Optimal designs for estimating individual coefficients in polynomial regression — a functional approach

Holger Dette
Ruhr-Universität Bochum
Fakultät für Mathematik
44780 Bochum
Germany
email: holger.dette@ruhr-uni-bochum.de
FAX: +49 2 34 70 94 559

Viatcheslav B. Melas
St. Petersburg State University
Department of Mathematics
St. Petersburg
Russia
email: v.melas@pobox.spbu.ru

Andrey Pepelyshev
St. Petersburg State University
Department of Mathematics
St. Petersburg
Russia
email: andrey@ap7236.spbu.edu

December 19, 2000

Abstract

In this paper the optimal design problem for the estimation of the individual coefficients in a polynomial regression on an arbitrary interval $[a,b](-\infty < a < b < \infty)$ is considered. Recently, Sahm (2000) demonstrated that the optimal design is one of four types depending on the symmetry parameter $s = (a+b)/(a-b)$ and the specific coefficient which has to be estimated. In the same paper the optimal design was identified explicitly in three cases. It is the basic purpose of the present paper to study the remaining open fourth case. It will be proved that in this case the support points and weights are real analytic functions of the boundary points of the design space. This result is used to provide a Taylor expansion for the weights and support points as functions of the parameters a and b, which can easily be used for the numerical calculation of the optimal designs in all cases, which were not treated by Sahm (2000).

1991 AMS Subject Classification: Primary 62K05, Secondary 41A10
Key words and phrases: polynomial regression, c-optimal design, implicit function theorem, extremal polynomial, estimation of individual coefficients

1 Introduction

Consider the common polynomial regression model with homoscedastic error

$$(1.1)\qquad \begin{aligned} E[Y(t)] &= \sum_{i=0}^{d} \beta_i t^i = f^T(t)\beta, \\ V[Y(t)] &= \sigma^2 > 0, \end{aligned}$$

where the explanatory variable t varies in a compact interval, say $[a, b](-\infty < a < b < \infty)$, $\beta = (\beta_0, \dots, \beta_d)^T$ is the vector of unknown parameters, $f(t) = (1, t, \dots, t^d)^T$ is the vector of regression functions and different observations are assumed to be uncorrelated. An approximate design is a probability measure on the interval $[a, b]$ with finite support [see e.g. Kiefer (1974)]

$$\xi = \begin{pmatrix} t_1, \dots, t_n \\ w_1, \dots, w_n \end{pmatrix}$$

where the support points $t_1, \dots, t_n$ give the positions in the interval $[a, b]$ at which observations are taken and the weights give the relative proportions of total observations taken at the corresponding support points. An optimal design minimizes (or maximizes) a specific convex (or convave) function of the information matrix

$$(1.2)\qquad M(\xi) = \int_a^b f(t) f^T(t) d\xi(t)$$

and there are numerous optimality criteria proposed in the literature, which can be used for the determination of efficient designs [see e.g. Silvey (1980) or Pukelsheim (1993)].
In this paper we are studying the optimal designs minimizing the variance of the least squares estimator for the individual coefficients in the model (1.1), a special case of c-optimality [see e.g. Pukelsheim (1993), Chapter 2]. To be precise let $e_k \in \mathbb{R}^{d+1}$ denote the $(k+1)$th unit vector, then a design ξ is called e_k-optimal or optimal for estimating the kth coefficient β_k in the polynomial regression (1.1) if $\beta_k = e_k^T \beta$ is estimable by ξ [i.e. $e_k \in \text{Range}(M(\xi))$] and ξ minimizes the function

$$(1.3)\qquad \Phi_k(\xi) = e_k^T M^-(\xi) e_k$$

where A^- denotes a generalized inverse of the matrix A. The problem of determining e_k-optimal designs in polynomial regression has been considered by many authors mainly concentrating on the interval $[-1, 1]$ [see e.g. Studden (1968), Kiefer and Wolfowitz (1959) or Hoel and Levine (1964)]. It is well known that in contrast to the famous D-optimality criterion the problem of minimizing the criterion (1.3) is not scale invariant and the solution of the optimal design of the experiment for estimating the individual coefficients in polynomial regression on arbitrary intervals was open for a long time.
Recently, Sahm (2000) made substantial progress and showed that the optimal design for estimating an individual coefficient is essentially of one of four types. The specific type depends on the location of the parameter

$$(1.4)\qquad s = s(b) = \frac{a+b}{a-b} \in \mathbb{R}$$

and the optimal design can be determined explicitly in three cases. In the remaining case an explicit solution of e_k-optimal design problem seems to be intractable, even numerically [see Sahm (2000)].

It is the purpose of the present paper to study this open problem in more detail. Section 2 gives a brief review of Sahm's (2000) results, which is the basis for our approach. In Section 3 we deal with the remaining open cases, which can be described by $d-k$ intervals for the parameter s in (1.4). We consider the weights and support points of the e_k-optimal design as functions of the boundary points of the design space. Implementing a technique similar as in Melas (1978, 2000) we introduce a differential equation for these functions, which is used to prove that the weights and support points are real analytic functions of the bounds of the design space. These results are used to derive in each of the $d-k$ intervals a Taylor expansion for the weights and support points of the optimal design using a specific point for which the solution is known. We derive recursion formulas for the coefficients of this expansion which can be easily used to determine the e_k-optimal design numerically in all remaining open cases. Finally the applicability of our approach is demonstrated by several examples in Section 4.

2 e_k-optimal designs

In this section we briefly review the known results about e_k-optimal designs which form the basis for our analytic approach in the following section. Because the case $k=0$ (estimation fo the intercept) and $k=d$ (estimation of the highest coefficient) are well know [see e.g. Sahm (2000) of Studden (1980a)] we restrict ourselves to the case $1 \leq k \leq d-1$. Sahm (2000) introduced the sets

$$\begin{aligned} A_i &= (-\nu_{d-k+1-i}, \nu_{i+1}) \quad & i = 0, \ldots, d-k \\ B_{1,i} = -B_{2,i} &= [\nu_i, \rho_i] \quad & i = 1, \ldots, d-k \\ C_i &= (\rho_i, -\rho_{d-k+1-i}) \quad & i = 1, \ldots, d-k \end{aligned} \tag{2.1}$$

where $\nu_{d-k+1} = \infty$ and $\nu_1, \ldots, \nu_{d-k}$ are the roots of the k-th derivative of the polynomial

$$(x+1)U_{d-1}(x) \tag{2.2}$$

and $U_j(x) = \sin((j+1)\arccos x)/\sin(\arccos x)$ is the j-th Chebyshev polynomial of the second kind. The points ρ_i are obtained from these roots via the transformation

$$\rho_i = \nu_i + (1+\nu_i)\frac{1-\cos(\pi/d)}{1+\cos(\pi/d)}.$$

Note that the union of these sets defines a partition of the real axis and Sahm (2000) proved that the location of the parameter s defined in (1.1) determines the structure of the optimal design as follows. If

$$s \in \bigcup_{i=0}^{d-k} A_i$$

the e_k-optimal design is supported at $d+1$ points including the boundary points a and b. If

