Robust designs for polynomial regression by maximizing a minimum of D- and D_1-efficiencies

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Abstract

In the common polynomial regression of degree m we determine the design which maximizes the minimum of the D-efficiency in the model of degree m and the D_1-efficiencies in the models of degree $m-j, \ldots, m+k$ ($j, k \geq 0$ given). The resulting designs allow an efficient estimation of the parameters in the chosen regression and have reasonable efficiencies for checking the goodness-of-fit of the assumed model of degree m by testing the highest coefficients in the polynomials of degree $m-j, \ldots, m+k$.

Our approach is based on a combination of the theory of canonical moments and general equivalence theory for minimax optimality criteria. The optimal designs can be explicitly characterized by evaluating certain associated orthogonal polynomials.

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1 Introduction

Consider the common polynomial regression model of degree $m \in \mathbb{N}$

$$y = f_m^T(x)\vartheta_m + \varepsilon \qquad (1.1)$$

where $f_m(x) = (1, x, \ldots, x^m)^T$ denotes the vector of monomials up to the order $m, \vartheta_m = (\vartheta_{m0}, \ldots, \vartheta_{mm})^T$ is the vector of unknown parameters, ε is a random error with mean 0 and constant variance and the explanatory variable varies in a compact interval, say $\mathcal{X}$. An approximate design is a probability measure ξ with finite support in $\mathcal{X}$ [see Kiefer (1974)], where the masses represent the relative proportion of total observations taken at the corresponding design points. The Fisher information matrix of an approximate design in the polynomial regression of degree m is proportional to

$$M_m(\xi) = \int_{\mathcal{X}} f_m(x) f_m^T(x) d\xi(x) \tag{1.2}$$

and an optimal (approximate) design maximizes an appropriate (concave) real valued function of the matrix $M_m(\xi)$, which is called optimality criterion. There are numeruous optimality criteria proposed in the literatur [see e.g. Silvey (1980) or Pukelsheim (1993)], which can be used to discriminate between different designs, and the solution of the optimal design problem for the polynomial regression model has been found in many cases [see e.g. Hoel (1958), Guest (1958), Kiefer and Wolfowitz (1959), Studden (1980, 1982a, 1982b, 1989), Pukelsheim and Studden (1993)].

Nevertheless many authors point out that these designs are not robust with respect to the model assumption and cannot be used for checking any departures from the assumed model [see for example Box and Draper (1959), Läuter (1974), Huber (1975), Studden (1982b), Wiens (1992), Wong (1994) among many others]. For example, an optimal design with respect to the classical criteria advises the experimenter to take observations at $m+1$ points and can therefore not be used for checking higher degree polynomials. There are several proposals in the literature to incorporate the problem of model adequacy in the construction of optimal designs. Stigler (1971) proposed to use a model of higher degree, say $m+k \quad (k \geq 0)$, and to determine the D-optimal design for the model of degreee m subject to a guaranteed efficiency for testing the highest k coefficients in the model of degree $m+k$ [see also Studden (1982b)]. Similary, Läuter (1974) proposed the maximization of a weighted geometric mean of D-optimality criteria for the models of degree $1, \ldots, m+k$, in order to obtain robustness against misspecification of the degree [see also Dette (1990) for a complete solution of Läuter 's problem in the polynomial case and Wong (1994) for a robustness study in this case]. A different approach was suggested by Wiens (1992) who obtained (minimax) designs which are robust against "small" contaminations of the polynomial regression of degree m. Spruill (1990) and Dette (1995) proposed optimal designs for identifying the degree of the regression by maximizing the minimum of D_1-criteria in the models up to degree $m+k$. In the present paper we use a different criterion for the determination of robust designs which are efficient for parameter estimation and for testing the goodness-of-fit of the assumed regression model. We assume that the experimenter has some preference for the model of degree m, but also wants an efficient design for checking higher and lower degree models. We propose to maximize a weighted minimum of the D-efficiency in the (assumed) model of degree m (in order to obtain an efficient design for estimating the parameters in the assumed model) and of the D_1-efficiencies in the polynomial regression models of degree $m-j, \ldots, m+k$ (in order to obtain an efficient design for testing the highest coefficients in the polynomials of degree $m-j, \ldots, m+k$). Section 2 introduces the criterion and gives some basic results on the theory of canonical moments which was introduced by Skibinsky (1967) and used by Studden (1980, 1982a, 1982b, 1989) in the context of optimal design for polynomial regression. In Section 3 we combine these results with some general equivalence theorems for maximin criteria [see Pukelsheim (1993)] and obtain a characterization of the optimal design by a system of nonlinear equations for its canonical moments. Section 4 discusses the most important case where all efficiencies are equally weighted. Here we are able to describe the optimal design analytically by evaluating certain linear combinations of associated orthogonal polynomials [see Grosjean (1986) or Lasser (1994)], which allows a simple calculation of the support points and weights using standard software as Maple or Mathematica.

2 Maximizing the minimum of D- and D_1-efficiencies

The D-efficiency of a design ξ in the polynomial regression of degree m is defined by

$$\text{eff}_m^D(\xi) = \frac{|M_m(\xi)|^{1/(m+1)}}{\sup\limits_{\eta} |M_m(\eta)|^{1/(m+1)}} \tag{2.1}$$

where $|\cdot|$ denotes the determinant and the *sup* in the denominator is taken over the set of all designs such that $|M_m(\eta)| \not= 0$ [see Pukelsheim (1993)]. The$D$-optimal design ξ_m^D has D-efficiency equal to one and minimizes the volume of the confidence ellipsoid for the parameter ϑ_m. The D-optimal design for the polynomial regression model of degree m has been independently found by Hoel (1958) and Guest (1958). Similary, the D_1-efficiency in the model of degree m is defined by

$$\text{eff}_m^{D_1}(\xi) = \frac{|M_m(\xi)|}{|M_{m-1}(\xi)|} \cdot \Big(\sup_{\eta} \frac{|M_m(\eta)|}{|M_{m-1}(\eta)|}\Big)^{-1} \tag{2.2}$$

A D_1-optimal design has D_1-efficiency equal to 1 and maximizes the power of the t-test for the significance of the highest coefficient in the polynomial of degree m. The D_1-optimal design has been found by Kiefer and Wolfowitz (1959) [see also Studden (1968, 1980)].
For the definition of our robust criterion let $m > j \geq 0, k \geq 0$, $w_{m-j}, \ldots, w_{m+k}, w_m^*$ denote positive weights and define

$$\Psi_{m,j,k}^w(\xi) := \min\{w_{m-j}\text{eff}_{m-j}^{D_1}(\xi), \ldots, w_{m+k}\text{eff}_{m+k}^{D_1}(\xi), w_m^*\text{eff}_m^D(\xi)\} \tag{2.3}$$

as a weighted minimum of D- and D_1- efficiencies. The weights reflect the importance of the different goals of the experiment, i.e. estimation of the parameters in the model of degree m and discrimination between the models of degrees $l-1$ and l, where $l = m-j, \ldots, m+k$. Note that increasing the weight decreases the importance of the corresponding efficiency [because we are forming the minimum in (2.3)] and that the efficiency $\text{eff}_l^{D_1}(\xi)$ for polynomial regression of degree l is excluded in the maximin criterion (2.3) by defining the corresponding weight as $w_l = \infty$. A design maximizing the criterion $\Psi_{m,j,k}^w$ is expected to have good properties for estimating the parameters in the assumed regression of degree m and for testing the adequacy of polynomials of higher or lower degree.
Note that the criterion (2.3) is invariant with respect to affine transformations of the design space $\mathcal{X}$ and we assume from now on without loss of generality $\mathcal{X} = [-1,1]$. Designs maximizing the criterion (2.3) on different design spaces are obtained from the results of this paper by an affine transformation onto the given design space. Moreover, strict concavity of the maximin criterion $\Psi_{m,j,k}^w$ implies that the maximin optimal design must be symmetric. An important tool for determining optimal designs for polynomial regression is the theory of canonical moments which was introduced by Studden (1980, 1982a, 1982b) in this context [see also Lau (1983,

1988), Skibinsky (1986) and the recent monograph of Dette and Studden (1997)]. Roughly speaking every probability measure on the interval $[-1,1]$ is uniquely determined by a sequence $(p_1, p_2, \ldots)$ whose elements vary independently in the interval $[0,1]$. For a given probability measure on the interval $[-1,1]$ the element p_j of the corresponding sequence is called the jth canonical moment of the measure ξ. If j is the first index for which $p_j \in \{0,1\}$, then the sequence of canonical moments terminates at p_j, the measure is supported at a finite number of points and can be determined by evaluating certain orthogonal polynomials [see Skibinsky (1986) or Lau (1988)]. Moreover, a measure ξ is symmetric if and only if all canonical moments of odd order are equal 1/2 and for a symmetric measure we obtain for the determinant of the information matrix

$$|M_m(\xi)| = \prod_{i=1}^{m} (q_{2i-2}p_{2i})^{m-i+1} \tag{2.4}$$

where $p_2, p_4, \ldots, p_{2m}$ denote the canonical moments of the symmetric design ξ and $q_{2j} = 1 - p_{2j}$ $(j = 1, \ldots, m)$. Observing this identity we can easily identify the canonical moments of the D-optimal design for the polynomial regression of degree m, that is

$$p_{2l} = \frac{m-l+1}{2(m-l)+1}; \quad p_{2l-1} = \frac{1}{2}; \qquad l = 1, \ldots, m; \tag{2.5}$$

