Some explicit solutions of c-optimal design problems for polynomial regression

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Abstract

In this paper we consider the optimal design problem for extrapolation and estimation of the slope at a given point, say z, in a polynomial regression with no intercept. We provide explicit solutions of these problems in many cases and characterize those values of z, where this is not possible.

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1 Introduction

Consider the common linear regression model

$$Y_i = \theta^\top f(x_i) + \varepsilon_i, \qquad i = 1, \dots, N, \tag{1.1}$$

where $\varepsilon_1, \dots, \varepsilon_N$ denote uncorrelated random variables with $\mathrm{E}[\varepsilon_i] = 0$; $\mathrm{Var}(\varepsilon_i) = \sigma^2 > 0$ $(i = 1, \dots, N)$, $\theta \in \mathbb{R}^d$ is an vector of unknown parameters, $f(x) = (f_1(x), \dots, f_d(x))^\top$ is the vector of regression functions and x varies in the design space $\mathcal{X} \subset \mathbb{R}$. Optimal design problems in the case, where the regression functions are polynomials, i.e. $f_i(x) = x^{k_i}$, have been studied intensively in the literature and numerous elegant solutions are available describing the optimal designs in a very elegant form. A large portion of the literature has its focus on the D-optimality criterion and starting with the seminal paper of Hoel (1958) numerous authors have received explicit solutions of optimal design problems with respect to various determinant type criteria [see Studden (1980); Dette (1990); Dette and Franke (2001); Zen and Tsai (2004) among many others]. Another type of criterion for which explicit solutions of the optimal design problem for polynomial regression are available is the E-optimality criterion [see Pukelsheim and Studden (1993); Dette (1993); Heiligers (1994)]. The E-optimal design problem is actually feasible, if the minimum eigenvalue of the information matrix of the optimal design has multiplicity 1. In this case the problem is equivalent to a c-optimal design problem for a specific vector $c \in \mathbb{R}^m$, which determines the design such that the variance of the best linear estimate of the linear combination $c^\top\theta$ becomes minimal [see Dette and Studden (1993)].
A rather complete characterization of the c-optimal design problem for regression models with basis functions forming a Chebychev system can be found in the seminal paper of Studden (1968). However, in this reference it is also indicated that in general the solution of the c-optimal design problem is an extremely difficult one. For this reason explicit solutions of the c-optimal design problem are mainly available for models with a small number of parameters, where they are usually determined by geometric arguments using Elfving's theorem [see Elfving (1952)].
The purpose of the present contribution is to provide more explicit solutions for this challenging optimal design problem in polynomial type regression models, where we concentrate on optimal designs for extrapolation and for estimating the slope. The problem of designing experiments for extrapolation in polynomial regression has been solved a long time ago by Hoel and Levine (1964) and several authors have discussed optimal extrapolation designs

from several perspectives problem [see Dette and Wong (1996); Dette and Huang (2000) or Celant and Broniatowski (2016) among others]. Similarly, optimal designs for estimating the slope of a regression function have found considerable attention in the literature [see Atkinson (1970); Ott and Mendenhall (1972); Murthy and Studden (1972); Myres and Lahoda (1975); Hader and Park (1978); Mukerjee and Huda (1985); Mandal and Heiligers (1992); Pronzato and Walter (1993); Melas et al. (2003) or Dette et al. (2010)]. In this paper we add new explicit results to the literature by finding optimal designs for extrapolation and estimating the slope in polynomial regression models with no intercept.
The remaining part of this paper is organized as follows. In Section 2 we introduce the basic optimal design problem and review a geometric characterization of the optimal designs. Section 3 is devoted to the determination of optimal designs for extrapolation in a polynomial regression with no intercept. Finally, Section 4 considers the problem of optimally designing experiments for the estimation of the slope in this model, while Section 5 contains a technical result, which is used several times in the proofs of our main statements.

2 Preliminaries

Following Kiefer (1974) we call a discrete probability measure

$$\xi = \begin{pmatrix} x_1 & \cdots & x_m \\ \omega_1 & \cdots & \omega_m \end{pmatrix}$$

with support points $x_1, \ldots, x_m$ and weights $\omega_1, \ldots, \omega_m$ an approximate design in the linear regression model (1.1). If N observations can be taken this means that the quantities $N\omega_i$ are rounded to integers, say n_i, with $\sum_{i=1}^m n_i = N$ and n_i observations are taken at each experimental condition x_i $(i = 1, \ldots, m)$. For an approximate design ξ we denote by

$$M(\xi) = \int_{\mathcal{X}} f(x) f^\top(x) \xi(dx)$$

its information matrix in model (1.1). The covariance matrix of the least squares estimate, say $\hat{\theta}$, can be approximated (if $N \to \infty$, $n_i/N \to \omega_i$) by $\sigma^2/NM^{-1}(\xi)$ and an optimal design minimizes an appropriate real valued function of the matrix $M^{-1}(\xi)$. In this paper we are interested in designs which minimize the asymptotic variance of the best linear unbiased estimate $c^\top\hat{\theta}$ of the linear combination $c^\top\theta$ for a given vector $c \in \mathbb{R}^d$. To be precise, we call a design ξ c-optimal in the regression model (1.1), if it minimizes the function

$$\Phi(\xi) = \begin{cases} c^\top M^-(\xi)c, & \text{if there exists a vector} v \in \mathbb{R}^d \text{ such that } c = M(\xi)v; \\ \infty, & \text{otherwise,} \end{cases}$$

where $M^-(\xi)$ is a generalized inverse for the matrix $M(\xi)$. In the first case the design ξ is called *admissible for estimating the linear combination* $c^\top\theta$ in the regression model (1.1) and the value of the quadratic form does not depend on the choice of the generalized inverse [see Pukelsheim (2006)]. An important case is obtained by the choice $c^\top = (f_1(z), \dots, f_d(z))$ for some z, which corresponds to the minimization of the variance of the best unbiased prediction of the function $\theta^\top f(x)$ at the point z. If $z \in \mathcal{X}$ the optimal design is called *optimal interpolation design*, if $z \notin \mathcal{X}$ *optimal extrapolation design*. If $\mathcal{X} \subset \mathbb{R}$, the vector f differentiable and $c^\top = (f_1'(z), \dots, f_d'(z))$ for some $z \in \mathbb{R}$ the *optimal design will be called optimal design for estimating derivative at the point* z.
A useful tool for the determination of c-optimal designs is a geometric characterization of the c-optimal design and called Elfving's theorem [see Elfving (1952)]. We formulate it here in a slightly different form, which can be directly used to check optimality of a given design [see Dette et al. (2004) for details].

Theorem 2.1 *An admissible design ξ^* for estimating the linear combination $c^\top\theta$ with support points $x_1, x_2, \dots, x_m$ and weights $\omega_1, \omega_2, \dots, \omega_m$ is c-optimal if and only if there exists a vector $p \in \mathbb{R}^d$ and a constant h such that the following conditions are satisfied:*

(1) $|p^\top f(x)| \le 1$ *for all* $x \in \mathcal{X}$*;*

(2) $|p^\top f(x_i)| = 1$ *for all* $i = 1, 2, \dots, m$ *;*

(3) $c = h\sum_{i=1}^m f(x_i)\omega_i p^\top f(x_i)$.

Moreover, in this case we have $c^\top M^-(\xi^*)c = h^2$.

The function $p^\top f(x)$ will be *called extremal polynomial* throughout this paper.