$$s \in \bigcup_{i=0}^{d-k} B_{1,i}$$

the optimal design for estimating the parameter β_k is supported at d points including the boundary point a and the case

$$s \in \bigcup_{i=1}^{d-k} B_{2,i}$$

is essentially obtained by symmetry arguments interchanging the role of a and b. In these cases the e_k-optimal design can be described explicitly in terms of transformed Chebyshev points $t_j = \cos(\pi_j/d)$ and we refer to Sahm (2000),Theorem 3.2 for more details. In the remaining case

$$s \in \bigcup_{i=1}^{d-k} C_i \tag{2.3}$$

the situation is substantially more difficult. Here the design is supported at d points including both boundary points of the design space but an explicit representation of the weights and support points is not available. Sahm (2000) characterized the solution for this case by a constrained optimization problem, which is difficult to use for the numerical construction of the optimal design. Additionally he proved the existence of points

$$\mu_i \in C_i \qquad i = 1, \ldots, d-k, \tag{2.4}$$

for which the solution of the design problem can be found explicitly. The points μ_i are the zeros of the k-th derivative of the polynomial

$$(x^2 - 1)U_{d-2}(x) \tag{2.5}$$

and for $s = \mu_i$ the e_k-optimal design is obtained as the optimal design for estimating β_k in a polynomial regression of degree $d-1$ where the case $s \in \cup_{i=0}^{d-k-1} A_i$ is applicable [see Section 3 for more details]. In the next section we will propose an analytic approach which allows the (numerical) determination in all cases specified by (2.3) and therefore closes the final gap in the solution of the e_k-optimal design problem on arbitrary intervals.

3 Analytical properties of e_k-optimal designs

Throughout this section we restrict ourselves to the (unsolved) case (2.3), for which Sahm (2000) showed that the optimal design is of the form

$$\xi_k^* = \begin{pmatrix} a, t_2^*, \ldots, t_{d-1}^*, b \\ \omega_1^*, \omega_2^*, \ldots, \omega_{d-1}^*, \omega_d^* \end{pmatrix}. \tag{3.1}$$

If a is fixed and we vary b such that (2.3) is satisfied the weights and support points in (3.1) are functions of the right boundary point b, i.e. $t_j^* = t_j^*(b)$, $j = 2, \ldots, d-1$,

$w_j^* = w_j^*(b)$, $j = 1, \dots, d$. We collect the information given by the e_k-optimal design ξ_k^* in the vector

$$\tau^* = \tau^*(b) = (t_2^*(b), \dots, t_{d-1}^*(b), w_2^*(b), \dots, w_d^*(b)) \tag{3.2}$$

and note that this function is well defined due to the uniqueness of the e_k-optimal design ξ_k^* in (3.1) for $1 \le k \le d$ [see Sahm (2000), Lemma 2.5]. Note that formally the optimality criterion (1.3) could be considered as a function of nontrivial weights and support points

$$\tau = (t_2, \dots, t_{d-1}, w_2, \dots, w_d), \tag{3.3}$$

where the points t_i and w_i correspond to the support points and weights of a design of the form (3.1), and the optimal design is implicitly determined as a solution of the equations

$$\frac{\partial}{\partial \tau} \Phi_k = 0.$$

However, a direct differentiation of the optimality criterion with respect to support points and weights seems to be intractable due to the nonsingularity of the corresponding information matrix of the d-point design. In order to circumvent this problem we will relate the design problem to a dual extremal problem for polynomials. This duality is used to derive a necessary and sufficient condition for the parameters of the design and the coefficients of the extremal polynomial by differentiating an appropriate function. We begin with a slightly different formulation of the equivalence theorem for e_k-optimal designs as it is usually stated in the literatur [see e.g. Pukelsheim (1993)].

Lemma 3.1. *Let $f_k(t) = (1, t, \dots, t^{k-1}, t^{k+1}, \dots, t^d)^T$ denote the vector obtained from $f(t) = (1, t, \dots, t^d)^T$ by omitting the monomial t^k. A design ξ_k^* is e_k-optimal on the interval $[a, b]$ if and only if there exist a positive number h_k and a vector $q^* \in \mathbb{R}^d$ such that the polynomial $\varphi_k(t) = t^k - f_k^T(t) q^*$ satisfies the following conditions*

(1) $h_k \varphi_k^2(t) \le 1 \quad \forall\, t \in [a, b]$

(2) $supp(\xi_k^*) \subset \{t \in [a, b] \mid h_k \varphi_k^2(t) = 1\}$

(3) $\int \varphi_k(t) f_k(t) d\xi_k^*(t) = 0 \in \mathbb{R}^d$.

Moreover, in this case $h_k = \Phi_k(\xi_k^*)$.

Proof. Let ξ_k^* denote the optimal design for estimating β_k and q^* denote the solution of the generalized Chebyshev problem

$$\inf_{q \in \mathbb{R}^d} \sup_{x \in [a,b]} |x^k - f_k^T(x) q|, \tag{3.4}$$

then we obtain

$$h = e_k^T M^-(\xi_k^*) e_k \;=\; \inf_{\xi} \sup_{d \in \mathbb{R}^{d+1}} \frac{e_k^T d}{d^T M(\xi) d}$$

$$
\begin{aligned}
&= \Big\{ \inf_{d^T e_k = 1} \sup_{\xi} \int_a^b |d^T f(t)|^2 d\xi(t) \Big\}^{-1} \\
(3.5) \qquad & \\
&= \{ \inf_{q \in \mathbb{R}^d} \sup_{t \in [a,b]} |t^k - f_k^T(t) q|^2 \}^{-1} \\
&= \{ \sup_{t \in [a,b]} |t^k - f_k^T(t) q^*|^2 \}^{-1}
\end{aligned}
$$

If ξ_k^* is optimal for estimating the parameter β_k we define $\varphi_k(t) = t^k - f_k^T(t)q^*$ which obviously satisfies (1). The inclusion (2) follows by discussing equality in the fourth equation of (3.5), which means that the L^2-norm is equal to the sup-norm if and only if the support of ξ_k^* is contained in the set of extreme points of the optimal polynomial $\varphi_k(t)$. In order to show (3) we discuss the equality in the first equation of (3.5) which is a simple consequence of Cauchy's inequality. For a d-dimensional vector q let d_q denote a $(d+1)$-dimensional vector with $(k+1)$th component equal to one where the vector $-q$ is obtained from d_q by omitting this component i.e. $d_q^T f(t) = t^k - q^T f_k(t)$. Discussing equality in Cauchy's inequality yields

$$
\begin{aligned}
e_k = M(\xi_k^*) d_{q^*} &= \int_a^b f(t)(f^T(t) d_{q^*}) d\xi_k^*(t) \\
&= \int_a^b f(t) \varphi_k(t) d\xi_k^*(t)
\end{aligned}
$$

which implies (3). On the other hand, if ξ_k^* and q^* satisfy conditions (1) - (3) of Lemma 3.1, the same calculations show that we have found a saddle point (ξ_k^*, q^*) such that there is equality in

$$
(3.6) \qquad \inf_{\xi} e_k^t M^-(\xi) e_k = \{ \inf_{q \in \mathbb{R}^d} \sup_{t \in [a,b]} |t^k - f_k^T(t) q|^2 \}^{-1}
$$

which establishes optimality of ξ_k^* for the e_k-optimal design problem and optimality of the vector q^* for the extremal problem (3.4).