(note that the D-optimal design must be symmetric which determines the canonical moments of odd order) which gives for the D-efficiency of a symmetric design ξ

$$\mathrm{eff}_m^D(\xi) = \frac{1}{b_m} \prod_{j=1}^{m} (q_{2j-2}p_{2j})^{(m-j+1)/(m+1)} \tag{2.6}$$

where the constant b_m is given by

$$b_m = \Big(\Big(\frac{m}{2m-1}\Big)^m \prod_{i=2}^{m} \Big(\frac{(m-i+1)^2}{(2(m-i)+1)(2(m-i)+3)} \Big)^{m+1-i} \Big)^{\frac{1}{m+1}}. \tag{2.7}$$

Similary, the D_1-efficiency of a symmetric design ξ in the polynomial regression of degree m is given by

$$\mathrm{eff}_m^{D_1}(\xi) = 2^{2(m-1)} \prod_{j=1}^{m} q_{2j-2}p_{2j}. \tag{2.8}$$

We finally note that the maximin optimal designs for the weights $w^0 := (w_{m-j}, \ldots, w_{m+k}, w_m^*)$ with $w_m^* = \infty$ (in other words we are maximizing the minimum of D_1-efficiencies) have been found by Dette (1995) who showed that the maximin optimal design has canonical moments

$$p_{2l} = \frac{1}{2}, \qquad l = 1, \ldots, m-j-1, \tag{2.9}$$

$$p_{2m+2k} = 1 \tag{2.10}$$

$$p_{2l} = \max\Big\{ 1 - \frac{w_l}{2^{2(m+k-l)} w_{m+k} \prod_{i=l+1}^{m+k-1} p_{2i}(1-p_{2i})}, \frac{1}{2} \Big\}, \tag{2.11}$$

$l = m+k-1, \ldots, m-j$. It will be demonstrated in Section 3 and 4 that the constrained optimal design (with respect to the maximin criterion (2.3) can be described explicitly by a system of (nonlinear) equations for its canonical moments. The measure corresponding to the ,,optimal“ canonical moments specified by this system can then be determined numerically by standard methods [see Dette and Studden (1997), Section 3]. Moreover, in important special cases the maximin optimal designs can be found analytically

3 Maximin optimal designs - the general case

A basic tool for determining the optimal design maximizing the criterion in (2.3) is the following equivalence theorem, which characterizes the maximin optimal design by a simple inequality.

Theorem 3.1. *A design ξ^* maximizes the minimum of efficiencies in the optimality criterion (2.3) if and only if there exist nonnegative numbers $\alpha_{m-j}, \dots, \alpha_{m+k}, \alpha_m^*$ with sum equal to one such that the following conditions are satisfied:*

$$\alpha_l w_l \,\mathrm{eff}_l^{D_1}(\xi^*) \;=\; \alpha_l \Psi^w_{m,j,k}(\xi^*) \qquad l = m-j, \dots, m+k \tag{3.1}$$

$$\alpha_m^* w_m \,\mathrm{eff}_m^{D}(\xi^*) \;=\; \alpha_m^* \Psi^w_{m,j,k}(\xi^*) \tag{3.2}$$

$$\sum_{l=1}^{m} \frac{\alpha^*}{m+1} \frac{(e_l^T M_l^{-1}(\xi) f_l(x))^2}{e_l^T M_l^{-1}(\xi) e_l} + \sum_{l=m-j}^{m+k} \alpha_l \frac{(e_l^T M_l^{-1}(\xi) f_l(x))^2}{e_l^T M_l^{-1}(\xi) e_l} \le 1 - \frac{\alpha^*}{m+1} \tag{3.3}$$

for all $x \in [-1, 1]$.

Proof. Using general equivalence theory [see e.g. Pukelsheim (1993)] we obtain that a design maximizes the criterion (2.3) if and only if there exists nonnegative numbers $\alpha_{m-j}, \dots, \alpha_{m+k}, \alpha_m^*$ with sum equal to one such that (3.1), (3.2) are satisfied and the inequality

$$\frac{\alpha^*}{m+1} f_m^T(x) M_m^{-1}(\xi) f_m(x) + \sum_{l=m-j}^{m+k} \alpha_l \frac{(e_l^T M_l^{-1}(\xi) f_l(x))^2}{e_l^T M_l^{-1}(\xi) e_l} \le 1 \tag{3.4}$$

holds for all $x \in [-1, 1]$. If $e_l = (0\,, \dots, 0, 1)^T \in \mathbb{R}^{l+1}$ denotes the $(l+1)$th unit vector it is easy to see that for a design ξ with nonsingular information matrix $M_m(\xi)$ the polynomials

$$P_l(x, \xi) = \frac{e_l^T M_l^{-1}(\xi) f_l(x)}{(e_l^T M_l^{-1}(\xi) e_l)^{1/2}} \qquad l = 0\,, \dots, m$$

are orthonormal with respect to the design ξ and that the vector $P(x) = (\,P_0(x, \xi), \dots, P_m(x, \xi))^T$ satisfies

$$P(x) = A f_m(x)$$

for a nonsingular matrix $A \in \mathbb{R}^{m+1 \times m+1}$. This implies for any design such that $|M_m(\xi)\,| \neq 0$

$$f_m^T(x) M_m^{-1}(\xi) f_m(x) = \sum_{l=0}^{m} P_l^2(x, \xi) = \sum_{l=0}^{m} \frac{(e_l^T M_l^{-1}(\xi) f_l(x))^2}{e_l^T M_l^{-1}(\xi) e_l}$$

which gives in a combination with (3.4) the assertion of the theorem. □

Theorem 3.2.
(a) *Let η^* denote the design with canonical moments given by (2.9) - (2.11). If*

$$(3.5) \qquad w_m^* \operatorname{eff}_m^D(\eta^*) \geq \min\{w_l \operatorname{eff}_l^{D_1}(\eta^*) | l = m-j, \ldots, m+k\}$$

then the design η^* also maximizes the criterion $\Psi^w_{m,j,k}$ defined in (2.3)

(b) *If the design η^* defined by the canonical moments in (2.9) - (2.11) does not satisfy the inequality (3.5), the canonical moments of even order of the optimal design η^* maximizing (2.3) are uniquely determined and obtained as follows (all canonical moments of odd order are equal $\frac{1}{2}$) : $p_{2m+2k} = 1$.*

b(i) *In the case $k \geq 1$, there exists a positive integer $n \in \{\, m-j-1, \ldots, m\}$ such that $(p_2, \ldots, p_{2m+2k-2}) \in [\frac{1}{2}, 1)^{m+k-1}$ is the unique solution of the system of nonlinear equations*

$$(3.6) \qquad p_{2l} = \max\Big\{1 - \frac{w_l}{2^{2(m+k-l)} w_{m+k} \prod_{i=l+1}^{m+k-1} p_{2i}(1-p_{2i})}, \frac{1}{2}\Big\},$$

$(l = m+k-1, m+k-2, \ldots, m+1)$

$$(3.7) \qquad p_{2l} = 1 - \frac{2^{-2(m+k-l)} w_l}{w_{m+k} \prod_{i=l+1}^{m+k-1} p_{2i}(1-p_{2i})},$$

$(l = m, m-1, \ldots, n+1)$

$$(3.8) \quad p_{2l} = \max\Big\{1 - \frac{2^{-2(m+k-l)} w_l}{w_{m+k} \prod_{i=l+1}^{m+k-1} p_{2i}(1-p_{2i})}, 1 - \Big[2 + \frac{2p_{2n}-1}{p_{2n}} \prod_{i=l+1}^{n-1} \frac{1-p_{2i}}{p_{2i}}\Big]^{-1}\Big\},$$

$(l = n-1, n-2, \ldots, m-j-1)$

$$(3.9) \qquad p_{2l} = \frac{(2(m-j-l)-1)p_{2(m-j-1)} - m + j + l + 1}{4(m-j-l-1)p_{2(m-j-1)} - 2(m-j-l) + 3},$$