3 Optimal extrapolation designs

It is well known that for the common polynomial regression model, i.e. $f(x) = (1, x, \dots, x^n)^\top$ on the interval $[-1, 1]$ the optimal extrapolation design for a point z with $|z| > 1$ is unique and supported at the extremal points $s_{1,n}, \ldots, s_{n+1,n}$ of the Chebyshev polynomial of the first kind

$$T_n(x) = \cos(n \arccos(x)) \tag{3.1}$$

[see Hoel and Levine (1964)]. In our notation this polynomial is the unique extremal polynomial (up to a sign) and the vector p in Theorem 2.1 is given by coefficients of the polynomial T_n. The points $s_{i,n}$ are explicitly given by

$$s_{i,n} = \cos\left(\tfrac{(n+1-i)\pi}{n}\right), \qquad i = 1, 2, \ldots, n+1, \tag{3.2}$$

and the weights of the optimal extrapolating design are obtained by

$$\omega_i = \frac{|L_i(z)|}{\sum_{j=1}^{n+1} |L_j(z)|}, \ i = 1, \ldots, n+1, \tag{3.3}$$

where

$$L_i(x) = \frac{\prod_{j \neq i}(x - s_{j,n})}{\prod_{j \neq i}(s_{i,n} - s_{j,n})}, \ i = 1, \ldots, n+1$$

are the Lagrange basis interpolation polynomials corresponding to the nodes $s_{1,n}, \ldots, s_{n+1,n}$. In this section we investigate the optimal extrapolation designs for a polynomial regression model on the interval $[-1, 1]$ without intercept. More precisely, we consider the vector of regression functions

$$f(x) = (x, x^2, \ldots, x^n)^\top. \tag{3.4}$$

in model (1.1). If the degree n in (3.4) is odd the Chebyshev polynomial is a polynomial without intercept and therefore it remains the unique extremal polynomial in Elfving's theorem. Consequently, the design with support points and weights given by (3.2) and (3.3), respectively is again an optimal extrapolation design. However, the optimal design is not unique anymore. Nevertheless we can describe all optimal extrapolation designs in this case. If the degree of the polynomial regression with no intercept is even the situation is different. The optimal extremal polynomial is again unique and can be found explicitly. Interestingly, the corresponding extremal polynomial in Elfving's theorem is not a Chebyshev polynomial. We first discuss the case where the degree in the regression model (1.1) with vector of regression functions given by (3.4) is odd, that is $n = 2k + 1$.

Theorem 3.1 *In the case $n = 2k + 1$ there exist exactly two optimal extrapolation designs with $2k + 1$ support points for the polynomial regression model of degree $2k + 1$ without* *intercept on the interval* $[-1, 1]$. *One of the designs is supported at the* $2k+1$ *smallest extremal points* $t_i^* = \cos\big(\frac{\pi(2k+2-i)}{2k+1}\big)$ $(i = 1, \dots, 2k+1)$ *of the Chebyshev polynomial* $T_{2k+1}(x)$ *in the interval* $[-1, 1)$ *and the other one is supported at the* $2k+1$ *largest extremal points* $t_{i-1}^* = \cos\big(\frac{\pi(2k+2-i)}{2k+1}\big)$ $(i = 2, \dots, 2k+2)$ *of* $T_{2k+1}(x)$ *in the interval* $(-1, 1]$. *The corresponding weights* $\omega_i^*, \dots \omega_{2k+1}^*$ *at these points are given by*

$$\omega_i^* = \omega_i^*(z) = \frac{|\bar{L}_i(z)|}{\sum_{j=1}^n |\bar{L}_j(z)|} \qquad (i = 1, \dots, n), \tag{3.5}$$

where

$$\bar{L}_i(x) = \frac{x \prod_{j \neq i}(x - t_j^*)}{t_i^* \prod_{j \neq i}(t_i^* - t_j^*)} \tag{3.6}$$

is the ith Lagrange basis interpolation polynomial without intercept corresponding to the nodes $t_1^*, \dots, t_{2k+1}^*$ $(i = 1, \dots, 2k+1)$.

Proof: Recall the definition of the vector f (with $n = 2k+1$) in (3.4) and note that the extremal polynomial in Theorem 2.1 is given by $p^\top f(x) = \pm T_{2k+1}(x)$. Consequently, by this characterization the support of the optimal extrapolation design is a subset of the extremal points

$$\big\{\cos\big(\tfrac{\pi(2k+2-i)}{2k+1}\big) : i = 1, \dots, 2k+2\big\}$$

of the polynomial $-T_{2k+1}(x)$ on the interval $[-1, 1]$. It will be shown below that it is possible to satisfy all conditions of Theorem 2.1 using all interior support points and exactly one of the boundary points. We assume without loss of generality that $t_1^* = -1$ and $z > 1$, all other cases can be proved by similar arguments.
Define the vector $\beta = (\beta_1, \dots, \beta_{2k+1})^T$ by $\overline{\beta}_i = \omega_i(p^\top f(t_i^*))$, $i = 1, \dots, 2k+1$, where $p^\top f(x) = -T_{2k+1}(x)$ is the extremal polynomial in Theorem 2.1 and $\omega_1, \dots, \omega_{2k+1}$ are weights. Note that

$$p^\top f(t_i^*) = -T_{2k+1}(t_i^*) = (-1)^{2k+1-i}, \quad i = 1, \dots, 2k+1 \tag{3.7}$$

and that condition (3) in Theorem 2.1 can be rewritten as

$$c = (z, \dots, z^n)^\top = hF\beta, \tag{3.8}$$

where

$$F = ((t_j^*)^i)_{i,j=1}^{2k+1} = (f(t_1^*), \dots, f(t_{2k+1}^*)) \in \mathbb{R}^{2k+1 \times 2k+1}.$$

We will show that there exists a solution with respect to the nonnegative weights $\omega_1, \ldots, \omega_{2k+1}$ with $\sum_{i=1}^{2k+1} \omega_i = 1$ which is given by (3.5). As the conditions (1) and (2) in this theorem are obviously satisfied this yields the assertion of Theorem 3.1.
In order to investigate condition (3.8) note that the identity $F^{-1}F = I_{2k+1}$ (here I_{2k+1} is the identity matrix) implies

$$e_i^\top F^{-1} f(t_j^*) = \delta_{ij} \quad (i, j = 1, \ldots, 2k+1),$$

where δ_{ij} is the Kroneker symbol. As these equations characterize the ith Lagrange basis interpolation polynomial $\bar{L}_i(z) = a_i^T f(z)$ with nodes $t_1^*, \ldots, t_{2k+1}^*$ we have

$$e_i^\top F^{-1} f(z) = \bar{L}_i(z), \ i = 1, \ldots, 2k+1,$$

or equivalently

$$F^{-1} f(z) = (\bar{L}_1(z), \ldots, \bar{L}_{2k+1}(z))^\top.$$

Therefore we obtain for the solution of (3.8)

$$h\beta = (\bar{L}_1(z), \ldots, \bar{L}_{2k+1}(z))^\top$$

or equivalently (since $\beta_i = \omega_i(p^\top f(x_i^*))$)

$$h\beta_i = h\omega_i(-1)^{2k+1-i} = \bar{L}_i(z) \ , \quad i = 1, \ldots, 2k+1 \tag{3.9}$$

Note that it follows immediately from formula (3.6) that for $z > 1$ the sign of $\bar{L}_i(z)$ is given by $(-1)^{2k+1-i}$ which implies that the weights are given by $\omega_i = |L_i(z)|/h$ with $h = \sum_{j=1}^n |\bar{L}_j(z)|$ and proves the result. □

Our next result specifies the optimal extrapolation designs for a polynomial regression model of even degree with no intercept. In this case the structure of the optimal design changes substantially.