□

Note that Lemma 3.1 (and its proof) relate the optimal design problem to an extremal problem for polynomials [see e.g. Karlin and Studden (1966), Section 10.8, or Studden (1980b)]. Moreover, the solution of the extremal problem (3.3) is unique, because the optimal polynomial $\rho_k(x) = x^k - f_k^T(x)q^*$ must attain its extremal values at the support points of the e_k-optimal design ξ_k^*, which is unique, whenever $1 \leq k \leq d$. In the following we will solve both problems simultaneously. To this and let

$$
(3.7) \quad T = \Big\{ (t_2, \ldots, t_{d-1}, \omega_2, \ldots, \omega_d)^T \mid a < t_1 < \ldots < t_{d-1} < b; \quad \omega_i > 0; \sum_{j=2}^d \omega_j < 1 \Big\},
$$

define for any $\tau \in T$ the design ξ_τ by

$$
(3.8) \qquad \xi_\tau = \begin{pmatrix} a, t_2, \ldots, t_{d-1}, b \\ \omega_1, \omega_2, \ldots, \omega_{d-1}, \omega_d \end{pmatrix} ,
$$

where $\omega_1 = 1 - \sum_{j=2}^{d} \omega_j$, and recall the definition of the vector $d_q \in \mathbb{R}^{d+1}$ for $q \in \mathbb{R}^d$ introduced in the proof of Lemma 3.1, i.e.

$$f^T(t) d_q = t^k - f_k^T(t) q \quad (q \in \mathbb{R}^d). \tag{3.9}$$

It follows from the proof of Lemma 3.1 that

$$\Phi_k(\xi_\tau) = \Big\{ \min_{q \in \mathbb{R}^d} \Psi(q, \tau, b) \Big\}^{-1} \tag{3.10}$$

for any $\tau \in T$, where

$$\Psi(q, \tau, b) = d_q^T M(\xi_\tau) d_q, \tag{3.11}$$

and the optimal design ξ_{τ^*} satisfies

$$\Psi^{-1}(q^*, \tau^*, b) = \min_{\tau \in T} \max_{q \in \mathbb{R}^d} \Psi^{-1}(q, \tau, b) = \max_{q \in \mathbb{R}^d} \min_{\tau \in T} \Psi^{-1}(q, \tau, b), \tag{3.12}$$

where q^* is the optimal solution of the extremal problem. Note that formally the minimum has to be taken over the set of all vectors $\tau \in T$ such that e_k is estimable by the design ξ_τ, i.e. $e_k \in \text{Range}(M(\xi_\tau))$. However, it is straightforward to see that in the case $e_k \notin \text{Range}(M(\xi_\tau))$ we have

$$\max_{q \in \mathbb{R}^d} \Psi^{-1}(q, \tau, b) = \infty$$

[see also Studden (1968)]. Consequently the optimization over the slightly bigger set T in (3.7) will yield a solution τ^*, q^* such that e_k is estimable by the design ξ_{τ^*}, even if this restriction is not incorporated in the definition of the set T. This observation will be crucial throughout the following discussion.

Lemma 3.2. *The design ξ_{τ^*} is e_k-optimal and the vector q^* corresponds to the solution of the generalized Chebyshev problem (3.4) if and only if the point $(q^*, \tau^*) \in \mathbb{R}^d \times T$ is the unique solution of the system*

$$\begin{aligned} \frac{\partial}{\partial \tau} \Psi(q, \tau, b) &= 0 \\ \frac{\partial}{\partial q} \Psi(q, \tau, b) &= 0 \end{aligned} \tag{3.13}$$

in the set of all pairs $(q, \tau) \in \mathbb{R}^d \times T$ such that e_k is estimable by the design ξ_τ and such that

$$|d_q^T f(t)|^2 = |t^k - q^T f_k(t)|^2 \le d_q^T M(\xi_\tau) d_q \qquad \text{for all } t \in [a, b].$$

Here $\frac{\partial}{\partial \tau}\Psi$ and $\frac{\partial}{\partial q}\Psi$ denote the gradient of Ψ with respect to $\tau \in T$ and $q \in \mathbb{R}^d$, respectively.

Proof. The necessary part follows directly from the known conditions for an extremum, the representation (3.12) and the fact that the solution of the design problem and extremal problem are unique. In order to prove sufficiency we note that it follows by a direct calculation from (3.13)

(i) $(M(\xi_\tau)d_q)_- = 0$

(ii) $(d_q^T f(t_i))^2 = (d_q^T f(a))^2 \quad i = 2, \dots, d$

(iii) $d_q^T f(t_i) \cdot d_q^T f'(t_i) = 0 \quad i = 2, \dots, d-1$

where $t_d = b$ and for $c \in \mathbb{R}^{d+1}$ the vector $c_- \in \mathbb{R}^d$ is obtained from c by deleting the $(k+1)$th component. Now let (q^*, τ^*) denote a solution of the system (i) — (iii) (obtained from (3.13)) such that $e_k \in$ Range$(M(\xi_{\tau^*}))$ and

$$|d_{q^*} f(t)| \leq d_{q^*} M(\xi_{\tau^*}) d_{q^*}$$

for all $t \in [a, b]$. Define $\delta = d_{q^*}^T f(a)$. Note that by condition (ii)

$$\delta^2 = d_{q^*}^T M(\xi_{\tau^*}) d_{q^*} \neq 0,$$

because otherwise this would yield $M(\xi_{\tau^*})d_{q^*} = 0$ which implies by identity (i) $M(\xi_{\tau^*})e_k = 0$ contradicting to the estimability of β_k by the design ξ_{τ^*}. Observing the identity (ii) we find that $\varphi(t) = d_{q^*}^T f(t)$ is a polynomial of degree d such that

$$|\varphi(t)|^2 \leq \delta^2 \quad \forall\ t \in [a, b].$$

Defining $h = 1/\delta$ we have identified a triple (h, q^*, φ) such that the condition (1) of Lemma 3.1 is satisfied. Condition (2) of this Lemma is obvious from the construction of the polynomial φ and the third condition follows from (i) which implies

$$\begin{aligned} 0 \ &= \ (M(\xi_\tau)d_{q^*})_- = \Big(\sum_{i=1}^{d} w_i f(t_i) f^T(t_i) d_{q^*}\Big)_- \\ &= \ \Big(\int_a^b f(t)\varphi(t) d\xi_\tau(t)\Big)_- = \int_a^b f_k(t)\varphi(t) d\xi_\tau(t). \end{aligned}$$

Therefore Lemma 3.1 and its proof show that the design $\xi_{\tau*}$ is the e_k-optimal design and that the vector q^* corresponds to a solution of the generalized Chebyshev problem.