$(l = m-j-2, m-j-3, \ldots, 1)$

$$(3.10) \quad w_{m+k} 2^{2(m+k-1)} \prod_{l=1}^{m+k-1} p_{2l}(1-p_{2l}) = \frac{w_m^*}{b_m} \Big(\prod_{l=1}^{m} p_{2l}^{m-l+1}(1-p_{2l})^{m-l}\Big)^{1/(m+1)}$$

such that the inequalities

$$(3.11) \qquad w_n \geq 2^{2(m+k-n)} w_{m+k}(1-p_{2n}) \prod_{l=n+1}^{m+k-1} p_{2l}(1-p_{2l}),$$

$$(3.12) \qquad \frac{2p_{2n}-1}{1-p_{2n}} \leq \Big(\prod_{i=n+1}^{l-1} \frac{1-p_{2i}}{p_{2i}}\Big) \frac{2p_{2l}-1}{p_{2l}}, \qquad l = n+1, \ldots, m;$$

are satisfied, where b_m is defined by (2.7) and the convention $w_{m-j-1} = \infty$ is used.

b(ii) *If, in the case $k = 0$,the D-optimal design ξ_m^D for the polynomial regression model of degree m satisfies*

$$\Psi^w_{m,j,k}(\xi^D_m) = w^*_m \,\mathrm{eff}^D_m(\xi^D_m) = w^*_m$$

then ξ_m^D is also maximin optimal with respect to the criterion (2.3). Otherwise there exist integers $z \in \{ m- j, \dots, m\}$ and $n = n(z) \in \{ m- j - 1, \dots, z - 1\}$ such that the canonical moments $(p_2, \dots, p_{2m-2})$ of even order of the maximin optimal design are the unique solution in the cube $[\frac{1}{2}, 1)^{m-1}$ of the system of nonlinear equations: $p_{2m} = 1$,

$$p_{2l} = \frac{m-l+1}{2(m-l)+1}, \tag{3.13}$$

$l = m-1, m-2, \dots, z+1;$

$$p_{2l} = 1 - \frac{2^{-2(z-l)} w_l}{w_z p_{2z} \prod_{i=l+1}^{z-1} p_{2i}(1-p_{2i})}, \tag{3.14}$$

$l = z-1, z-2, \dots, n+1;$

$$\frac{2p_{2n}-1}{1-p_{2n}} = \prod_{l=n+1}^{m-1} \frac{1-p_{2l}}{p_{2l}} \tag{3.15}$$

(if $z < m$ and $n > 0$)

$$p_{2l} = \max\Big\{1 - \frac{2^{-2(z-l)} w_l}{w_z p_{2z} \prod_{i=l+1}^{z-1} p_{2i}(1-p_{2i})}, 1 - \Big(2 + \frac{2p_{2n}-1}{p_{2n}} \prod_{i=l+1}^{n-1} \frac{1-p_{2i}}{p_{2i}}\Big)^{-1}\Big\}, \tag{3.16}$$

$l = n-1, n-2, \dots, m-j-1;$

$$p_{2l} = \frac{(2(m-j-l)-1)p_{2(m-j-1)} - m + j + l + 1}{4(m-j-l-1)p_{2(m-j-1)} - 2(m-j-l) + 3}, \tag{3.17}$$

$l = m-j-2, m-j-3, \dots, 1$

$$w_z 2^{2(z-1)} p_{2z} \prod_{l=1}^{z-1} p_{2l}(1-p_{2l}) \;=\; \frac{w^*_m}{b_m} \Big(\prod_{l=1}^{m} p_{2l}^{m-l+1}(1-p_{2l})^{m-l}\Big)^{1/(m+1)} \tag{3.18}$$

such that the inequalities

$$w_n \;\geq\; 2^{2(z-n)} w_z (1-p_{2n}) \prod_{l=n+1}^{z-1} p_{2l}(1-p_{2l}), \tag{3.19}$$

$$w_z \;\leq\; 2^{2(l-z)} w_l (1-p_{2z}) \prod_{i=z+1}^{l-1} p_{2i}(1-p_{2i}), \qquad l = z+1\,, z+2\,, \dots, m, \tag{3.20}$$

$$\frac{2p_{2n}-1}{1-p_{2n}} \;\leq\; \Big(\prod_{i=n+1}^{l-1} \frac{1-p_{2i}}{p_{2i}}\Big) \frac{2p_{2l}-1}{p_{2l}}, \qquad l = n+1\,, n+2\,, \dots, z, \tag{3.21}$$

are satisfied, where b_m is defined by (2.7), $w_{m-j-1} = \infty$ and in the case $n = 0$ the inequalities (3.21) have to be replaced by the system

$$\frac{2p_{2l}-1}{1-p_{2l}} \geq \prod_{i=l+1}^{m-1} \frac{1-p_{2i}}{p_{2i}}, \qquad l = 1\,,\ldots,z. \tag{3.22}$$

Remark 3.3. Note that we do not claim the uniqueness of the constants z and n in Theorem 3.2. However, the canonical moments of the maximin optimal design are unique, because the optimization problem (2.3) has a unique solution. It is also worthwhile to mention that Theorem 3.2 guarantees the existenc of a z (and $n = n(z)$) such that the system of nonlinear equations has a solution $p_2, \ldots, p_{2m+2k-2}$ in the cube $[\frac{1}{2}, 1)^{m+k-1}$.

Proof of Theorem 3.2. A standard arguments of optimal theory shows the existence of a maximin optimal design. Because the maximin criterion (2.3) is strictly concave it follows from the results of Section 2 that the optimal design is unique and all canonical moments of odd order of the optimal design are equal 1/2.

(a) By the discussion in Section 2 the design η^* with canonical moments given by (2.9) - (2.11) maximizes

$$\Phi^w_{m,j,k} := \min\{w_l \,\mathrm{eff}_l^{D_1}(\xi) | l = m-j, \ldots, m+k\}$$

and it follows from (3.5)

$$\max_\xi \Psi^w_{m,j,k}(\xi) \leq \max_\xi \Phi^w_{m,j,k}(\xi) = \Phi^w_{m,j,k}(\eta^*) = \Psi^w_{m,j,k}(\eta^*)$$

which also proves optimality of η^* with respect to the maximin criterion $\Psi^w_{m,j,k}$.

(b) Assume that (3.5) is not satisfied and that $k > 0$. Observing Theorem 3.1 of this paper and Theorem 6.3.2 in Dette and Studden (1997) (for $p = 0$) it follows that η^* maximizes the criterion (2.3) if and only if there exists a prior $(\beta_1, \ldots, \beta_{m+k})$ for the class of polynomials of degreee $1, \ldots, m+k$ with $\beta_{m+k} > 0$ such that the equations

$$\beta_l = \beta_1, \tag{3.23}$$

$l = 2\,, \ldots, m-j-1,$

$$(\beta_l - \min_{i=1,\ldots,m} \beta_i) w_l \mathrm{eff}_l^{D_1}(\eta^*) = (\beta - \min_{i=1,\ldots,m} \beta_i)\Psi^w_{m,j,k}(\eta^*), \tag{3.24}$$

$l = m-j, \ldots, m,$

$$\beta_l w_l \mathrm{eff}_l^{D_1}(\eta^*) = \beta_l \Psi^w_{m,j,k}(\eta^*)\ , \tag{3.25}$$

$$(\min_{i=1,\ldots,m} \beta_i) w_{m^*} \mathrm{eff}_m^{D}(\eta_*) = (\min_{i=1,\ldots,m} \beta_i)\Psi^w_{m,j,k}(\eta^*)$$

$l=m+1,\ldots,m+k$, are satisfied and such that the design η^* maximizes the weighted geometric mean of D_1-efficiencies

$$\sum_{l=1}^{m+k} \beta_l \log \mathrm{eff}_l^{D_1}(\xi). \tag{3.26}$$

This follows directly by identifying the corresponding weights in the equivalence theorems for both criteria. Additionally we obtain

$$\beta_1 = \min_{i=1,\ldots,m} \beta_i$$

whenever $j \le m-2$. Now Theorem 6.2.6 in Dette and Studden (1997) expresses the weights β_l of the criterion (3.26) in terms of the canonical moments of the maximin optimal design η^*, i.e.

$$\beta_l = \prod_{j=1}^{l-1} \frac{q_{2j}}{p_{2j}}(1-\frac{q_{2l}}{p_{2l}}) \qquad l = 1\,,\ldots,m+k. \tag{3.27}$$

From $\beta_{m+k} > 0$ and (3.25) we have

$$w_{m+k}\,\mathrm{eff}_{m+k}^{D_1}(\eta^*) = \Psi_{m,j,k}^{w}(\eta^*) = w_m^*\,\mathrm{eff}_m^{D}(\eta^*) \tag{3.28}$$

[note that (3.5) is not satisfied in case (b)] which implies (3.10) observing (2.6) and (2.8). A further application of (3.25) and (2.8) for $l=m+k-1$ yields

$$\frac{\beta_{m+k-1}}{4q_{2m+2k-2}} = \frac{\beta_{m+k-1}\mathrm{eff}_{m+k-1}^{D_1}(\eta^*)}{\mathrm{eff}_{m+k}^{D_1}(\eta^*)} = \beta_{m+k-1}\frac{w_{m+k}}{w_{m+k-1}} \tag{3.29}$$