Theorem 3.2 *For $i = 1, \ldots, k$ define*

$$x_i^* = -\sqrt{\frac{\cos\frac{(i-1)\pi}{k} + \cos\frac{\pi}{2k}}{1 + \cos\frac{\pi}{2k}}} \ , \ x_{2k+1-i}^* = \sqrt{\frac{\cos\frac{(i-1)\pi}{k} + \cos\frac{\pi}{2k}}{1 + \cos\frac{\pi}{2k}}} \ . \tag{3.10}$$

Then the design with support points $x_1^*, \ldots, x_{2k}^*$ and weights $\omega_1, \ldots, \omega_{2k}$ determined by (3.5) is the unique optimal extrapolation design in the polynomial regression model of degree $2k$ without intercept on the interval $[-1, 1]$.

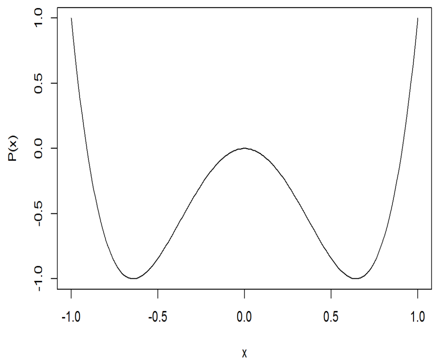

Figure 1: *The extremal polynomial in the proof of Theorem 3.2 in the case* $n = 4$ $(k = 2)$.

Proof. A simple calculation shows that the points $x_1^*, x_2^*, \ldots, x_{2k}^*$ in (3.10) are the extremal points of the polynomial

$$P(x) = T_k\left((x^2(1 + \cos\frac{\pi}{2k}) - \cos\frac{\pi}{2k})\right). \tag{3.11}$$

Consequently, $P(x)$ is an extremal polynomial, which can be used in Theorem 2.1 to prove the optimality of the design. Observing that $P(x_i^*) = (-1)^{i+1}$, if $i = 1, \ldots, k$ and $P(x_i^*) = (-1)^i$ if $i = k+1, \ldots, 2k$ we see that condition (1) and (2) of Theorem 2.1 are satisfied. The verification of condition (3) follows by the same arguments as given in the proof of Theorem 3.1 and is omitted for the sake of brevity.

The uniqueness of the optimal design follows from the fact that the polynomial P in (3.11) is the unique (up to a sign) polynomial of degree $2k$ with no intercept that achieves its sup-norm on the interval $[-1, 1]$ exactly $2k$ times. The proof of this property can be obtained by the same arguments as the proof of a similar extremal property of the Chebyshev polynomial of the first kind. □.

Example 3.3 In the case $n = 4$ (that is $k = 2$) we have $\cos\frac{\pi}{2k} = \cos\frac{\pi}{4} = \frac{1}{\sqrt{2}}$ and the extremal polynomial in (3.11) is given by

$$P(x) = 2[x^2(1 + \tfrac{1}{\sqrt{2}}) - \tfrac{1}{\sqrt{2}}]^2 - 1 = (3 + 2\sqrt{2})x^4 - (2 + 2\sqrt{2})x^2.$$

The extremal polynomial $P(x)$ in (3.11) is depicted in Figure 1 and a straightforward calculation shows that the optimal extrapolation design at the point $z = 2$ is given by

$$\xi = \begin{pmatrix} -1 & -0.6436 & 0.6436 & 1 \\ 0.083 & 0.227 & 0.442 & 0.248 \end{pmatrix}. \tag{3.12}$$

4 Optimal designs for estimating the slope

In this section we consider optimal designs for estimating the slope of a polynomial regression with no intercept on the interval $[-1, 1]$ at a given point, say $z \in \mathbb{R}$. As pointed out in the previous sections, this problem corresponds to a c-optimal design problem in model (1.1) with $f^\top(x) = (x, \ldots, x^n)$ and vector $c = (1, 2z, \ldots, nz^{n-1})^\top$. For the common polynomial model with intercept this problem has recently been studied in Dette et al. (2010), who showed that there exists three different types of optimal designs, depending on the location of the point z. Only in one of these cases the corresponding extremal polynomial is a Chebyshev polynomial.

For the polynomial with no intercept we begin with a result regarding the general structure of the optimal design for estimating derivative at a given point. The proof is similar to the proof of the corresponding result with intercept [see Dette et al. (2010)] and therefore omitted.

Theorem 4.1 *The optimal design for estimating the slope in the polynomial regression of degree n with no intercept has either $m = n$ or $m = n - 1$ support points $t_1^*, \ldots, t_m^*$. The weights at these points are given by*

$$\omega_i = \frac{|\bar{L}_i'(z)|}{\sum_{j=1}^m |\bar{L}_j'(z)|} \ , \ i = 1, \ldots, m, \tag{4.1}$$

where $\bar{L}_1, \ldots, \bar{L}_m$ are the Lagrange basis interpolation polynomials without intercept defined in (3.6) corresponding to the nodes $t_1^*, \ldots, t_m^*$ and $\bar{L}_i'$ denotes the derivative of $\bar{L}_i$.

We now discuss the case of even and odd degree separately starting with the odd degree. that is $n = 2k + 1$.

4.1 Polynomials of odd degree

For the linear model through the origin (that is $k = 0$, $n = 1$) it is easy to see using Elfving's theorem that (independently of the point z) there exist an infinite number of optimal designs of the form

$$\xi^* = \alpha\delta_{-1} + (1 - \alpha)\delta_1$$

where $\alpha \in [0, 1]$ and δ_x denotes the Dirac measure at the point x. However, in the case $k \geq 1$ the situation is more complicated. In order to describe the optimal design in the case $n = 2k+1$ explicitly we recall the notation

$$s_{i,2k+1} = \cos(\tfrac{(2k+2-i)\pi}{2k+1}) \ , \quad i = 1, \dots, 2k+2 \tag{4.2}$$

for the extremal points of the Chebyshev polynomial $T_{2k+1}(x) = \cos((2k+1)\arccos x)$ of the first kind and denote by

$$U_{2k}(x) = \frac{\sin((2k+1)\arccos x)}{\cos(\arccos x)}$$

the $2k$th Chebyshev polynomial of the second kind. It can be checked by a direct calculation that the leading coefficient of $U_{2k}(x)$ is 2^{2k} and that $T'_{2k+1}(x) = (2k+1)U_{2k}(x)$. Therefore we obtain the representation

$$U_{2k}(x) = 2^{2k} \prod_{l=2}^{2k+1} (x - s_{l,2k+1}). \tag{4.3}$$

Based on the polynomial $U_{2k}(x)$ we now consider four basic polynomials of degree $2k+1$

$$R(x) = \frac{x(x+1)U_{2k}(x)}{x - s_{k+1,2k+1}}, \tag{4.4}$$

$$R_1(x) = \frac{x(x-1)U_{2k}(x)}{x - s_{k+2,2k+1}}, \tag{4.5}$$

$$R_2(x) = \frac{x(x-1)U_{2k}(x)}{x - s_{k+1,2k+1}}, \tag{4.6}$$

$$R_3(x) = \frac{x(x+1)U_{2k}(x)}{x - s_{k+2,2k+1}}, \tag{4.7}$$

and denote the roots of their derivatives by

$$\nu_1 < \nu_2 < \cdots < \nu_{2k}, \tag{4.8}$$

$$\mu_1 < \mu_2 < \cdots < \mu_{2k}, \tag{4.9}$$

$$\rho_1 < \rho_2 < \cdots < \rho_{2k} \tag{4.10}$$

$$\tau_1 < \tau_2 < \cdots < \tau_{2k}, \tag{4.11}$$

respectively. In order to study the roots of the derivatives of these polynomials we will make use of the following two auxiliary results.