□

Note that Lemma 3.2 generates a vector differential equation, which implicitly determines τ^*, q^* as vector valued function of the boundary point b such that (2.3) is satisfied (where the left boundary of the design space has been fixed). In the following discussion we will show that the Jacobian matrix of the equation (3.13) is nonsingular, which allows the application of the implicit function theorem to study the functions $\tau^*(b)$ and $q^*(b)$ as analytic functions of the right boundary b such that (2.3) is satisfied. To this end define

$$\begin{aligned} \Theta \ &= \ (\Theta_1, \dots \Theta_{3(d-1)}) = (q^T, \tau^T), \\ \Theta^*(b) \ &= \ (q^{*T}(b), \tau^{*T}(b)) \end{aligned} \tag{3.14}$$

as the vector containing the parameters of the e_k-optimal design and the coefficients of the solution of the corresponding Chebyshev problem and

$$\bar{\Psi}(\Theta, b) = \Psi(q, \tau, b),$$

then the basic equation (3.13) can be rewritten as

$$\frac{\partial}{\partial \Theta} \bar{\Psi}(\Theta, b) = 0 \in \mathbb{R}^{3(d-1)}. \tag{3.15}$$

Finally, if U denotes an open set in $\mathbb{R}^n$, we call a function $f : U \to \mathbb{R}$ real analytic if for any point $u_0 \in U$ there exists a neighbourhood $U_0 \subset U$ of u_0 such that $f|_{U_0}$ can be expanded in a convergent Taylor series.

Theorem 3.3. *For any fixed $a \in \mathbb{R}$ define $s(b) = (a+b)/(a-b)$ and $B_i = s^{-1}(C_i)$ the components of the function*

$$\Theta^* : \begin{cases} \bigcup_{i=1}^{d-k} B_i & \to \mathbb{R}^{3(d-1)} \\ b & \to \Theta^*(b) \end{cases}$$

are real analytic functions. Moreover, the vector function Θ^* is a solution of the system

$$G(\Theta(b), b) \cdot \Theta'(b) = Q(\Theta(b), b) \tag{3.16}$$

with initial conditions

$$\Theta(b_0) = \Theta^*(b_0), \tag{3.17}$$

where b_0 is any arbitrary point such that (2.3) is satisfied for $s_0 = s(b_0)$ and the functions G and Q are defined by

$$G(\Theta, b) = \Big(\frac{\partial^2}{\partial \Theta_i \partial \Theta_j} \bar{\Psi}(\Theta, b) \Big)_{i,j=1}^{3(d-1)} \tag{3.18}$$

$$Q(\Theta, b) = \Big(\frac{\partial^2}{\partial b \partial \Theta_i} \bar{\Psi}(\Theta, b) \Big)_{i=1}^{3(d-1)}. \tag{3.19}$$

Proof. We will prove that the Jacobi matrix

$$J(b) = G(\Theta^*(b), b) \in \mathbb{R}^{3(d-1) \times 3(d-1)} \tag{3.20}$$

is nonsingular. The assertion of Theorem 3.1 then follows by a straightforward application of the implicit function theorem [see e.g. Gunning and Rossi (1965)]. For this Jacobi matrix we obtain the representation

$$J = J(b) = 2 \begin{pmatrix} D & B_1^T & B_2^T \\ B_1 & E & 0 \\ B_2 & 0 & 0 \end{pmatrix}_{-} \tag{3.21}$$

where A_{-} denotes the $3(d-1) \times 3(d-1)$ matrix obtained from $A \in \mathbb{R}^{(3d-2) \times (3d-2)}$ by deleting the $(k+1)$th row and $(k+1)$th column. The matrices D, B_1, B_2 and E in (3.21) are defined as follows ($t_1^* = a, t_d^* = b$)

$$
\begin{aligned}
D &= M(\xi_{\tau^*}) \in \mathbb{R}^{d+1\times d+1} \\
B_1^T &= \Big(w_2^* f'(t_2^*) \cdot d_{q^*}^T f(t_2^*), \ldots, w_{d-1}^* f'(t_{d-1}^*) \cdot d_{q^*}^T f(t_{d-1}^*) \Big) \\
&= \Delta \Phi^{-1/2}(\xi_{\tau^*}) \cdot \Big(w_2^* f(t_2^*), -w_3^* f(t_3^*), \ldots, (-1)^{d-1} w_{d-1}^* f'(t_{d-1}^*) \Big) \in \mathbb{R}^{d+1\times d-2} \\
&\quad (3.22) \\
B_2^T &= \Big(d_{q^*}^T f(t_2^*) \cdot \{ f(t_2^*) - f(t_1^*) \}, \ldots, d_{q^*}^T f(t_d^*) \cdot \{ f(t_d^*) - f(t_1^*) \} \Big) \\
&= \Delta \Phi^{-1/2}(\xi_{\tau^*}) \cdot \Big(f(t_2^*) - f(t_1^*), (-1)\{ f(t_3^*) - f(t_1^*) \} \}, \ldots, (-1)^d \{ f(t_d^*) - f(t_1^*) \} \Big) \in \mathbb{R}^{d+1\times d-1} \\
E &= \operatorname{diag}\Big(w_2^* d_{q^*}^T f(t_2^*) \cdot d_{q^*}^T f''(t_2^*), \ldots, w_{d-1}^* d_q^* f(t_{d-1}^*) \cdot d_q^* f''(t_{d-1}^*) \Big) \\
&= \operatorname{diag}\Big(w_2^* \varphi''(t_2^*) \varphi(t_2^*), w_3^* \varphi''(t_3^*) \varphi(t_3^*), \ldots, w_{d-1}^* \varphi''(t_{d-1}^*) \varphi(t_{d-1}^*) \Big) \in \mathbb{R}^{d-2\times d-2}
\end{aligned}
$$

where $\Delta \in \{-1, 1\}$ is a fixed constant and the polynomials φ is defined by $\varphi(t) = d_{q^*}^T f(t)$ (all other entries in the matrix J are 0). The Jacobi matrix J in (3.21) is essentially obtained by direct differentiation and the properties of the extremal polynomial $\varphi(t) = d_{q^*}^T f(t)$. For example, consider the calculation of B_1^T and let $I_- \in \mathbb{R}^{d+1\times d}$ denote the identity matrix with deleted $(k+1)$th column. We obtain by straightforward calculation

$$
\begin{aligned}
\frac{\partial^2 \Psi}{\partial t \partial q} &= \frac{\partial}{\partial t} 2 I_-^T M(\xi_\tau) dq \\
&= 2 I_-^T \cdot \Big(w_{j+1} d_q^T f'(t_{j+1}) \cdot f(t_{j+1}) + w_{j+1} d_q^T f(t_{j+1}) \cdot f'(t_{j+1}) \Big)_{j=1}^{d-2} \in \mathbb{R}^{d\times d-2}.
\end{aligned}
$$

Now for $q = q^*$ we have $\varphi(t_j^*) = d_{q^*}^T f(t_j^*) = \Delta(-1)^j \Phi^{-1/2}(\xi_{\tau^*})$ $(j = 2, \ldots, d)$ for some $\Delta \in \{-1, 1\}$. This follows from Lemma 3.1 which shows that φ is equioscillating which implies $\varphi'(t_j^*) = d_{q^*}^T f'(t_j^*) = 0$. Consequently we obtain

$$
B_1^T = \frac{2 \cdot \Delta}{\Phi_k^{1/2}(\xi_{\tau^*})} \Big((-1)^{j+1} w_{j+1}^* f'(t_{j+1}^*) \Big)_{j=1}^{d-2}
$$

which proves the representation of the block B_1^T in (3.21). The other cases are treated similary and left to the reader.

