. The optimal product design for $\mathscr{F}_n$ with respect to the prior $\beta(z) \in B_n$ over the class Ξ is given by $\tilde{\eta}_{q,n,z} = \tilde{\xi}^{(1)}_{q,n,z} \times \cdots \times \tilde{\xi}^{(q)}_{q,n,z}$. For $i = 1, \dots, q$ the measure $\tilde{\xi}^{(i)}_{q,n,z}$ is supported by the zeros of the polynomial*

$$(1+y)^{1-u_i}(1-y)^{1-v_i}P_{n-1+u_i+v_i}^{((z+q)/2-v_i,\,(z+q)/2-u_i)}(y).$$

The design $\tilde{\xi}^{(i)}_{q,n,z}$ concentrates equal mass on all the support points which are in the interior of $[-1, 1]$, $i = 1, \dots, q$. If there are any support points of $\tilde{\xi}^{(i)}_{q,n,z}$ at the boundary (this depends on u_i, v_i) their masses are $(z + q)/2$ times bigger than the masses at the interior points of $\tilde{\xi}^{(i)}_{q,n,z}$, $i = 1, \dots, q$.

Acknowledgments. This paper is based on a part of the author's thesis written at the Universität Hannover. The author wishes to thank Dr. N. Henze, Professor Dr. F. Pukelsheim and Professor Dr. E. Weber for suggesting the problem and for stimulating discussions. Furthermore, the author is indebted to the Associate Editor and the referees for various suggestions which improved the presentation of the results.

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