Lemma 4.2 *The roots $\nu_1 < \nu_2 < \cdots < \nu_{2k}$ and $\mu_1 < \mu_2 < \cdots < \mu_{2k}$ of the polynomials $R'(x)$ and $R_1'(x)$ satisfy*

$$\nu_{2k+1-i} = -\mu_i \quad , i = 1, \ldots, 2k \ .$$

The roots $\rho_1 < \rho_2 < \cdots < \rho_{2k}$ and $\tau_1 < \tau_2 < \cdots < \tau_{2k}$ of the polynomials $R_2'(x)$ and $R_3'(x)$ satisfy

$$\rho_{2k+1-i} = -\tau_i \quad , i = 1, \ldots, 2k \ .$$

Lemma 4.2 is a simple consequence of the facts $s_{k+1,2k+1} = -s_{k+2,2k+1}$ and $U_{2k}(-x) = U_{2k}(x)$, which implies $R(-x) = R_1(x)$, $R_2(-x) = R_3(x)$.

Lemma 4.3 *Let $P_1(x)$ and $P_2(x)$ be polynomials of degree n with n distinct roots $t_{(1,1)} < t_{(2,1)} < \ldots < t_{(n,1)}$ and $t_{(1,2)} < t_{(2,2)} < \ldots < t_{(n,2)}$, respectively. Assume that the roots are interlacing in the following sense:*

$$t_{(1,1)} \leq t_{(1,2)} < t_{(2,1)} \leq t_{(2,2)} < \ldots < t_{(n,1)} \leq t_{(n,2)}$$

where at least one of the inequalities $t_{(\ell,1)} \leq t_{(\ell,2)}$ ($\ell = 1, \ldots n$) is strict.
Then the roots $v_{(1,1)} \leq v_{(2,1)} \leq \ldots \leq v_{(n-1,1)}$ and $v_{(1,2)} \leq v_{(2,2)} \leq \ldots \leq v_{(n-1,2)}$ of the derivatives $P_1'(x)$ and $P_2'(x)$ are strictly interlacing, that is

$$v_{(1,1)} < v_{(2,1)} < \ldots < v_{(1,n-1)} < v_{(2,n-1)}.$$

The proof can be found in the PhD thesis of Sahm (1998) and is given in the Appendix for the sake of completeness. The following lemma provides the interlacing property for the roots of the first derivatives of the polynomials $R(x), R_1(x), R_2(x)$ and $R_3(x)$.

Lemma 4.4 *The points defined by (4.8) - (4.11) satisfy*

$$\mu_i < \rho_i, \mu_i < \tau_{i+1}, \tau_i < \nu_i, \rho_i < \nu_{i+1}, \ i = 1, \ldots, 2k \ ,$$

where $\nu_{2k+1} = \infty, \tau_{2k+1} = \infty$.

Proof. The proof is a direct consequence of Lemma 4.3. Exemplarily, consider the roots of the polynomials $R_1(x)$ and $R_2(x)$, which are given by

$$\begin{array}{l} s_{2,2k+1} < \ldots < s_{k,2k+1} < s_{k+1,2k+1} < \quad 0 \quad < s_{k+3,2k+1} < \ldots < s_{2k+1,2k+1}, \\ s_{2,2k+1} < \ldots < s_{k,2k+1} < \quad 0 \quad < s_{k+2,2k+1} < s_{k+3,2k+1} < \ldots < s_{2k+1,2k+1}, \end{array}$$

respectively. Consequently Lemma 4.3 with $P_1(x) = R_1(x)$ and $P_2(x) = R_2(x)$ is applicable and implies for the roots μ_i and ρ_i of the derivatives R_1' and R_2' the interlacing properties

$$\mu_1 < \rho_1 < \mu_2 < \rho_2 < \ldots < \mu_{2k} < \rho_{2k} \ .$$

As all other cases are treated similarly, the assertion of Lemma 4.4 follows. □

For the statement of our first main result we define a sequence of designs $\xi_1, \ldots, \xi_{2k+2}$ supported at $2k+1$ points, where the weights are defined by (4.1) for the different the support points. Note that these weights are positive by definition. For the design ξ_1 the support points are given by

$$s_{2,2k+1}, s_{3,2k+1}, \ldots, s_{2k+2,2k+1} \tag{4.12}$$

If $i \in \{2, \ldots 2k+1\}$ the support points of the design ξ_i are given by

$$s_{1,2k+1}, \ldots s_{i-1,2k+1}, s_{i+1,2k+1}, \ldots, s_{2k+2,2k+1},$$

and the support points of the design ξ_{2k+2} are given by

$$s_{1,2k+1}, s_{2,2k+1}, \ldots, s_{2k+1,2k+1}.$$

Note that the designs are obtained by omitting one of the points $s_{1,2k+1}, \ldots, s_{2k+2,2k+1}$. In the following result we show that for many values of z one of the designs $\xi_1, \xi_{k+1}, \xi_{k+2}$ or ξ_{2k+2} is optimal for estimating the slope in a polynomial regression with no intercept.

Theorem 4.5 *The optimal design on the interval $[-1, 1]$ for estimating the slope of a polynomial regression with no intercept at the point z has at most $2k+1$ points in the set $\{s_{1,2k+1}, \ldots, s_{2k+2,2k+1}\}$ if and only if $z \in \cup_{i=1}^{2k+1} A_i$, where the set A_i is defined by $A_i = (-\nu_{2k+2-i}, \nu_i)$, $i = 1, \ldots, 2k+1$. Moreover,*

(1) The design ξ_1 is the optimal design if and only if z is in one of the intervals $(\mu_i, \rho_i), i = 1, \ldots, 2k$. If $z = \rho_i, i = 1, \ldots, 2k$ the optimal is supported at the $2k$ points

$$s_{2,2k+1}, \ldots, s_{k,2k+1}, s_{k+2,2k+1}, \ldots, s_{2k+2,2k+1}$$

with weights defined by (4.1).

(2) *The design* ξ_{k+1} *is the optimal design if and only if* z *is in one of the intervals* $(-\infty, \nu_1), (\rho_{2k}, \infty)$ *or* (ρ_i, ν_{i+1}), $i = 1, \dots, 2k-1,$. *If* $z = \nu_i, i = 1, \dots, 2k$ *the optimal is supported at the* $2k$ *points*

$$s_{1,2k+1}, \dots, s_{k,2k+1}, s_{k+2,2k+1}, \dots, s_{2k+1,2k+1}$$

with weights defined by (4.1).

(3) *The design* ξ_{k+2} *is the optimal design if and only if* z *is in one of the intervals* $(-\infty, \tau_1)$, (μ_{2k}, ∞) *or* $(\mu_i, \tau_{i+1}), i = 1, \dots, 2k-1$. *If* $z = \mu_i, i = 1, \dots, 2k$ *the optimal is supported at the* $2k$ *points*

$$s_{2,2k+1}, \dots, s_{k+1,2k+1}, s_{k+3,2k+1}, \dots, s_{2k+2,2k+1}$$

with weights defined by (4.1).

(4) *The design* ξ_{2k+2} *is the optimal design if and only if* z *is in one of the intervals* $(\tau_i, \nu_i), i = 1, \dots, 2k$. *If* $z = \tau_i, i = 1, \dots, 2k$ *the optimal is supported at the* $2k$ *points*

$$s_{1,2k+1}, \dots, s_{k+1,2k+1}, s_{k+3,2k+1}, \dots, s_{2k+1,2k+1}$$

with weights defined by (4.1).