On the basis of the representation (3.21) the proof of the nonsingularity of the Jacobi matrix $J(b)$ is straightforward. Note that the matrix D_- is nonnegative definite, because it is obtained from the nonnegative definite matrix $M(\xi_{\tau^*})$ by deleting the $(k+1)$th row and column. Similary, the matrix E defined in (3.22) is negative definite, which follows, because it essentially contains the second derivatives $\varphi''(t_i)$ $(i = 2, \ldots, d-1)$ of the extremal polynomial $\varphi(t) = t^k - f_k^T(t) q^*$ specified in Lemma 3.1. To be precise we note that the results of Theorem 4.3 in Sahm (2000) show that for the case $b = \mu_i$ this polynomial is of degree $d-1$ while in the case $b \in C_i \backslash \{\mu_i\}$ the polynomial is of degree d with one extremum outside the interval $[a, b]$. A careful counting of the multiplicities of the zeros of the polynomial $\varphi^2(t) - 1$ shows

$$
\varphi''(t_i) = d_{q^*}^T f''(t_i) \neq 0 \quad i = 2, \ldots, d-1. \tag{3.23}
$$

Moreover, by the oscillating property of the extremal polynomial the second derivative must alternate in sign yielding $\varphi''(t_i)\varphi(t_i) < 0 \quad (i = 2, \dots, d-1)$ and the definition of the matrix E in (3.22) shows that this matrix has negative diagonal elements.
From these auxiliary results it follows that the matrix

$$D_- - \tilde{B}_1^T E^{-1} \tilde{B}_1$$

is positive definite where $\tilde{B}_1^T$ denotes the matrix obtained from B_1^T by deleting the $(k+1)$th row. Similary, let $\tilde{B}_2^T$ obtained from B_2^T by deleting the $(k+1)$th row, then it follows by the Frobenius formula and the representation (3.21)

$$\begin{aligned}
\det J(b) &= \det \begin{pmatrix} D_- & \tilde{B}_1^T & \tilde{B}_2^T \\ \tilde{B}_1 & E & 0 \\ \tilde{B}_2 & 0 & 0 \end{pmatrix} \\
&= -\det \begin{pmatrix} D_- & \tilde{B}_1^T \\ \tilde{B}_1 & E \end{pmatrix} \cdot \det\Big\{ (\tilde{B}_2 \mid 0) \begin{pmatrix} D_- & \tilde{B}_1^T \\ \tilde{B}_1 & E \end{pmatrix}^{-1} \begin{pmatrix} \tilde{B}_2^T \\ 0 \end{pmatrix} \Big\} \\
&= -\det E \cdot \det(D_- - \tilde{B}_1^T E^{-1} \tilde{B}_1) \cdot \det\{ \tilde{B}_2 (D_- - \tilde{B}_1^T E^{-1} \tilde{B}_1)^{-1} \tilde{B}_2^T \}.
\end{aligned} \tag{3.24}$$

Now the matrix $\tilde{B}_2^T$ is of rank $d-1$ (because of the Chebyshev property of the polynomials $1, x, \dots, x^d$) and the matrix $D_- - \tilde{B}_1^T E^{-1} \tilde{B}_1$ is positive definite by the preceding discussion. Consequently all determinants in (3.24) are different from zero which proves the nonsingularity of the Jacobi matrix $J(b)$.

□

Theorem 3.4. *Let $b_0 \in B_i = s^{-1}(C_i)$ for some $i = 1, \dots, d-k$, and Θ^* be the function defined in Theorem 3.3, then the coefficients in the Taylor expansion*

$$\Theta^*(b) = \Theta^*(b_0) + \sum_{j=1}^{\infty} \Theta^*(j, b_0)(b - b_0)^j$$

in a neighbourhood of the point b_0 can be obtained recursively by the formulas

$$\Theta^*(s+1, b_0) = -J^{-1}(b_0) (\frac{d}{db})^{s+1} g(\Theta^*_{(s)}(b), b) \Big|_{b=b_0} \qquad s = 0, 1, 2, \dots \tag{3.25}$$

where the polynomial $\Theta^*_{(s)}$ of degree s is defined by

$$\Theta^*_{(s)}(b) = \Theta^*(b_0) + \sum_{j=1}^{s} \Theta^*(j, b_0)(b - b_0)^j$$

and the function g is given by

$$g(\Theta, b) = \frac{\partial}{\partial \Theta} \bar{\Psi}(\Theta, b) \mid_{\Theta = \tilde{\Theta}} . \tag{3.26}$$

Proof. By Theorem 3.3 the function $\Theta^* : \cup_{i=1}^{d-k} B_i \to \mathbb{R}^{3(d-1)}$ has real analytic components and its Taylor expansion exists locally for any $b_0 \in \cup_{i=1}^{d-k} B_i$. Note that

$$\frac{d}{db} g(\Theta^*(b), b) = \frac{\partial}{\partial \Theta} g(\Theta, b)\Big|_{\Theta=\Theta^*(b)} \cdot \Theta^{*'}(b) + \frac{\partial}{\partial b} g(\Theta, b)\Big|_{\Theta=\Theta^*(b)}$$

and a repeated application of this formula gives

$$\left(\frac{d}{db}\right)^{s+1} g(\Theta^*(b), b) = \frac{\partial}{\partial \Theta} g(\Theta, b)\Big|_{\Theta=\Theta^*(b)} \cdot \Theta^{*(s+1)}(b) + h_s(\Theta^*(b), b), \tag{3.27}$$

where $\Theta^{*(j)}$ denotes the jth derivative of the function Θ^* and the function h_s contains higher order derivatives of g with respect to Θ and derivatives of the function $\Theta^*(b)$ up to the order s. If

$$\Theta^*(b) = \sum_{j=0}^{\infty} \Theta^*(j, b_0)(b - b_0)^j \tag{3.28}$$

denotes the Taylor expansion of Θ at the point b_0 we obtain from (3.27) for $b \to b_0$

$$\begin{aligned} \left(\frac{d}{db}\right)^{s+1} g(\Theta^*(b), b)\Big|_{b=b_0} &= \frac{\partial}{\partial \Theta} g(\Theta, b_0)\Big|_{\Theta=\Theta^*(0,b_0)} \cdot (s+1)!\Theta^*(s+1, b_0) \\ &+ \tilde{h}_s(\Theta^*(0, b_0), \ldots, \Theta^*(s, b_0)), \end{aligned} \tag{3.29}$$

where the function $\tilde{h}_s$ depends only on the first $s+1$ coefficients $\Theta^*(0, b_0), \ldots, \Theta^*(s, b_0)$ of the Taylor expansion (3.28). If we use the polynomials

$$\Theta^*_{(k)}(b) := \Theta^*(b_0) + \sum_{j=1}^{k} \Theta^*(j, b_0)(b - b_0)^j$$

for $k = s+1$ and s in (3.29) we obtain

$$\begin{aligned} \left(\frac{d}{db}\right)^{s+1} g(\Theta^*(b), b)\Big|_{b=b_0} &= \left(\frac{d}{db}\right)^{s+1} g(\Theta^*_{(s+1)}(b), b)\Big|_{b=b_0} \\ = (s+1)!\Theta^*(s+1, b_0) \cdot \frac{\partial}{\partial \Theta} g(\Theta, b) &\ |_{\Theta=\Theta^*(0,b_0)} + \tilde{h}_s(\Theta^*(0, b_0), \ldots, \Theta^*(s, b_0)) \end{aligned}$$