This gives either $p_{2m+2k-2} = \frac{1}{2}$ (equivalently $\beta_{m+k-1}=0$) or

$$p_{2m+2k-2} = 1 - \frac{w_{m+k-1}}{4w_{m+k}}.$$

Because

$$w_{m+k-1}\mathrm{eff}_{m+k-1}^{D_1}(\eta^*) \ge \Psi_{m,j,k}^{w}(\eta^*) = w_m^*\mathrm{eff}_m^{D}(\eta^*) = w_{m+k}\mathrm{eff}_{m+k}^{D_1}(\eta^*)$$

and $\beta_{m+k-1} \ge 0$ we obtain from (2.8) and (3.27) the identity (3.6) for $l=m+k-1$. Repeating these arguments yields the remaining equations in (3.6) for $l=m+k-2,\ldots,m+1$. From (3.23) and (3.27) we directly obtain (3.9), by induction. If we define

$$n = \max\{l \in \{\,1,\ldots,m\,\}\ |\beta_l = \min_{i=1,\ldots,m} \beta_i\}, \tag{3.30}$$

then (3.7) follows directly observing (3.24) and (2.8), because for $l=n+1\,,\ldots,m$ the corresponding factors $\beta_l - \min_{i=1,\ldots,m}\beta_i$ in (3.24) are all positive. Similary we derive from $\beta_n < \beta_l$ $(l=n+1\,,\ldots,m\,)$ and (3.27) the inequalities (3.12). The system of equations in (3.8) is also obtained from (3.24) as follows. If $\beta_l > \beta_n$ for $l=n-1,n-2,\ldots,m-j$ we have from (3.24)

$$w_l\mathrm{eff}_l^{D_1}(\eta^*) = w_{m+k}\mathrm{eff}_{m+k}^{D_1}(\eta^*)$$

which gives by (2.8)

$$p_{2l} = 1 - \frac{2^{-2(m+k-l)}w_l}{w_{m+k}\prod_{i=l+1}^{m+k-1} p_{2i}1-p_{2i}}.$$

Otherwise the equation $\beta_n = \beta_l$ and (3.27) imply

$$p_{2l} = 1 - [2 + \frac{2p_{2n} - 1}{p_{2n}} \prod_{i=l+1}^{n-1} \frac{q_{2i}}{p_{2i}}]^{-1}.$$

Because

$$w_l \text{eff}_l^{D_1}(\eta^*) \geq w_{m+k} \text{eff}_{m+k}^{D_1}(\eta^*)$$

and $\beta_l \geq \beta_n$ we obtain that the optimal value for p_{2l} is the corresponding maximum of these expressions for $l = n-1, \ldots, m-j$. If $j \leq m-2$ the remaining case $l = m-j-1$ in (3.8) follows from $\beta_1 = \beta_n = \min_{l=1}^m \beta_l$ and (3.23) using the convention $w_{m-j-1} = \infty$. Finally, the inequality (3.11) is obtained from (2.8) and (3.28) which implies $w_{m+k}\, \text{eff}_{m+k}^{D_1}(\eta^*) \leq w_n \text{eff}_n^{D_1}(\eta^*)$. This shows that in the case $k > 0$ the canonical moments of the maximin optimal design with respect to the criterion $\Psi_{m,j,k}^w$ in (2.3) satisfy the conditions specified by part b(i) of Theorem 3.2.

Reversing these arguments shows that any design with canonical moments satisfying the system of equations and inequalities in Theorem 3.2 b(i) also satisfies the conditions (3.1) – (3.3) of Theorem 3.1, which proves its optimality with respect to the criterion $\Psi_{m,j,k}^w$. Thus the class of maximin optimal designs (with respect to the criterion $\Psi_{m,j,k}^w$) is characterized by the system of nonlinear equations for the corresponding canonical moments in part b(i) of Theorem 3.2 and the assertion follows because the optimization problem (2.3) has a unique solution. The assertion for the case $k = 0$ in part b(ii) is proved similary [see Franke (2000)] and its proof therefore omitted.

□

4 Two special cases

In this section we discuss a special but very important situation in the optimality criterion (2.3), where all weights w_l, w_m^* are equal. In this case the maximin optimality criterion reduces to

(4.1) $$\Psi_{m,j,k}(\xi) = \min\{\text{eff}_m^D(\xi), \text{eff}_{m-j}^{D_1}(\xi), \ldots, \text{eff}_{m+k}^{D_1}(\xi)\}$$

Similary, if $w_m = \infty$ and all other weights are equal the maximin criterion (2.3) yields

(4.2) $$\chi_{m,j,k}(\xi) = \min\{\text{eff}_m^D(\xi), \text{eff}_{m-j}^{D_1}(\xi), \ldots, \text{eff}_{m-1}^{D_1}(\xi), \text{eff}_{m+1}^{D_1}(\xi), \ldots, \text{eff}_{m+k}^{D_1}(\xi)\}.$$

Note that for the choice $k = j = 0$ the criterion $\chi_{m,0,0}$ gives the D-optimality criterion for which the optimal design was explicitly found by Hoel (1958). For the criterion (4.1) and (4.2) the optimal designs can also be found analytically using the associated ultraspherical polynomials, which are defined recursively by

(4.3)
$$C_{-1}^{(\lambda)}(x,\nu) = 0 \;, \qquad C_0^{(\lambda)}(x,\nu) = 1 \;,$$
$$(n+\nu+1)\, C_{n+1}^{(\lambda)}(x,\nu) = 2(n+\nu+\lambda)x C_n^{(\lambda)}(x,\nu) - (n+\nu+2\lambda-1) C_{n-1}^{(\lambda)}(x,\nu),$$

$n \geq 0$, (see Grosjean (1986) or Lasser (1994)). We will frequently make use of the monic form of these polynomials defined by

$$\hat{C}_n^{(\lambda)}(x, \nu) = \frac{(\nu+1)_n}{2^n(\nu+\lambda)_n} C_n^{(\lambda)}(x, \nu), \tag{4.4}$$

where $(\alpha)_0 := 1$; $(\alpha)_n := \alpha(\alpha+1)\ldots(\alpha+n-1)$ if $n \geq 1$. These polynomials satisfy the recursion

$$\begin{aligned} \hat{C}_0^{(\lambda)}(x, \nu) &= 1 \ , \quad \hat{C}_1^{(\lambda)}(x, \nu) = x, \\ \hat{C}_{n+1}^{(\lambda)}(x, \nu) &= x\hat{C}_n^{(\lambda)}(x, \nu) - \frac{(n+\nu+2\lambda-1)(n+\nu)}{4(n+\nu+\lambda-1)(n+\nu+\lambda)} \hat{C}_{n-1}^{(\lambda)}(x, \nu), \quad n \geq 1. \end{aligned} \tag{4.5}$$

Theorem 4.1. *If $j = k = 0$ and $m \geq 2$ the maximin optimal design η^* with respect to the criterion (4.1) has canonical moments $p_{2m} = 1; p_{2l-1} = \frac{1}{2}$, $l = 1, \ldots, m$;and $(p_2, \ldots, p_{2m-2})$ is the unique solution of the the system of equations*

$$p_{2(m-1-l)} = \frac{(2l+1)\, p_{2(m-1)} - l}{4l p_{2(m-1)} - 2l + 1}, \qquad l = 1, \ldots, m-2, \tag{4.6}$$

$$1 = b_m^{m+1} 2^{2(m^2-1)} \prod_{l=1}^{m-1} p_{2l}^l (1-p_{2l})^{l+1}. \tag{4.7}$$

in the cube $[\frac{1}{2}, 1)^{m-1}$. The support points $x_0, \ldots, x_m$ are given by the zeros of the polynomial

$$(x^2-1) C_{m-1}^{(3/2)}(x, \nu-1)$$

and the masses are obtained as

$$\eta^*(x_l) = \frac{(\nu+m-1)\left[\frac{x_l}{\nu} C_{m-1}^{(1/2)}(x_l, \nu-1) - \frac{1}{\nu+1} C_{m-2}^{(1/2)}(x_l, \nu+1)\right]}{\frac{d}{dx}(x^2-1) C_{m-1}^{(3/2)}(x, \nu-1)\Big|_{x=x_l}}$$

$(l = 0, \ldots, m)$ where the parameter ν is defined by

$$\nu = \frac{1-p_{2m-2}}{2p_{2m-2}-1}$$

and p_{2m-2} is obtained from (4.6) and (4.7).