Proof. We begin with the proof of the statements (1) - (4), where we restrict ourselves to the case (1), as the other cases can be shown similarly. The basic idea is the following. The polynomial $T_{2k+1}(x)$ will serve as extremal polynomial in Theorem 2.1. Consequently, the points $s_{i,2k+1}$ in (4.2) are potential support points of the optimal design and conditions (1) and (2) of Theorem 2.1 are satisfied. It now remains to characterize those values of z such that the system of equations defined by condition (3) in Theorem 2.1 admits a solution with nonnegative weights ω_i satisfying $\sum_{i=1}^m \omega_i = 1$. Observing the representation (4.3) it is easy to see that the polynomials $R(x), R_1(x), R_2(x)$ and $R_3(x)$ are special cases (up to a constant) of the polynomials

$$\bar{L}_{i,j}(x) = \frac{x \prod_{\ell \neq i,j}(x - s_{\ell,2k+1})}{s_{j,2k+1} \prod_{\ell \neq i,j}(s_{j,2k+1} - s_{\ell,2k+1})} \ , \ j = 1, 2, \dots, i-1, i+1, \dots 2k+2 \tag{4.13}$$

(note that $\bar{L}_{i,j}(x)$ is a polynomial of degree $2k+1$ as the index ℓ runs over the set $\{1, 2, \dots, 2k+2\} \setminus \{i, j\}$). More precisely we have

$$\begin{aligned} R(x) = c\bar{L}_{2k+2,k+1}(x) \ , \quad R_1(x) = c_1\bar{L}_{1,k+2}(x) \ , \\ R_2(x) = c_2\bar{L}_{1,k+1}(x) \ , \quad R_3(x) = c_3\bar{L}_{2k+2,k+2}(x) \ , \end{aligned} \tag{4.14}$$

for appropriate constants c, c_1, c_2 and c_3. Note that in case (1) the Lagrange interpolation polynomial without intercept defined in (3.6) corresponding to the points in (4.12) is given by

$$\bar{L}_j(x) = \frac{x \prod_{\ell \neq 1,j}(x - s_{\ell,2k+1})}{s_{j,2k+1} \prod_{\ell \neq 1,j}(s_{j,2k+1} - s_{\ell,2k+1})} = \bar{L}_{1,j}(x)$$

$(j = 2, \ldots, 2k+2)$. If $z \to -\infty$ the sign of the derivatives $\bar{L}'_{1,j}(z)$ coincide with the sign of the polynomials $\bar{L}_{1,j}(z)$ and are equal to the sign of

$$(-1)s_{j,2k+1} \prod_{\ell \neq 1,j} (s_{j,2k+1} - s_{\ell,2k+1}) \ ,$$

which are denoted by t_j in the following $(j = 2, \ldots, 2k+2)$. Consequently we have

$$t_j = \begin{cases} (-1)^j & \text{if } j = 2, \ldots, k+1 \\ (-1)^{j+1} & \text{if } j = k+2, \ldots, 2k+2 \end{cases}$$

if z is negative and $|z|$ is sufficiently large.
Let us now consider the signs of the derivatives of the polynomials $\bar{L}_{1,j}(x)$ $(j = 2, \ldots, 2k+1)$ at a point $z \in (\mu_i, \rho_i)$ $(i = 1, \ldots, 2k+1)$. For this purpose we denote the roots of $\bar{L}'_{1,j}(x)$ by $u_{j,1}, \ldots, u_{j,2k}, j = 2, \ldots, 2k+2$. A straightforward calculation shows that the roots of the polynomials $\bar{L}_{1,j}$ and $\bar{L}_{1,l}$ for $j < l$ are interlacing and by Lemma 4.3 we have

$$u_{2k+2,1} < \ldots < u_{k+2,1} < u_{k+1,1} < \ldots < u_{2,1} <$$

$$< u_{2k+2,2} < \ldots < u_{k+2,2} < u_{k+1,2} < \ldots < u_{2,2} < \ldots < u_{2k+2,2k} < \ldots < u_{2,2k}.$$

Observing that μ_j and ρ_j are the roots of the polynomials R_1 and R_2, respectively and using the representation (4.14) it follows that

$$u_{k+2,j} = \mu_j, u_{k+1,j} = \rho_j, j = 1, \ldots, 2k.$$

Next we show that the quantities $\bar{L}'_{1,i}(z)(-1)^i$, $i = 1, 2, \ldots, 2k+1$ have the same sign if and only if z is in the one of the intervals $(\mu_i, \rho_i), i = 1, \ldots, 2k$. Note (see Figure 2) that each of the polynomials $\bar{L}_{1,j}$ $(j = 2k+2, \ldots, k+2)$ has exactly one root in the interval $(-\infty, u_{k+2,1} - \delta)$ (where $\delta > 0$ and arbitrarily small). Moreover $u_{k+2,1} = \mu_1, u_{k+1,1} = \rho_1$, and there are no roots between μ_1 and ρ_1 Consequently, the quantities $\bar{L}'_i(z)(-1)^i$, $i = 1, 2, \ldots, 2k+1$ have the same sign for $z \in (\mu_1, \rho_1)$.

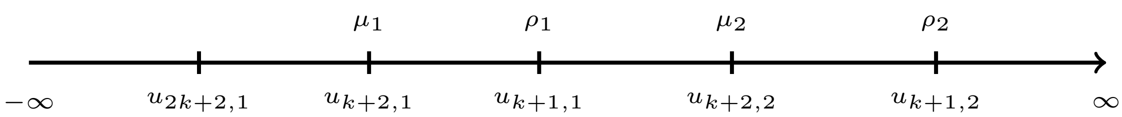

Figure 2: *Roots of the polynomials* $\bar{L}'_{1,j}(x)$, $j = 1, \ldots, 2k$. *There are no roots between* μ_1 *and* ρ_1.

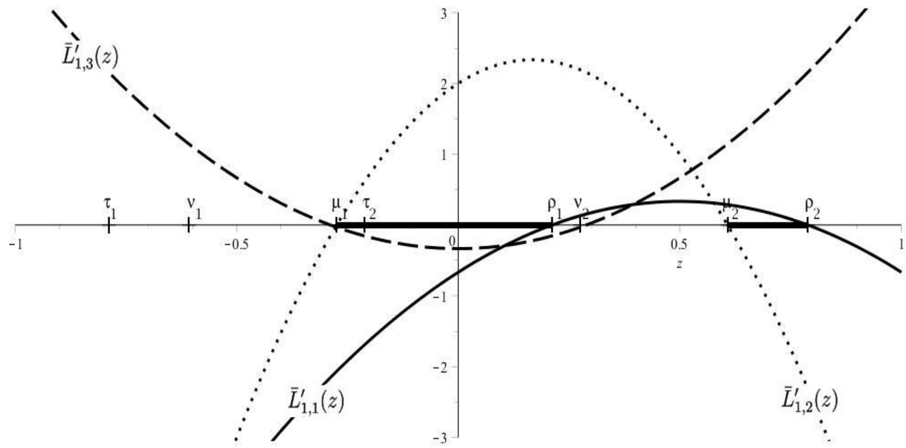

Figure 3: *The derivatives* $\bar{L}'_{1,j}(z)$ *as a function* $z \in \mathbb{R}$ *for* $j = 1, \ldots, n = 2k+1 = 3$ *(*$k = 1$*). The polynomials* $\bar{L}'_{1,1}(z), \bar{L}'_{1,2}(z)$ *and* $\bar{L}'_{1,3}(z)$ *alternate in sign if and only if* $z \in (\mu_1, \rho_1) \cup (\mu_2, \rho_2)$.