(if $k = s+1$) and

$$\left(\frac{d}{db}\right)^{s+1} g(\Theta^*_{(s)}(b), b)\Big|_{b=b_0} = \tilde{h}_s(\Theta^*(0, b_0), \ldots, \Theta^*(s, b_0))$$

(if $k = s$), which gives

$$\begin{aligned} \left(\frac{d}{db}\right)^{s+1} g(\Theta^*(b), b)\Big|_{b=b_0} &= (s+1)!\Theta^*(s+1, b_0) \cdot \frac{\partial}{\partial \Theta} g(\Theta, b)\Big|_{\Theta=\Theta^*(0,b_0)} \\ &+ (\frac{d}{db})^{s+1} g(\Theta^*_{(s)}(b), b)) \ |_{b=b_0} . \end{aligned} \tag{3.30}$$

By Theorem 3.3 the solution $b \to \Theta^*(b)$ is real analytic and satisfies

$$g(\Theta^*(b), b) = 0,$$

in a neighbourhood of $b_0 \in B_i$ which follows from (3.15) and the definition of g in (3.26). Consequently the left hand side of (3.30) vanishes and we obtain

$$\begin{aligned} -\Big(\frac{d}{db}\Big)^{s+1} g(\Theta^*_{(s)}(b), b)\Big|_{b=b_0} &= (s+1)!\Theta^*(s+1, b_0) \cdot \frac{\partial}{\partial\Theta} g(\Theta, b)\Big|_{\Theta=\Theta^*(0,b_0)} \\ &= (s+1)!\Theta^*(s+1, b_0) \cdot J(b_0) \end{aligned}$$

where the last identity follows from the definition of J and g by (3.20) and (3.26), respectively. But this equation is equivalent to (3.25) which proves the assertion of Theorem 3.4.

□

Example 3.5. The recursion of Theorem 3.4 can be easily explained for a function $g : \mathbb{R}^2 \to \mathbb{R}$ (although this case does not appear in the solution of the design problem). Consider for example the problem

$$g(\Theta(b), b) = \sin b - \log \Theta(b),$$

where we illustrate the application of the recurrence relation deriving the Taylor expansion of the solution $\Theta(b) = e^{\sin b}$. Note that $J(0) = -1/\Theta(0) = -1$, because $g(\Theta(0), 0) = 0$ yields $\Theta(0) = 1$. For $s = 0$ we obtain from (3.25)

$$\Theta(1, 0) = \frac{d}{db} g(1, b)\Big|_{b=0} = \cos 0 = 1$$

while the recursion for $s = 1, 2, 3, 4, 5$ yields

$$\begin{aligned} \Theta(2, 0) &= \frac{1}{2!}\Big(\frac{d}{db}\Big)^2 g(1 + b, b)\Big|_{b=0} = \frac{1}{2} \\ \Theta(3, 0) &= \frac{1}{3!}\Big(\frac{d}{db}\Big)^3 g(1 + b + \frac{b^2}{2}, b)\Big|_{b=0} = 0 \\ \Theta(4, 0) &= \frac{1}{4!}\Big(\frac{d}{db}\Big)^4 g(1 + b + \frac{b^2}{2}, b)\Big|_{b=0} = -\frac{3}{4!} = -\frac{1}{8} \\ \Theta(5, 0) &= \frac{1}{5!}\Big(\frac{d}{db}\Big)^5 (g(1 + b + \frac{b^2}{2} - \frac{b^4}{8}, b)\Big|_{b=0} = -\frac{8}{5!} = -\frac{3}{15} \end{aligned}$$

for the first six coefficients of the Taylor expansion

$$e^{\sin b} = \sum_{j=0}^{\infty} \Theta(j, 0) b^j.$$

In general Theorem 3.3 and 3.4 show that for any b_0 such that (2.3) is satisfied the functions

$$\begin{aligned} t_j^* : b \to t_j^*(b) \quad & j = 2, \ldots, d-1 \\ w_j^* : b \to w_j^*(b) \quad & j = 2, \ldots, d \\ q_j^* : b \to q_j^*(b) \quad & j = 1, \ldots, d \end{aligned}$$

(here q_j^* denotes the jth component of the vector of coefficients q^* of the extremal polynomial) can be expanded into Taylor series in a neighbourhood of the point b_0. The coefficients of these expansions can be directly computed from the recurrence formulas (3.25) and therefore the remaining case in the optimal design problem for estimating the individual coefficients in a polynomial regression on an arbitrary interval can be easily solved numerically, if we are able to find a point b_0 such that (2.3) is satisfied and for which the solution of the e_k-optimal design problem is known. But such a point has been identified by Sahm (2000) who showed that there exist $d-k$ points

$$\mu_i = s(b_i) = \frac{a+b_i}{a-b_i} \in C_i \quad i = 1, \dots, d-k$$

such that the optimal design for estimating the parameter β_k is supported at the points at the d Chebyshev points

$$t_j^*(b_i) = \frac{b_i - a}{2}\Big\{\cos\big(\frac{j-1}{d-1}\pi\big) - \mu_i\Big\} \quad j = 1, \dots, d \tag{3.31}$$

with weights

$$w_j^*(b_i) = 2\gamma_{j-1} \frac{\sum_{\ell=0}^{k}(d-\ell-1)\gamma_\ell \cos\big(\frac{(j-1)\ell}{d-1}\pi\big) C_{k-\ell}^{(d-k-1)}(\mu_i)}{C_k^{(d-k-1)}(\mu_i)}, \quad j = 1, \dots, d \tag{3.32}$$

where $\gamma_0 = \gamma_{d-1} = 1/2(d-1); \gamma_j = 1/(d-1) \quad j = 1, \dots, d-2$ and $C_n^{(\lambda)}(x)$ denotes the nth ultraspherical polynomial [see e.g. Szegö (1959)]. Moreover, the points μ_i (or equivalently b_i) are determined as the zeros of the polynomial in (2.5). For this reason we are able to find in each interval $s^{-1}(C_i)$ a Taylor expansion for the weights and support points of the e_k-optimal design, which is based on the location $b_i = s^{-1}(\mu_i)$ $(i = 1, \dots, d-k)$. This technique provides a numerical solution for the open design problem and will be illustrated for the case $d-k$ in the following section.

4 A numerical example

Consider the case $d = 4$. We are interested in the estimation of the coefficient of β_1, β_2 and β_3 in the case which cannot be treated by the results of Sahm (2000). We concentrate ourselves on the case $a = -1$ and vary the parameter b, which corresponds to the situation considered in Section 3. The general case can be reduced to this case by an appropriate scaling of the symmetry parameter $s = s(b) = (a+b)/(a-b)$.