Otherwise the support points $x_0, \ldots, x_{m+k}$ of the maximin optimal design with respect to the criterion (4.1) are given by the zeros of the polynomial

$$Q_{m+k+1}(x) := U_{m-j-1}(x) T_{k+j+2}(x) + (k+j) T_{k+m+1}(x) - U_{m+k-1}(x) \tag{4.8}$$

where $T_l(x)$ and $U_l(x)$ denote the Chebyshev polynomial of the first and second kind, respectively. The masses at the support points are obtained by

$$\eta^*(x_l) = \frac{(k+j+1)\, U_{m+k}(x_l) - U_{m-j-2}(x_l) U_{k+j}(x_l)}{\frac{d}{dx} Q_{m+k+1}(x) \mid_{x=x_l}} \tag{4.9}$$

$l = 0, \ldots, m+k$.

Proof. We start with an examination of the condition (3.5) in Theorem 3.2. Observing (2.9) - (2.11) it follows by a straightforward induction ($w_l = 1$, $l = m-j, \ldots, m+k$) that the design η^* specified in part (a) of Theorem 3.2 has canonical moments $p_{2l-1} = 1/2$, $l = 1, \ldots, m+k$; and

(4.10) $$p_{2l} = \begin{cases} \dfrac{1}{2} & \text{if } 1 \le l < m-j \\[2ex] \dfrac{m+k-l+2}{2(m+k-l)+2} & \text{if } m-j \le l \le m+k. \end{cases}$$

Now a straightforward but tedious calculation shows that for equal weights the inequality (3.5) in Theorem 3.2 can be rewritten as

$$\Big(\frac{m-\frac{1}{2}}{m}\Big)^m \prod_{l=2}^{m} \Big[\frac{(m+\frac{1}{2}-l)(m+\frac{3}{2}-l)}{(m-l+1)^2}\Big]^{m-l+1} \ge \Big(\frac{1}{2}\Big)^{m+1} \Big(\frac{k+j+2}{k+j+1}\Big)^{m-j}.$$

Elementary but cumbersome calculus shows that this inequality is always satisfied except in the case $k = j = 0$ and $m \ge 2$.

(i) Therefore the case $k = j = 0$ and $m \ge 2$ requires the application of part b(ii) of Theorem 3.2. More precisely, it is easy to see that the D-optimal design is not maximin optimal. With $z = m$ and $n = m-1$ the system of equations (3.13) - (3.18) reduces to (4.6) – (4.7) and the inequality (3.19) is satisfied (note that $w_{m-1} = \infty$ and that the inequality (3.20) does not appear in this case). Moreover, it is easy to see that (4.6) - (4.7) define a unique solution $(p_2, \ldots, p_{2m-2})$. Note that for $p_{2m-2} = \frac{2}{3}$ the equation (4.6) gives the canonical moments of the D-optimal design in (2.5), for which the left hand side of (4.7) is cleary greater than the right hand side. Moreover a straightforward calculation shows that (4.6) is increasing and the right hand side of (4.7) is decreasing with increasing p_{2m-2}, which proves that the canonical moments of the maximin optimal design are less or equal than the corresponding canonical moments of the D-optimal design. Especially we obtain $p_{2m-2} \le \frac{2}{3}$ which proves the remaining inequality (3.21).

By Theorem 3.4.1 in Dette and Studden (1997) the Stieltjes transform of the measure η^* is given by

$$\int_{-1}^{1} \frac{d\eta^*(z)}{x-z} = \sum_{l=0}^{m} \frac{\eta^*(\{x_l\})}{x-x_l} = \frac{\underline{P}_m(x,q)}{(x^2-1)\bar{Q}_{m-1}(x,p)}$$

where $\bar{Q}_{m-1}(x,p), \underline{P}_m(x,q)$ are the supporting polynomials of the sequences

$$\frac{1}{2}, p_2, \frac{1}{2}, \ldots, \frac{1}{2}, p_{2m-2}, \frac{1}{2}, 1;$$
$$\frac{1}{2}, q_2, \frac{1}{2}, \ldots, \frac{1}{2}, q_{2m-2}, \frac{1}{2}, 0;$$

respectively [and the canonical moments are obtained from (4.6) and (4.7)]. Note that $\bar{Q}_{m-1}(x,p)$ is also the supporting polynomial of the sequence

$$\frac{1}{2}, q_{2m-2}, \frac{1}{2}, \ldots, \frac{1}{2}, q_2, \frac{1}{2}, 1$$

[see Studden (1982a)] and obtained recursively as $\bar{Q}_{m-1}(x,p) = \bar{Q}_{m-1}(x)$,$\bar{Q}_{-1}(x) = 0$, $\bar{Q}_0(x) = 1$

$$\begin{aligned} \bar{Q}_{l+1}(x) &= x\bar{Q}_l(x) - p_{2m-2l-2}q_{2m-2l}\bar{Q}_{l-1}(x) \\ &= \bar{Q}_l(x) - \frac{(l + \frac{p_{2m-2}}{2p_{2m-2}-1})(l + \frac{2-3p_{2m-2}}{2p_{2m-2}-1})}{4(l + \frac{1}{2(2p_{2m-2}-1)})(l + \frac{3-4p_{2m-2}}{2(2p_{2m-2}-1)})}\bar{Q}_{l-1}(x) \end{aligned}$$

($l = 0, \ldots, m-2$) [see Dette and Studden (1997)]. Comparing this recursive relation with (4.4) and (4.5) yields

$$\bar{Q}_{m-1}(x,p) = \frac{(\nu)_{m-1}}{2^{m-1}(\nu+\frac{1}{2})_{m-1}}(x^2-1)C_{m-1}^{(3/2)}(x,\nu-1) .$$

A similar argument shows

$$\underline{P}_m(x,q) = \frac{(\nu+1)_{m-1}}{2^{m-1}(\nu+\frac{1}{2})_{m-1}}\Big[xC_{m-1}^{(1/2)}(x,\nu) - \frac{\nu}{\nu+1}C_{m-2}^{(1/2)}(x,\nu+1)\Big]$$

and the assertion follows by calculating the coefficients in the partial fraction expansion of the Stieltjes transform.

(ii) If $k + j \geq 1$ or $m = 1$ part a) of Theorem 3.2 shows that the design with canonical moments given by (4.10) is maximin optimal with respect to the criterion (4.1). The assertion now follows from Theorem 4.4 and equation (4.2) in Dette (1995) [with $k = m - j; n = m + k, \rho = \vartheta = 2$] observing the identities $U_l(1) = l + 1$ ($l \in \mathbb{N}$),

$$\begin{aligned} U_{i+l}(x) &= U_i(x)U_l(x) - U_{i-1}(x)U_{l-1}(x) \qquad (i, l \geq 0) \\ 2T_l(x) &= U_l(x) - U_{l-2}(x) \qquad (l \geq 2) \end{aligned} \tag{4.11}$$

□

Example 4.2. Consider a cubic regression model and assume that $j = k = 0$ .In other words we are searching for the design maximizing

$$\Psi_{3,0,0}(\xi) = \min\{\text{eff}_3^{D_1}(\xi), \text{eff}_3^{D}(\xi)\}.$$

From part a) of Theorem 4.1 and (2.7) we obtain that the design maximizing $\Psi_{3,0,0}$ has canonical moments $p_1 = p_3 = p_5 = 1/2; p_6 = 1$ and p_2, p_4 are determined from the equations

$$\begin{aligned} (4p_4 - 1)^3 c &= (3p_4 - 1)p_4^4(1-p_4)^3 \\ p_2 &= \frac{3p_4 - 1}{4p_4 - 1} \end{aligned}$$

where $c = 5^5/2^{20}$. The numerical solution of this system yields

$$p_2 = 0.548724 \qquad p_4 = 0.56052$$

and the maximin optimal design η^* has masses $0.203, 0.297, 0.297, 0.203$ at the point $-1, -0.491, 0.491$ and 1, respectively [see Dette and Studden (1997), p. 106]. This design produces equal efficiencies, i.e.

$$\text{eff}_3^D(\eta^*) = \text{eff}_3^{D_1}(\eta^*) = 0.97599.$$

We finally note that the D-optimal design ξ_3^D for the cubic model has D_1-efficiency $\text{eff}_3^{D_1}(\xi_3^D) = 0.8533$ while the D_1-optimal design in this model has D-efficiency 0.9346.