Consider now the intervals $(\mu_i, \rho_i), i = 2, \ldots, 2k$. Note that the derivatives $\bar{L}'_{1,j}(z)$ $(j = 1, \ldots, 2k+1)$ change their signs exactly once as z is passing from ρ_i to μ_{i+1} and that there are no roots between μ_i and ρ_i (see Figure 3, where we show these functions for $k = 1$). This part is still a little unclear to me ! Thus the signs of the quantities $\bar{L}'_{1,j}(z)$ coincide with the signs of $(-1)^{i-1}T_{2k+1}(s_{j,2k+1})$ if z is in the interval (μ_i, ρ_i) and they do not coincide with the signs of $T_{2k+1}(s_{j,2k+1})$ or $-T_{2k+1}(s_{j,2k+1})$ if z is outside these intervals $(i = 2, \ldots, 2k+1)$. Using these observations we obtain in the same manner as in the proof of Theorem 3.1 that

$$c^\top = (1, 2z, \ldots, (2k+1)z^{2k})^\top = F \cdot (\bar{L}'_{1,1}(z), \ldots, \bar{L}'_{1,2k+1}(z))^\top = hF\beta,$$

where

$$F = (s^i_{j+1,2k+1})^{2k+1}_{i,j=1} \in \mathbb{R}^{2k+1 \times 2k+1},$$

$h = \sum_{j=1}^{2k+1} |\bar{L}'_{1,j}(z)|$, $\beta_i = \omega_i T_{2k+1}(s_{i+1,2k+1})$ and $\omega_i = |\bar{L}'_{1,i}(z)| \geq 0$ $(i = 1, \ldots, 2k+1)$. As these equations are equivalent to the condition (3) in Theorem 2.1 the optimality of the

design ξ_1 in part (1) of Theorem 4.5 follows. The optimality of the designs ξ_{k+1}, ξ_{k+2} and ξ_{2k+2} in part (2), (3) and (4) is shown by the same arguments.
Next we consider the remaining case $z = \rho_i, i = 1, 2, \dots, 2k$ in part (1) of Theorem 4.5. For this purpose we use the obvious identities

$$\begin{aligned} (\mu_i, \rho_i) \cup (\rho_i, \nu_{i+1}) \cup \{\rho_i\} &= (\mu_i, \nu_{i+1}), i = 1, \dots, 2k, \\ (\mu_i, \tau_{i+1}) \cup (\tau_{i+1}, \nu_{i+1}) \cup \{\tau_{i+1}\} &= (\mu_i, \nu_{i+1}), i = 1, \dots, 2k, \end{aligned} \tag{4.15}$$

and $(-\infty, \tau_1) \cup (\tau_1, \nu_1) \cup \{\tau_1\} = (\mu_0, \nu_1)$, where $\mu_0 = -\infty$. The assertion about the case $z = \rho_i, i = 1, 2, \dots, 2k$ follows considering the limit $z \to \rho_i$ (the designs ξ_1 and ξ_{k+1} must converge to the same limit). The remaining statements for $z = \nu_i, \mu_i$ and τ_i are treated similarly. Finally, it can be also verified that designs ξ_i can not be optimal if i is outside the set $\{1, k+1, k+2, 2k+1\}$.
Due to Lemma 4.2 we have $\nu_{2k+1-i} = -\mu_i, i = 1, \dots, 2k$. Thus from (1) - (4) it follows that the optimal design on the interval $[-1, 1]$ for estimating the slope of a polynomial regression with no intercept at the point z is supported at exactly $2k + 1$ points in the set $\{s_{1,2k+1}, \dots, s_{2k+2,2k+1}\}$ if and only if $z \in \cup_{i=1}^{2k+1} A_i$, which completes the proof of Theorem 4.5.

Remark 4.6
(a) It also follows from the proof of Theorem 4.5 that ξ_j can not be optimal if $j \notin \{1, k + 1, k + 2, 2k + 2\}$.
(b) It follows from the proof of Theorem 4.5 that for any $z \in \cup_{i=1}^{2k+1} A_i$ there exist exactly two optimal designs for estimating the slope of a polynomial regression with no intercept which are supported at $2k+1$ points from the set of $2k+2$ points $\{s_{1,2k+1}, \dots, s_{2k+2,2k+1}\}$. Indeed, it follows from the identity (4.15) that each

$$z \in A_i = (-\nu_{2k+2-i}, \nu_i) = (\mu_{i-1}, \nu_i),\ i = 1, \dots, 2k + 1,$$

belongs to exactly two of the intervals determined in the cases (1) - (4) of Theorem 4.5. Similarly, the points $\rho_1, \dots, \rho_{2k}$ and $\tau_1, \dots, \tau_{2k}$ belong to exactly two of the intervals determined in the cases (1) - (4) of Theorem 4.5 (in this case there exists an optimal design with $2k$ and $2k + 1$ support points).

Example 4.7 In this example we illustrate potential applications of Theorem 4.5 determining optimal designs for estimating the slope of a cubic regression with no intercept (note that this corresponds to the case $k = 1$ in the previous result). In this case the extremal points in (4.2) are given by $\{-1, -1/2, 1/2, 1\}$ and the derivatives of the polynomials in (4.4) - (4.7) are given by

$$R'(x) = 12x^2 + 4x - 2 \ , \ R'_1(x) = 12x^2 - 4x - 2$$
$$R'_2(x) = 12x^2 - 12x + 2 \ , \ R'_3(x) = 12x^2 + 12x22$$

The corresponding roots are obtained as

$$\nu_1 = -0.608 \ , \quad \nu_2 = 0.274 \ , \quad \mu_1 = -0.274 \ , \quad \mu_2 = 0.608 \ ,$$
$$\rho_1 = 0.211 \ , \quad \rho_2 = 0.789 \ , \quad \tau_1 = -0.789 \ , \quad \tau_2 = -0.211 \ ,$$

and consequently the optimal design for estimating the slope of a polynomial regression without intercept at the point z is supported at 3 points from the set $\{-1, -1/2, 1/2, 1\}$ if and only if

$$z \in (-\infty, -0.608) \cup (-0.274, 0.274) \cup (0.608, \infty)$$

(1) The optimal design supported at the points $\{-1/2, 1/2, 1\}$ if

$$z \in (\mu_1, \rho_1) \cup (\mu_2, \rho_2) \approx (-0.274, 0.211) \cup (0.608, 0.789);$$

(2) The optimal design supported at the points $\{-1, 1/2, 1\}$ if

$$z \in (-\infty, \nu_1) \cup (\rho_1, \nu_2) \cup (\rho_2, \infty) \approx (-\infty, -0.608) \cup (0.211, 0.274) \cup (0.789, \infty);$$

(3) The optimal design supported at the points $\{-1, -1/2, 1\}$ if

$$z \in (-\infty, \tau_1) \cup (\mu_1, \tau_2) \cup (\mu_2, \infty) \approx (-\infty, -0.789) \cup (-0.274, -0.211) \cup (0.608, \infty);$$

(4) The optimal design supported at the points $\{-1, -1/2, 1/2\}$ if

$$z \in (\tau_1, \nu_1) \cup (\tau_2, \nu_2) \approx (-0.789, -0.608) \cup (-0.211, 0.274).$$

4.2 Polynomials of even degree

In this section we consider the problem of designing an experiment for the estimation of the slope of a polynomial regression of even degree with no intercept, that is $n = 2k$. We recall the definition of the polynomial $P(x)$ in (3.11), its corresponding extremal points $x_1^*, \dots x_{2k}^*$ in (3.10) and introduce the polynomials

$$\begin{aligned}
Q_1(x) &= x(x+1)\prod_{\ell=2}^{2k-1}(x-x_\ell^*) = x(x+1)P'(x),\\
Q_2(x) &= x(x-1)\prod_{\ell=2}^{2k-1}(x-x_\ell^*) = x(x-1)P'(x).\\
Q_3(x) &= x(x-1)\prod_{\ell=2}^{2k-1}(x-s_{\ell,2k-1}) = x(x-1)U_{2k-2}(x),\\
Q_4(x) &= x(x+1)\prod_{\ell=2}^{2k-1}(x-s_{\ell,2k-1}) = x(x+1)U_{2k-2}(x)
\end{aligned}$$

where $s_{1,2k-1}, s_{2,2k-1}, \dots, s_{2k,2k-1}$, are the extremal points of the Chebyshev polynomial $T_{2k-1}(x)$. Moreover, we define the sets

$$B = \cup_{i=0}^{2k-1}(-\nu_{2k-i}, \nu_{i+1}), \tag{4.16}$$

$$C = \cup_{i=1}^{2k-1}(-\rho_{2k-i}, \rho_i), \tag{4.17}$$

where $\nu_{2k} = \infty$ and $\nu_1 < \nu_2 < \cdots < \nu_{2k-1}$ are the roots of the first derivative of the polynomial $Q_1(x)$ and $\rho_1 < \rho_2 < \cdots < \rho_{2k-1}$ are the roots of the first derivative of the polynomial $Q_3(x)$. Note that the roots of the derivative of the polynomial $Q_2(x)$ are given by $-\nu_{2k-1}, \dots, -\nu_1$ because of the equality $Q_2(-x) = Q_1(x)$.