(a) If $k = 3$, we have one critical interval for the symmetry parameter s given by

$$C_1 = (\rho_1, -\rho_1) = (-0.1213, 0.1213),$$

and $\mu_1 = 0$, which corresponds in the b scale to the interval

$$B_1 = s^{-1}(C_1) = (0.7836, 1.2761) \tag{4.1}$$

and $b_1 = s^{-1}(0) = 1$. The first six coefficients in the Taylor expansion for the coefficients of the extremal polynomial, interior support poins and weights are listed in Table 4.1 and are calculated by the procedure described at the end of Section 3 using the recursive relation (3.25). For example, if $b = 1.2$ we obtain for the e_3-optimal design on the interval $[-1, 1.2]$

$$\xi_3^* = \begin{pmatrix} -1 & -0.595 & 0.395 & 1.2 \\ 0.239 & 0.412 & 0.261 & 0.088 \end{pmatrix}$$

and the extremal polynomial is given by

$$\varphi_3(t) = t^3 - 0.654t^4 + 0.685t^2 - 0.808t - 0.134.$$

Similary, the optimal design for estimating the coefficient of x^3 on the interval $[-1, 0.9]$ is given by

$$\xi_3^* = \begin{pmatrix} -1 & -0.406 & 0.506 & 0.9 \\ 0.121 & 0.290 & 0.379 & 0.210 \end{pmatrix}$$

and the extremal polynomial is

$$\varphi_3(t) = t^3 + 0.426t^4 - 0.333t^2 - 0.650t + 0.052.$$

– *insert Table 4.1 here* –

Figure 4.1 shows the interior support points (left figure) and weights in dependence of the parameter $b \in B_1$ which are obtained by the same reasoning. Note that the figure for the weights contains three lines, where two lines represent the weights $w_2^*(b)$ and $w_3^*(b)$ corresponding to the interior support points $t_2^*(b)$ and $t_3^*(b)$ and the third line corresponds to the weight $w_4^*(b)$ at the point b.

– *insert Figure 4.1a here* –

(b) If $k = 2$ we have two critical intervals for the symmetry parameter s given by

$$C_1 = (-0.5687, -0.1213); \quad C_2 = (0.1213, 0.5687)$$

and the specific points (where the solution is known) are $\mu_1 = -0.4564; \mu_2 = 0.4564$. This corresponds to the intervals

$$B_1 = s^{-1}(C_1) = (1.9677, 3.6374); \quad B_2 = s^{-1}(C_2) = (0.2749, 0.5082) \tag{4.2}$$

and the points $b_1 = s^{-1}(\mu_1) = 2.6794, b_2 = s^{-1}(\mu_2) = 0.3732$ for the parameter b, which can be used for the Taylor expansion in the respective intervals. The corresponding support points and weights are depicted in Figure 4.2a and 4.2b. For example, if $b = 2.2$ the optimal design for estimating the parameter β_2 on the interval $[-1, 2.2]$ is (approximately) obtained from Figure 4.2a as

$$\xi_2^* \approx \begin{pmatrix} -1 & 0.12 & 1.56 & 2.2 \\ 0.03 & 0.43 & 0.37 & 0.17 \end{pmatrix}$$

while the e_2-optimal design on the interval $[-1, 0.5]$ is approximately given by

$$\xi_2^* \approx \begin{pmatrix} -1 & -0.72 & 0.31 & 0.5 \\ 0.09 & 0.31 & 0.41 & 0.19 \end{pmatrix}$$

and obtained from Figure 4.2b (note that for $b = 1.5$ we have $s = 1/3$ which corresponds to the case $b \in B_2$).

– *insert Figure 4.2a and 4.2b here* –

Of course a better precision can be obtained by using a table of coefficients for the Taylor expansion of the weights and support points as a function of the parameter b as explained in the case $k = 1$. For the sake of completeness the first coefficients of the corresponding expansions are listed in Table 4.2a and 4.2b.

– *insert Table 4.2 a and 4.2b here* –

(c) If $k = 3$ the critical intervals for the symmetry parameter are given by

$$C_1 = (-0.8504, -0.6925); \quad C_2 = (-0.2060, 0.2060); \quad C_3 = (0.6925, 0.8504)$$

and the specific points (for which the solution is known) are $\mu_1 = 0.7906, \mu_2 = 0$ and $\mu_3 = 0.7906$, respectively. This gives in the b-scale the intervals

$B_1 = s^{-1}(C_1) = (5.5041, 12.369); \quad B_2 = s^{-1}(C_2) = (0.6583, 1.5190);$

$B_3 = s^{-1}(B_3) = (0.0808, 0.1817)$

and $b_1 = s^{-1}(\mu_1) = 8.5511, b_2 = s^{-1}(0) = 1$ and $b_3 = s^{-1}(\mu_3) = 0.1169$, respectively. The corresponding support points and weights as functions of the parameter b are depicted in Figure 4.3a, 4.3b and 4.3c for the different three cases and the coefficients in the corresponding Taylor expansions are listed in Table 4.3a, 4.3b and 4.3c. The interpretation of these graphs and tables is exactly the same as in the previous examples and therefore omitted.

– *insert Table 4.3 a-c and Figure 4.3 a-c here* –

Acknowledgements. This work was done while V.B. Melas was visiting the Ruhr-Universität Bochum. The authors are grateful to the DAAD for the financial support which made this visit possible. The work of H. Dette was supported by the SFB 475 (Komplexitätsreduktion in multivariaten Datenstrukturen). The authors would also like to thank M. Sahm for sending us his work before publication and I. Gottschlich, who typed this paper with considerable technical expertise.

References.

R.C. Gunning, H. Rossi (1965). Analytical Functions of Several Complex Variables. Prentice Hall, New York.

P.G. Hoel, A. Levine (1964). Optimal spacing and weighting in polynomial prediction. Ann. Math. Statist. 35, 1553-1560.

S. Karlin, W.J. Studden (1966). Tchebycheff Systems: With Applications in Analysis and Statistics. Wiley Interscience, New York.

J.C. Kiefer (1974). General equivalence theory for optimum designs (approximate theory). Ann. Statist. 2, 849-879.

J.C. Kiefer, J. Wolfowitz (1959). Optimum designs in regression problems. Ann. Math. Statist. 30, 271-294.

J.C. Kiefer, J. Wolfowitz (1965). On a theorem of Hoel and Levine on extrapolation designs. Ann. Math. Statist. 36, 1627-1655.

V.B. Melas (1978). Optimal designs for exponential regression. Math. Oper. Forsch. Stat., Ser. Statistics, 9, 45-59.

V.B. Melas (2000). Analytic theory of E-optimal designs for polynomial regression. Advances in stochastic simulation methods (eds. N. Balakrishnan, V.B. Melas, S. Ermarkov). Birkhäuser, Boston, 85-116.

F. Pukelsheim (1993). Optimal Design of Experiments. Wiley, New York.

M. Sahm (2000). Optimal designs for individual coefficients in polynomial regression. Tentatively accepted for publication in: Ann. Statist.