If we assume that $k = 0$, $j = 1$, we are interested in a design which has reasonable D-efficiency for estimating the parameters in the cubic regression model and reasonable efficiencies for testing the highest coefficients in the quadratic and cubic model. In this case we are looking for the design η^* which maximizes

$$\Psi_{3,1,0}(\eta) = \min\{\text{eff}_3^D(\xi), \text{eff}_3^{D_1}(\xi), \text{eff}_2^{D_1}(\xi)\}.$$

Observing that

$$U_1(x) = 2x, \quad U_2(x) = 4x^2 - 1, \quad T_3(x) = 4x^3 - 3x, \quad T_4(x) = 8x^4 - 8x^2 + 1$$

[see Szegö (1975)] we obtain for the polynomial $Q_4(x)$ in (4.8)

$$Q_4(x) = 2(8x^2 - 1)(x^2 - 1)$$

and the design η^* maximizing $\Psi_{3,1,0}$ is supported at the points $-1, -1/\sqrt{8}, 1/\sqrt{8}, 1$. The corresponding masses are obtained from (4.9) observing that the polynomial in the numerator is given by $2(8x^3 - 5x)$, which yields

$$\eta^*(\mp 1) = \frac{3}{14} \qquad \eta^*(\mp \frac{1}{\sqrt{8}}) = \frac{2}{7}.$$

This design has efficiencies

$$\text{eff}_l^{D_1}(\eta^*) = 0.75 \quad l = 2, 3 \quad \text{eff}_3^D(\eta^*) = 0.9625$$

in the quadratic and cubic model.

In the remaining part of this section we will concentrate on the maximin problem (4.2), where for each model exactly one efficiency appears in the maximin criterion.

Theorem 4.3. *The maximin optimal design η^* with respect to the criterion (4.2) can be characterized as follows.*

(a) *If $k = 0; j = m-1 \geq 1$ the maximin optimal design η^* is supported at the roots of the polynomial*

$$(x^2-1)C^{(2)}_{m-1}(x,\nu), \tag{4.12}$$

and the masses are given by

$$\eta^*(x_l) = \frac{(\nu+m)\left[U_m(x_l) - \frac{\nu}{\nu+2}U_{m-2}(x_l)\right]}{2(\nu+1)\frac{d}{dx}\left[(x^2-1)C^{(2)}_{m-1}(x,\nu)\right]\Big|_{x=x_l}}, \tag{4.13}$$

$l = 0, \ldots, m$, where

$$\nu = \frac{3-4p_{2(m-1)}}{2p_{2(m-1)}-1}, \tag{4.14}$$

and p_{2m-2} is the solution of the equation

$$2^{(m+1)(m-2)}b_m^{m+1} = \frac{(1-p_{2(m-1)})(4(m-2)p_{2(m-1)}-2(m-3))}{2(m-1)p_{2(m-1)}-(m-2)} \tag{4.15}$$

in the interval $[\frac{1}{2}, 1)$.

(b) *If $k = 0$, $j \geq 1, m-j \geq 2$ the maximin optimal design η^* has canonical moments $p_{2l-1} = 1/2$ ($l = 1, \ldots, m$), $p_{2m} = 1$ and $(p_2, \ldots, p_{2m-2}) \in [\frac{1}{2}, 1)^{m-1}$ is the unique solution of*

$$\begin{aligned}
p_{2(m-1-l)} &= \frac{2(l+1)\,p_{2(m-1)}-l}{4lp_{2(m-1)}-2(l-1)}, \qquad l = 1, \ldots, j-1, \\
p_{2(m-j-1-l)} &= \frac{(2l+1)\,p_{2(m-j-1)}-l}{4lp_{2(m-j-1)}-2l+1}, \qquad l = 1, \ldots, m-j-2, \\
p_{2(m-j-1)} &= \frac{1+\prod_{l=m-j}^{m-1}\frac{1-p_{2l}}{p_{2l}}}{2+\prod_{l=m-j}^{m-1}\frac{1-p_{2l}}{p_{2l}}}. \\
1-p_{2(m-1)} &= 2^{2m^2-2mj+j^2-j-4}b_m^{m+1}p_{2(m-j)}^{m-j}\prod_{l=1}^{m-j-1}p_{2l}^l(1-p_{2l})^{l+1}.
\end{aligned} \tag{4.16}$$

The support points of the maximin optimal design η^* are given by the zeros of the polynomial $(x^2-1)Q_{m-1}(x)$ where

$$Q_{m-1}(x) = \left[C^{(2)}_j(x,\nu)C^{(3/2)}_{m-j-1}(x,\eta_{j+1}-1) - \frac{\eta_{j+1}+1}{\eta_{j+1}}C^{(2)}_{j-1}(x,\nu)C^{(3/2)}_{m-j-2}(x,\eta_{j+1})\right],$$

and the weights are obtained by the formula

$$\eta^*(x_l) = \frac{P_m(x_l)}{\frac{d}{dx}(x^2-1)Q_{m-1}(x)|_{x=x_l}},$$

where

$$P_m(x) \;=\; \frac{(\eta_{j+1}+m-j-1)(\nu+j+1)}{2\eta_{j+1}(\nu+1)}\Big\{C^{(1/2)}_{m-j-1}(x,\eta_{j+1})\Big[U_{j+1}(x)-\frac{\nu}{\nu+2}U_{j-1}(x)\Big]$$
$$-\frac{\eta_{j+1}}{\eta_{j+1}+1}\cdot\frac{j+\nu+2}{j-\nu-3}\cdot C^{(1/2)}_{m-j-2}(x,\eta_{j+1}+1)\Big[U_j(x)-\frac{\nu}{\nu+2}U_{j-2}(x)\Big]\Big\},$$

ν is defined in (4.14), η_{j+1} given by

$$\eta_{j+1} \;=\; \frac{1-p_{2m-2j-2}}{2p_{2m-2j-2}-1}$$

and $p_{2m-2j-2}$, p_{2m-2} are obtained from the system (4.16).

(c) *If $k=1$, $j=0$ the maximin optimal design η^* is supported at the zeros of the polynomial*

(4.17) $$(x^2-1)C^{(3/2)}_m(x,\eta_0-1),$$

and the weights are given by

(4.18)
$$\eta^*(x_l) \;=\; \frac{x_l C^{(1/2)}_m(x_l;\eta_0)-\frac{\eta_0}{\eta_0+1}C^{(1/2)}_{m-1}(x_l;\eta_0+1)}{\frac{\eta_0}{\eta_0+m}\frac{d}{dx}\Big[(x^2-1)C^{(3/2)}_m(x,\eta_0-1)\Big]\Big|_{x=x_l}},$$

$l=0,\ldots,m+1$. Here $\eta_0=(1-p_{2m})/(2p_{2m}-1)$ and $p_{2m}\in[\frac{1}{2},1)$ is determined from the system

(4.19)
$$p_{2(m-l)} \;=\; \frac{(2l+1)\,p_{2m}-l}{4lp_{2m}-2l+1}, \qquad l=1,\ldots,m-1,$$
$$1 \;=\; b^{m+1}_m 2^{2m(m+1)}\prod_{l=1}^{m}p^l_{2l}(1-p_{2l})^{l+1}.$$

(d) *If $k=2$, $m=1$ the maximin optimal design η^* puts masses 0.2395 and 0.2605 at the points ∓ 1 and ∓ 0.3711, respectively.*

(e) *If $j=0$, $k\geq 3$ or $j=0$, $k=2$, $m\geq 2$ the maximin optimal design is supported at the zeros of the polynomial*

(4.20) $$H_{m+k+1}(x) \;=\; (x^2-1)[U_m(x)U'_k(x)-U_{m-1}(x)U'_{k-1}(x)],$$

and the masses are given by

(4.21) $$\eta^*(x_l)=\frac{kU_{m+k}(x_l)-U_{k-1}(x_l)U_{m-1}(x_l)}{H'_{m+k-1}(x_l)}, \qquad l=0,\ldots,m+k.$$

(f) *If $j \geq 1, k \geq 1$ the maximin optimal design η^* is supported at the zeros of the polynomial*

$$
\begin{aligned}
(4.22)\quad Q_{m+k+1}(x) \;=\; & (x^2-1)\Big[\big(\frac{k}{k+1}U'_{k+1}(x)+\frac{1}{k+1}U'_{k-1}(x)\big) \\
& \cdot\big(U_{m-j-1}(x)C_j^{(2)}(x,k-1)-U_{m-j-2}(x)C_{j-1}^{(2)}(x,k-1)\big) \\
& -\frac{k+2}{k}U'_k(x)\big(U_{m-j-1}(x)C_{j-1}^{(2)}(x,k)-U_{m-j-2}(x)C_{j-2}^{(2)}(x,k)\big)\Big]
\end{aligned}
$$

and the masses are obtained from

$$
(4.23)\qquad \eta^*(x_l) = \frac{(k+j)P_{m+k}(x_l)}{\frac{d}{dx}Q_{m+k+1}(x)\mid_{x=x_l}} \qquad l = 0\,,\ldots,m+k
$$

where the polynomial $P_{m+k}(x)$ is defined by

$$
\begin{aligned}
(4.24)\qquad P_{m+k}(x) = & \Big[\big(U_{k+1}(x)-\frac{1}{k}U_{k-1}(x)\big)\big(U_{m-1}(x)-\frac{1}{j+k}U_{m-j-2}(x)U_{j-1}(x)\big) \\
& -\frac{k}{k+1}U_k(x)\big(U_{m-2}(x)-\frac{1}{j+k}U_{m-j-2}(x)U_{j-2}(x)\big)\Big].
\end{aligned}
$$