Theorem 4.8

(1) There exists an optimal design for estimating the slope at the point z in a polynomial regression of degree $2k \geq 2$ with no intercept supported at the points $x_1^*, \dots x_{2k}^*$ in (3.10) if and only $z \in B$. In this case the optimal design is unique and the corresponding weights are given by (4.1) with m=2k.

(2) There exists an optimal design for estimating the slope at the point z in a polynomial regression of degree $2k \geq 2$ with no intercept supported at the extremal points $s_{1,2k-1}, s_{2,2k-1}, \dots, s_{2k,2k-1}$, of the Chebyshev polynomial $T_{2k-1}(x)$ if and only if $z \in C$. In this case the optimal design is unique and the corresponding weights are given by (4.1) with m=2k.

Proof. The proof is similar to that of Theorem 4.5 and therefore we only indicate a proof of part (1). As the polynomial $P(x)$ in (3.11) obviously satisfies the conditions of Theorem 2.1

it remains to show condition (3). It then follows that the weights coefficients are uniquely determined by (4.1) with $m = 2k$.

Similar to the proof of Theorem 3.1 condition (3) of Theorem 2.1 holds if the quantities $P(x_i^*)$ and $\bar{L}_i'(z)$ have the same sign for $i = 1, 2, \ldots, 2k$, where the polynomial $\bar{L}_i$ is given by

$$\bar{L}_i(x) = \frac{x \prod_{s \neq i}(x - x_s^*)}{x_i^* \prod_{s \neq i}(x_i^* - x_s^*)}, \; i = 1, 2, \ldots, 2k.$$

Note that the quantities $P(x_i^*)(-1)^i$, $i = 1, 2, \ldots, k$ and $-P(x_i^*)(-1)^i$, $i = k+1, k+2, \ldots, 2k$ have the same sign, and consequently it is sufficient to show that all the quantities $\bar{L}_i'(z)(-1)^i, i = 1, 2, \ldots, k$ and $-\bar{L}_i'(z)(-1)^i, i = k+1, k+2, \ldots, 2k$ have the same sign. We will show that this property holds if and only if $z \in B$, where the set B is defined in (4.16).

Obviously, the roots of the polynomials $\bar{L}_i(x)$ and $\bar{L}_{i+1}(x)$ satisfy the assumptions of Lemma 4.3. Note also that $Q_1(x) = c_1 \bar{L}_{2k}(x), Q_2(x) = c_2 \bar{L}_1(x)$ for some constants $c_1$and c_2. Consequently, if $v_{(i,1)} < \ldots, v_{(i,2k-1)}$ denote the roots of the derivative of $\bar{L}_i(x)$ $(i = 1, 2, \ldots, 2k)$, then an application of Lemma 4.3 shows that

$$\begin{aligned} \nu_1 = v_{(1,2k)} < \cdots < v_{(1,1)} = -\nu_{2k-1} < \\ \nu_2 = v_{(2,2k)} < \cdots < v_{(2,1)} = -\nu_{2k-2} < \nu_3 < \cdots < \\ \nu_{2k-1} = v_{(2k-1,2k)} < \cdots < v_{(2k-1,1)} = -\nu_1. \end{aligned}$$

First we consider the case $z < \nu_1$. If $z \to -\infty$ the sign of the derivatives $\bar{L}_i'(z)$ coincide with the sign of the polynomials $\bar{L}_i(z)$ and are equal to the sign of

$$-x_i^* \prod_{s \neq i}(x_i^* - x_s^*), \; i = 1, 2, \ldots, 2k.$$

which are denoted by t_i in the following $i = 1, \ldots, 2k$. Consequently we have

$$t_i = \begin{cases} (-1)^i & \text{if } i = 1, \ldots, k \\ (-1)^{i+1} & \text{if } i = k+1, \ldots, 2k. \end{cases}$$

if z is negative and $|z|$ is sufficiently large. Note that there are no zeros of the polynomial $\bar{L}_1'(z), \ldots, \bar{L}_{2k}'(z)$ for $z \in (-\infty, \nu_1)$. Therefore all the quantities $\bar{L}_i'(z)(-1)^i, i = 1, 2, \ldots, k$ and $-\bar{L}_i'(z)(-1)^i, i = k+1, k+2, \ldots, 2k$ have the same sign for $z \in (-\infty, \nu_1)$.

Next consider the case $z \in (-\nu_{2k-1}, \nu_2)$. In this case it follows from the above inequalities

that all polynomials $\bar{L}_i'(z)(-1)^i, i = 1, 2, \ldots, k$ and $-\bar{L}_i'(z)(-1)^i, i = k+1, k+2, \ldots, 2k$ have the same signs since all derivatives have exactly one sign change on the interval $(\nu_1, -\nu_{2k-1})$. Proceeding in the same way we can prove that the quantities $P(x_i^*)$ and $\bar{L}_i'(z)$ $(i = 1, 2, \ldots, 2k)$ have the same sign if and only if $z \in B$.
The uniqueness of the optimal design follows from the fact that the extremal polynomial $P(x)$ in (3.11) is unique in the sense that it is the unique polynomial of degree $2k$ with no intercept that achieve its extremal absolute value equal in the interval $[-1, 1]$ exactly $2k$ times. This completes the proof of the part (1) of the theorem. The part (2) can be proved in a similar way.

Example 4.9
(a) Consider the case $n = 2$, which corresponds to a quadratic regression model with no intercept. In order to apply part (2) of Theorem 4.8 note that in this case the extremal points of the Chebyshev polynomials $T_1(x)$ are given by $s_{1,1} = -1$ and $s_{2,1} = 1$ and $Q_3(x) = x(x-1)$. This gives for the root of its derivative $\rho_1 = 1/2$.
Consequently, the optimal design for estimating the slope in a quadratic regression model with no intercept is supported at the points -1 and 1 if and only if $z \in C = (-\frac{1}{2}, \frac{1}{2})$. Moreover, in this case the weights are given by

$$\frac{1}{2} - z \quad \text{and} \quad \frac{1}{2} + z,$$

respectively. It can be checked by a direct calculation that this statement remains correct in the case $z = -\frac{1}{2}$ of $z = \frac{1}{2}$.
Next we consider the situation corresponding to part (1) in Theorem 4.8, noting that in this case the polynomial P in (3.11) is given by $P(x) = x$, which yields $x_1^* = -1$ and $x_2^* = 1$ as support points of the potential optimal design. Moreover as $Q_1(x) = x(x+1)$ we have $\nu_1 = -1/2$ and $\nu_2 = 1/2$ and

$$B = (-\infty, -1/2) \cup (1/2, \infty)$$

Consequently, if $|z| > 1/2$, it follows by a straightforward calculation that the optimal design for estimating the slope in a quadratic regression has weights

$$1/2 - \frac{1}{4z} \quad \text{and} \quad 1/2 + \frac{1}{4z}$$

at the points -1 and 1, respectively.