Proof. In a first step we check if condition (3.5) in Theorem 3.2(a) is satisfied. It is easy to see that for $k=0$ the inequality (3.5) cannot be true. For the case $k>0$ we note that for $w_m=\infty$, $w_m^*=\infty$, $w_l=1$ ($l=m-j,\ldots,m-1,m+1\,,\ldots,m+k$) the canonical moments in (2.9) - (2.11) are given by $p_{2l-1}=\frac{1}{2}$ $\quad(l=1\,,\ldots,m+k)$

$$
(4.25)\qquad
\begin{aligned}
p_{2l} &= \frac{m+k-l+2}{2(m+k-l+1)}, && l=m+1\,,\ldots,m+k, \\
p_{2l} &= \frac{1}{2}, && l=1\,,\ldots,m-j-1,m, \\
p_{2l} &= \frac{m+k-l+1}{2(m+k-l)}, && l=m-j,\ldots,m-1.
\end{aligned}
$$

which implies

$$
\mathrm{eff}_l^{D_1}(\tilde\eta) = \frac{j+k+1}{2(j+k)} \qquad l=m-j,\ldots,m-1,m+1\,,\ldots,m+k
$$

for the design $\tilde\eta$ with canonical moments given by (4.25). For this design the D-efficiency is obtained as

$$
\mathrm{eff}_m^D(\tilde\eta) = \frac{1}{b_m}\Big[\Big(\frac{1}{2}\Big)^{m^2}\Big(\frac{k+j+1}{k+j}\Big)^{j+1}\frac{k}{k+1}\Big]^{1/(m+1)}
$$

and a straightforward but tedious calculation shows that condition (3.5) in Theorem 3.2 is satisfied whenever

(e) $j=0; k\geq 3$ or $j=0; k=2; m\geq 2$

(f) $j\geq 1; k\geq 1$

Here the design $\tilde\eta$ corresponding to the canonical moments in (4.25) is also maximin optimal with respect to the criterion $\chi_{m,j,k}$ and we will discuss the identification of the support points and weights for both cases separately.

(e) If $j = 0; k \geq 3$ or $j = 0$, $k = 2$, $m \geq 2$ it follows from (4.25) and Theorem 4.4 in Dette (1995) (using $\vartheta = \rho = 2$, $n = m + k, k = m + 1$ in his notation) that η^* is supported at the $m + k + 1$ zeros of the polynomial

$$\begin{aligned} Q_{m+k+1}(x) &= U_m(x)\{kU_{k+1}(x) - (k+2)\, U_{k-1}(x)\} \\ &\qquad - U_{m-1}(x)\{(k-1)U_k(x) - (k+1)\, U_{k-2}(x)\} \\ &= 2(x^2 - 1)[U_m(x)U_k'(x) - U_{m-1}(x)U_{k-1}'(x)] \end{aligned}$$

where the last identity is obtained from the trigonometric respresentation of the Chebyshev polynomials of the second kind [see e.g. Szegö (1975)]. The same result shows that the weights are given by

$$\eta^*(\{x_l\}) = \frac{kU_k(x_l)U_m(x_l) - (k+1)\, U_{k-1}(x_l)U_{m-1}(x_l)}{\frac{1}{2}\frac{d}{dx}Q_{m+k+1}(x)\ |_{x=x_l}}$$

and the representation (4.20) and (4.21) follow from (4.11) which proves the assertion of Theorem 4.3 for case (e).

(f) By Theorem 3.4.1 in Dette and Studden (1997) the Stieltjes transform of the measure η^* is given by

$$\int_{-1}^{1} \frac{d\eta^*(z)}{x - z} = \sum_{l=0}^{m+k} \frac{\eta^*(\{x_l\})}{x - x_l} = \frac{\underline{P}_{m+k}(x,q)}{(x^2-1)\bar{Q}_{m+k-1}(x,p)} \tag{4.26}$$

where $\bar{Q}_{m+k-1}(x,p), \underline{P}_{m+k}(x,q)$ are the supporting polynomials of the sequences

$$\frac{1}{2}, p_2, \frac{1}{2}, \ldots, \frac{1}{2}, p_{2m+2k-2}, \frac{1}{2}, 1; \tag{4.27}$$

$$\frac{1}{2}, q_2, \frac{1}{2}, \ldots, \frac{1}{2}, q_{2m+2k-2}, \frac{1}{2}, 0; \tag{4.28}$$

respectively. The assertion in part (f) of Theorem 4.3 therefore follows by showing the identities

$$\bar{Q}_{m+k-1}(x,p) = \frac{1}{(k+j)2^{m+k}} Q_{m+k-1}(x) \tag{4.29}$$

$$\underline{P}_{m+k}(x,q) = \frac{1}{2^{m+k}} P_{m+k}(x) \tag{4.30}$$

where $Q_{m+k-1}(x)$ and $P_{m+k}(x)$ are defined in (4.22) and (4.23), respectively. We will only prove the statement (4.29) regarding the polynomial $\bar{Q}_{m+k-1}(x,p)$; the equation (4.30) is shown similary and left to the reader. From Theorem 4.4.2 in Dette and Studden (1997) we obtain that

$$\bar{Q}_{m+k-1}(x,p) = G_k(x)H_{m-1}(x) - \frac{1}{4}\frac{k+2}{k+1}G_{k-1}(x)H_{m-2}(x) \tag{4.31}$$

where the polynomials $G_k(x)$ and $H_{m-1}(x)$ are the supporting polynomials of the sequences

$$(4.32) \qquad \begin{array}{l} \frac{1}{2}, p_{2m}\frac{1}{2}, \ldots, \frac{1}{2}, p_{2m+2k-2}, \frac{1}{2}, 1; \\ \\ \frac{1}{2}, p_2, \frac{1}{2}, \ldots, \frac{1}{2}, p_{2m-2}, \frac{1}{2}, 1; \end{array}$$

respectively. By Lemma 2.10 in Studden (1982a) and Corollary 2.3.6 in Dette and Studden (1997) the polynomial $G_k(x)$ is obtained recursively as $G_0(x) = 1$, $G_1(x) = x$,

$$\begin{aligned} G_{i+1}(x) &= xG_i(x) - q_{2m+2k-2i}p_{2m+2k-2i-2}G_{i-1}(x) \\ &= \begin{cases} xG_i(x) - \dfrac{i(i+3)}{4(i+1)(i+2)}G_{i-1}(x) & \text{if } i \le k-2 \\ \\ xG_{k-1}(x) - \dfrac{k-1}{4k}G_{k-2}(x) & \text{if } i = k-1. \end{cases} \end{aligned}$$

Comparing this recursion with the monic version of the recursive relation for the associated ultraspherical polynomials in (4.3) yields

$$(4.33) \qquad \begin{aligned} G_{k-1}(x) &= \frac{1}{k2^{k-1}}C_{k-1}^{(2)}(x,0) = \frac{1}{k2^k}U_k'(x) \\ G_k(x) &= \frac{1}{k2^k}\{2xC_{k-1}^{(2)}(x,0) - C_{k-2}^{(2)}(x,0)\} \\ &= \frac{1}{2^k(k+1)}\{C_k^{(2)}(x,0) + \frac{1}{k}C_{k-2}^{(2)}(x,0)\} \\ &= \frac{1}{(k+1)2^{k+1}}\{U_{k+1}'(x) + \frac{1}{k}U_{k-1}'(x)\} \end{aligned}$$

where $C_k^{(2)}(x,0) = C_k^{(2)}(x)$ denotes the classical ultraspherical polynomial [see e.g. Szegö (1975)] and we used the recursion (4.3) and the identity $U_l'(x) = 2\ C_{l-1}^{(2)}(x,0)$ [see e.g. Abramowitz and Stegun (1964)].

For the determination of the polynomials $H_{m-1}(x)$ corresponding to the second sequence in (4.32) we apply again Theorem 4.4.2 in Dette and Studden (1997) and obtain

$$(4.34) \qquad H_{m-1}(x) = \tilde{G}_j(x)\tilde{H}_{m-j-1}(x) - \frac{1}{4}\frac{k+j-1}{k+j}\tilde{G}_{j-1}(x)\tilde{H}_{m-j-2}(x)$$

where $\tilde{G}_j(x)$ and $\tilde{H}_{m-j-1}(x)$ correspond to the sequences

$$\begin{array}{l} \frac{1}{2}, p_{2m-2j}, \frac{1}{2}, \ldots, \frac{1}{2}, p_{2m-2}, \frac{1}{2}, 1; \\ \frac{1}{2}, \frac{1}{2}, \ldots, \frac{1}{2}, 1; \end{array}$$

respectively. From Corollary 4.3.3 in Dette and Studden (1997) we have

$$\tilde{H}_l(x) = \frac{1}{2^l} U_l(x) \qquad l = m-j-1, m-j-2 \tag{4.35}$$

and Theorem 2.5.1 and Corollary 2.3.6 in the same reference show that the polynomials $\tilde{G}_j(x)$ can be obtained recursively from

$$\tilde{G}_0(x) = 1 \; \tilde{G}_1(x) = x$$

$$\tilde{G}_{l+1}(x) = x\tilde{G}_l(x) - q_{2m-2l} p_{2m-2l-2} \tilde{G}_{l-1}(x) = x\tilde{G}_l(x) - \frac{1}{4} \frac{(k+l-1)(k+l+2)}{(k+l)(k+l+1)} \tilde{G}_{l-1}(x)$$

$(l = 1, \ldots, j-1)$. Comparing this recurrence relation with (4.4) and (4.5) shows that

$$\tilde{G}_l(x) = \frac{k}{2^l(k+l)} C_l^{(2)}(x, k-1) \qquad l = j-1, j \tag{4.36}$$

[note that $2^l(k+l)/k$ is the leading coefficient of the polynomial $C_l^{(2)}(x, k-1)$]. Observing (4.34), (4.35) yields

$$H_{m-1}(x) = \frac{k}{(k+j)2^{m-1}} \{U_{m-j-1}(x) C_j^{(2)}(x, k-1) - U_{m-j-2}(x) C_{j-1}^{(2)}(x, k-1)\}$$

and similar arguments show

$$H_{m-2}(x) = \frac{k+1}{(k+j)2^{m-2}} \{U_{m-j-1}(x) C_{j-1}^{(2)}(x, k) - U_{m-j-2}(x) C_{j-2}^{(2)}(x, k)\}.$$

Finally a combination of these representations with (4.33), (4.34) and (4.31) yields the assertion (4.29). The proof of the remaining statement (4.30) is similar and therefore omitted. This completes the proof of part (f) of Theorem 4.3.

In the remaining cases

(a) $k = 0; j = m-1 \geq 1$
(b) $k = 0; j \geq 1; m-j \geq 2$
(c) $k = 1; j = 0$
(d) $k = 2$, $m = 1$

condition (3.5) of Theorem 3.2 is not satisfied and the other parts of this theorem apply. We will only give a proof for (a) and (b). The proofs of the other cases are very similar and therefore omitted.

(a), (b): If $k = 0; j \geq 1$ it is easy to see that the D-optimal design ξ_m^D satisfies

$$\text{eff}_{m-1}^{D_1}(\xi_m^D) < \text{eff}_m^D(\xi_m^D),$$

which shows that ξ_m^D is not maximin-optimal and that the maximin optimal design η^* is determined by the conditions (3.13) – (3.21) in Theorem 3.2 b(ii). In the case (a)

$(k = 0\ , j = m-1 \geq 1)$ we use $z = m-1$ and $n = 0$ and obtain from (3.14) and induction the recursion

$$p_{2(m-1-l)} = \frac{2(l+1)\, p_{2(m-1)} - l}{4l p_{2(m-1)} - 2(l-1)}, \qquad l = 1\ , \ldots , m-2, \tag{4.37}$$

which implies

$$p_{2l+2}q_{2l} = \frac{1}{4} \qquad l = 1\ , \ldots , m-2$$

Using this identity in (3.18) yields the equation (4.15) for p_{2m-2}. For the calculation of the support points we use Theorem 2.5.1 and Corollary 2.3.6 in Dette und Studden (1997) and it follows that the support of the maximin optimal design is given by the zeros of the polynomial $(x^2-1)Q_{m-1}(x)$, where $Q_{m-1}(x)$ is the supporting polynomial of the sequence

$$\frac{1}{2}, q_{2m-2}, \frac{1}{2}, \ldots , \frac{1}{2}, q_2, \frac{1}{2}, 1$$

and obtained recursively as

$$\begin{aligned} Q_{l+1}(x) &= xQ_l(x) - q_{2m-2l}p_{2m-2l-2}Q_{l-1}(x) \\ &= xQ_l(x) - \frac{1}{4}\frac{(2(l+1)\, p_{2m-2} - l)(2(l-2)p_{2m-2} - l + 3)}{(2lp_{2m-2} - l + 1)(2(l-1)p_{2m-2} - l + 2)}Q_{l-1}(x). \end{aligned}$$

A straightforward calculation shows that this is the recurrence relation for the monic version of the associated ultraspherical polynomials defined in (4.4) and (4.5) for $\lambda = 2$ and ν given in (4.14), i.e.

$$Q_{m-1}(x) = \frac{(\nu + 1)}{2^{m-1}(\nu + m)} C^{(2)}_{m-1}(x, \nu)$$

which proves the assertion regarding the support points. A similar argument shows for the polynomial in the numerator of (4.26)

$$\underline{P}_m(x, q) = \frac{1}{2^m}[U_m(x) + (4\, p_{2m-2} - 3)U_{m-2}(x)]$$

and the assertion in the case $k = 0; j = m-1 \geq 1$ follows as in case (f).

The remaining case $k = 0\ , m-j \geq 2$ is essentially treated in the same way, where $z = m-1$ and $n = m-j-1$ in Theorem 3.2 b(ii). From (3.14) we obtain the first equation in (4.16) which yields

$$\text{eff}^{D_1}_l(\eta^*) = \text{eff}^{D_1}_{m-1}(\eta^*) \qquad l = m-2, m-3, \ldots , m-j.$$

This implies for the equation in (3.18)

$$(\text{eff}^D_m(\eta^*))^{m+1} = (\text{eff}^{D_1}_{m-1}(\eta^*))^{m+1} = (\text{eff}^{D_1}_{m-j}(\eta^*))^{m-j+1}\text{eff}^{D_1}_{m-1}(\eta^*) \prod_{l=m-j+1}^{m-1} \text{eff}^{D_1}_l(\eta^*)$$

and a straightforward calculation shows [observing (2.6) and (2.8)] that this is equivalent to the fourth equation in (4.16). The second and the third equation are obtained from (3.17) and (3.15), respectively. Finally, the statement regarding the weights and support points follows by similar arguments as given for the proof of case (a) and is left to the reader. □

Example 4.4.

(a) Consider the case $m = k = 2$, $j= 1$,where part (f) of Theorem 4.3 applies. We obtain that the support points of the maximin optimal design are given by the zeros of

$$Q_5(x) = x(x^2 - 1)(48x^2 - 22)$$

where we have used $U_0(x) = 1$, $U_1(x) = 2\,x$, $U_2(x) = 4\,x^2 - 1$, $U_3(x) = 8\,x^3 - 4x$ and

$$C_1^{(2)}(x, \nu) = \frac{2(\nu + 2)}{\nu + 1}x,$$

which follows from the recurrence relation (4.3) for the associated ultraspherical polynomials. Consequently the design η^* maximizing the criterion $\chi_{2,1,2}$ in (4.2) is supported at the points $-1, -\sqrt{\frac{11}{24}}, 0, \sqrt{\frac{11}{24}}, 1$. A similar calculation shows

$$P_4(x) = 16\,x^4 - \frac{38}{3}x^2 + \frac{2}{3}$$

and we obtain from (4.23) for the weights

$$\eta^*(\{\mp 1\}) = \frac{3}{13}, \quad \eta^*(\{\mp\sqrt{11/24}\}) = \frac{32}{11 \cdot 13}, \quad \eta^*(\{0\}) = \frac{1}{11}.$$

(b) In the case $m = 3$, $k= 0$, $j= 2$ the maximin optimal design (with respect to the criterion $\chi_{3,2,0}$) is obtained from part (a) of Theorem 4.3. For the calculation of the support points we use (4.3) which gives

$$C_2^{(2)}(x, \nu) = \frac{4(\nu + 3)}{\nu + 1}x^2 - \frac{\nu + 4}{\nu + 2}$$

where ν is defined in (4.14) for $m = 3$ and p_4 is the solution of the equation

$$2^4 b_3^4 = \frac{4(1 - p_4)p_4}{4p_4 - 1}$$

in the interval $[\frac{1}{2}, 1)$ [note that $b_3^4 = 2^4/5^5$, by (2.7)], i.e. $p_4 \approx 0.93987$. This gives $\nu \approx -\ 0.8633$ and the maximin optimal design with respect to the criterion $\chi_{3,2,0}$ is the supported at the points ∓ 1 and ∓ 0.2101. The corresponding masses are obtained from (4.13) and a straightforward calculation, i.e.

$$\eta^*(\mp 1) \approx 0.36086 \qquad \eta^*(\mp 0.2101) \approx 0.13914.$$

Note that this design has equal efficiencies for all criteria appearing in $\chi_{3,0,2}$, that is

$$\text{eff}_1^{D_1}(\eta^*) = \text{eff}_2^{D_1}(\eta^*) = \text{eff}_3^{D}(\eta^*) = p_2 \approx 0.73401.$$

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