(b) For polynomials of larger degree the situations gets substantially more complicated. Consider exemplarily the case $n = 2k = 4$. The extremal polynomial in part (1) of Theorem 4.8 is given by (3.11). The optimal design for estimating the slope in the polynomial of degree $n = 4$ with no intercept is supported at the extremal points $-1, -0.6436, 0.6436$ and 1 of this polynomial if and only if z belongs to one of the following intervals

$$(-\infty, -0.8503), \ (-0.4027, -0.3023), \ (0.3023, 0.4027), \ (0.8503, \infty).$$

Part (2) of Theorem 4.8 is applicable if and only if z belongs to one of the intervals

$$(-0.804, -0.663), (-0.235, 0.235), (0.663, 0.804).$$

In this case the optimal design for estimating the slope is supported at the extremal points $1, -0.5, 0.5$ and 1 of the third Chebyshev polynomial $T_3(x) = 4x^3 - 3x$.

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5 Proof of Lemma 4.3

The proof of this result can be found in the PhD thesis of Sahm (1998). As it is difficult to get access to this thesis, we repeat his arguments here for the sake of completeness. We begin with two statements, from which the proof of Lemma 4.3 will easily follow.

Lemma 5.1 *Let $Q(x) = \prod_{i=1}^{n}(x - q_i)$ and $P(x) = \prod_{i=1}^{m}(x - p_i)$ denote two polynomials of degree n and m, respectively,where $m = n - 1$ or $m = n$. Assume that $P \neq Q$ and set $q_{n+1} = -\infty$. If*

$$q_i \geq p_i \geq q_{i+1}, i = 1, \ldots, m, \tag{5.1}$$

then we have

$$R(x) := (P(x)/Q(x))' < 0,$$

whenever the polynomial $R(x)$ is defined.

Proof. In the case $n = 1$ the result is nearly obvious: if $m = n - 1 = 0$ we have $R(x) = -Q^{-2}(x) < 0$ and for $m = n = 1$

$$R(x) = \frac{p_1 - q_1}{(x - q_1)^2} < 0 \quad \text{for all } x \neq q_1$$

Now we turn to the case $n > 1$ and assume that the pair (P, Q) form a counterexample of minimal degree. This implies in particular that $P(x)$ and $Q(x)$ cannot have a root in common (otherwise their degree would not be minimal). Furthermore all roots of $P(x)$ and $Q(x)$ must be simple. As the pair (P, Q) is a counterexample there exists some $z \in \mathbb{R}$ where $R(z) \geq 0$.

The idea is following. Move the polynomial P up (or down) without changing the property $R(z) \geq 0$ until one of the zeros of $P(x)$ and $Q(x)$ coincide. Then divide the polynomials by this factor and produce a counterexample of smaller degree, which contradicts the assumption of minimality. For this purpose we have to consider the two cases $Q'(z) \geq 0$ and $Q'(z) < 0$ separately.

We restrict ourselves to the case $Q'(z) \geq 0$ and mention that the case $Q'(z) < 0$ can be obtained by exactly the same arguments. To be precise define

$$\epsilon := \sup\{\delta > 0 | \text{ the roots of the polynomials } P(x) - \delta \text{ and } Q(x) \text{ interlace } \}.$$

This set is not empty due to the continuity of the roots of the polynomial $P(x) - \delta$ with respect to δ. Now let $\bar{P}(x) = P(x) - \epsilon$. Then it is clear from the definition of ϵ that $\bar{P}(x)$ has m zeros $\bar{p}_1, \ldots, \bar{p}_m$, which interlace with those of $Q(x)$, and $\bar{P}(x)$ and $Q(x)$ have at least one zero in common. Furthermore, since $\bar{P}'(x) = P'(x)$ we have

$$\bar{R}(z) = (\bar{P}/Q)'(z) = R(z) + \frac{\epsilon Q'(z)}{Q^2(z)} \geq 0;$$

Before we divide $\bar{P}(x)$ and $Q(x)$ by the factors that they have in common, note that $\bar{P}$ cannot equal Q because in this case we would have $P(x) = Q(x) + \epsilon$, which contradicts the interlacing property for $n > 1$. Now let $\tilde{P}(x)$ and $\tilde{Q}(x)$ denote the polynomials obtained by dividing $\bar{P}(x)$ and $Q(x)$ by their greatest common denominator. These polynomials still have the interlacing property, are of degree smaller than n and are not equal. For the corresponding ratio we find

$$\hat{R}(z) = (\tilde{P}/\tilde{Q})'(z) = (\bar{P}/Q)'(z) = \bar{R}(z) \geq 0$$

which contradicts the assumption that the pair (P, Q) forms a counterexample of minimal degree. □

Theorem 5.2 *Consider two polynomials* $Q(x) = \prod_{i=1}^{n}(x - q_i)$*, and* $P(x) = \prod_{i=1}^{m}(x - p_i)$*, of degree* n *and* m*, where* $m \leq n \leq m+1$*, the roots* $q_1 > \cdots > q_n$*,* $p_1 > \cdots > p_m$*, fulfil condition (5.1) and* $P \neq Q$*. Then the zeros of* $q'_1 > \cdots > q'_{n-1}$ *and* $p'_1 > \cdots > p'_{m-1}$*, the derivatives* $Q'(x)$ *and* $P'(x)$ *satisfy*

$$q'_i > p'_i > q'_{i+1} \quad \text{for } i = 1, \ldots, m-1$$

(here q'_n *id defined as* $q'_n = -\infty$*). In other words, if the polynomials* $P \neq Q$ *have only simple roots, which interlace, then the roots of their derivatives strictly interlace.*

Proof. We first consider the case where the polynomial $P(x)$ has degree $m = n - 1$. From Lemma 5.1 for $i = 1, \ldots, n-1$

$$0 > R(q'_i) = \left(\frac{P}{Q}\right)'(q'_i) = \frac{P'(q'_i)Q(q'_i) - P(q'_i)Q'(q'_i)}{Q(q'_i)^2} = \frac{P'(q'_i)}{Q(q'_i)}.$$

Since the denominator alternates in sign (the roots of Q' interlace with those of Q) and the leading coefficient is 1 it follows that $\operatorname{sign}(Q(q'_i)) = (-1)^i$. This implies that the numerator must also alternate in sign, i.e.

$$\operatorname{sign}(P'(q'_i)) = (-1)\operatorname{sign}(P'(q'_{i+1})) = (-1)^{i-1} \quad (i = 1, \ldots, n-2)\ .$$

This means that between any pair of consecutive roots q'_i, q'_{i+1} of $Q'(x)$ there is a root of $P'(x)$, which proves the Theorem 5.2 for $n = m + 1$.
If both polynomials $P(x)$ and $Q(x)$ have the same degree m, note that

$$\lim_{x \to -\infty} \operatorname{sign}(P'(x)) = (-1)^{m-1} = (-1)P'(q'_{m-1})\ .$$

Consequently, $P'(x)$ also has a root in the interval $(-\infty, q'_{m-1})$, which completes the proof of Theorem 5.2 . ☐

Proof of Lemma 4.3. Without loss of generality we assume that the leading coefficients of the polynomial P_1 and P_2 are equal to 1. With the notation

$$\begin{aligned} P(x) = P_2(x),\ Q(x) = P_1(x) \\ p_i = t_{(n-i+1,2)}, i = 1. \ldots, n \\ q_i = t_{(n-i+1,1)}, i = 1. \ldots, n \end{aligned}$$

the proposition of Lemma 4.3 follows from Theorem 5.2. ☐

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