S.D. Silvey (1980). Optimal design. Chapman and Hall, London.

W.J. Studden (1968). Optimal design on Tchebycheff points. Ann. Math. Statist. 39, 1435-1447.

W.J. Studden (1980a). D_s-optimal designs for polynomial regression using continued fractions. Ann. Statist. 8, 1132-1141.

W.J. Studden (1980b). On a problem of Chebyshev. J. Approx. Theory 29, 253-260.

G. Szegö (1959). Orthogonal polynomials. Am. Math. Soc. Colloqu. Publ. 23. Providence, RI.

	0	1	2	3	4	5
q_1^*	0.0000	-0.6250	-0.6250	5.4688	0.0000	-87.2500
q_2^*	-0.7500	-0.7500	2.5625	0.0000	-8.0000	8.0000
q_3^*	0.0000	3.5000	0.0000	-18.0000	18.0000	314.5000
q_4^*	0.0000	-4.0000	4.0000	13.0000	-30.0000	-217.2500
t_2^*	-0.5000	-0.7500	2.0000	-1.0000	-15.5000	23.7500
t_3^*	0.5000	-0.2500	-2.0000	1.0000	15.5000	-23.7500
w_2^*	0.3333	0.4444	-0.0741	-2.2099	1.4053	26.1485
w_3^*	0.3333	-0.4444	0.3704	1.9136	-5.0021	-18.6588
w_4^*	0.1667	-0.4444	0.0741	2.2099	-1.4053	-26.1485

Table 4.1: First six coefficients of the Taylor expansions of the coefficients of the extremal polynomial $t^3 + q_4^* t^4 + q_3^* t^2 + q_2^* t + q_1^*$ and the interior support points t_2^*, t_3^* and weights w_2^*, w_3^*, w_4^* of the e_3-optimal design in a polynomial regession of degree 4 on the interval $[-1, b]$, where $b \in (0.8836, 1.2761)$. The center of the expansion is $b_1 = 1$.

	0	1	2	3	4	5
q_1^*	-0.6111	-0.0837	0.2284	-0.2006	-0.0144	0.1035
q_2^*	0.1679	0.6556	-0.3245	-0.1527	-0.0306	0.5245
q_3^*	-0.3970	-0.6202	0.4635	-0.0246	-0.0262	-0.3029
q_4^*	0.0000	0.2550	-0.2492	0.0956	-0.0232	0.0922
t_2^*	-0.0801	-0.2936	0.2332	0.0121	-0.1175	-0.0640
t_3^*	1.7596	0.2064	-0.4092	-0.0212	0.3126	0.0944
w_2^*	0.4550	0.0679	-0.0338	-0.0097	-0.0004	0.0283
w_3^*	0.2116	-0.1159	0.0804	0.0117	-0.0308	-0.0320
w_4^*	0.0450	-0.0679	0.0338	0.0097	0.0004	-0.0283

Table 4.2a: First six coefficients of the Taylor expansions of the coefficients of the extremal polynomial $t^2 + q_4^* t^4 + q_3^* t^3 + q_2^* t + q_1^*$ and the interior support points t_2^*, t_3^* and weights w_2^*, w_3^*, w_4^* of the e_2-optimal design in a polynomial regession of degree 4 on the interval $[-1, b]$, where $b \in (1.9677, 3.6374)$. The center of the expansion is $b_1 \approx 2.6794$.

	0	1	2	3	4	5
q_1^*	-0.0851	-0.3725	1.2528	10.3417	-33.0375	-172.2301
q_2^*	-0.0627	1.5888	6.2421	-37.8069	188.1016	2915.9334
q_3^*	1.0636	-14.7798	7.5615	212.6852	-1336.5488	-10635.3851
q_4^*	0.0000	-13.1439	13.4439	168.2561	-1132.4771	-7551.2227
t_2^*	-0.6567	-1.2064	7.8709	-24.0211	-237.7108	2949.0192
t_3^*	0.0299	-0.7064	-4.4867	13.6928	75.3346	-1269.9645
w_2^*	0.2116	0.8321	1.9158	-20.5706	26.1568	1026.1537
w_3^*	0.4550	-0.4878	-0.4334	9.4172	-57.9234	-266.3371
w_4^*	0.2884	-0.8321	-1.9158	20.5706	-26.1568	-1026.1537

Table 4.2b: First six coefficients of the Taylor expansions of the coefficients of the extremal polynomial $t^2 + q_4^* t^4 + q_3^* t^3 + q_2^* t + q_1^*$ and the interior support points t_2^*, t_3^* and weights w_2^*, w_3^*, w_4^* of the e_2-optimal design in a polynomial regession of degree 4 on the interval $[-1, b]$, where $b \in (0.2749, 0.5082)$. The center of the expansion is $b_2 \approx 0.3732$.

	0	1	2	3	4	5
q_1^*	0.4194	0.0500	-0.0170	0.0043	-0.0010	0.0002
q_2^*	-0.4415	-0.0418	0.0141	-0.0035	0.0008	-0.0002
q_3^*	0.0390	0.0191	-0.0072	0.0019	-0.0004	0.0000
q_4^*	0.0000	-0.0020	0.0009	-0.0002	0.0000	0.0000
t_2^*	1.3874	-0.0492	0.0098	-0.0012	0.0002	-0.0000
t_2^*	6.1623	0.4508	-0.0652	-0.0073	0.0004	0.0003
w_2^*	0.4935	0.0036	-0.0011	0.0002	-0.0001	0.0000
w_3^*	0.0250	-0.0094	0.0028	-0.0006	0.0001	-0.0000
w_4^*	0.0065	-0.0036	0.0011	-0.0002	0.0001	-0.0000

Table 4.3a: First six coefficients of the Taylor expansions of the coefficients of the extremal polynomial $t + q_4^* t^4 + q_3^* t^3 + q_2^* t^2 + q_1^*$ and the interior support points t_2^*, t_3^* and weights w_2^*, w_3^*, w_4^* of the e_1-optimal design in a polynomial regession of degree 4 on the interval $[-1, b]$, where $b \in (5.5034, 12.371)$. The center of the expansion is $b_1 \approx 8.5511$.

	0	1	2	3	4	5
q_1^*	0.0000	0.3333	0.0000	-1.9861	1.9861	13.8105
q_2^*	0.0000	-2.1667	2.1667	6.3472	-14.8611	-39.4690
q_3^*	-1.3333	1.3333	-4.1389	6.9444	-5.2697	-0.8854
q_4^*	0.0000	3.3333	-6.6667	2.7639	8.3750	23.5284
t_2^*	-0.5000	-0.3750	0.7813	-0.0234	-3.5313	3.2778
t_3^*	0.5000	0.1250	-0.7813	0.7578	2.7969	-6.6050
w_2^*	0.4444	0.1481	-0.0247	-0.6039	0.5056	3.8814
w_3^*	0.4444	-0.1481	0.1235	0.5051	-1.2320	-2.3298
w_4^*	0.0556	-0.1481	0.0247	0.6039	-0.5056	-3.8814

Table 4.3b: First six coefficients of the Taylor expansions of the coefficients of the extremal polynomial $t + q_4^* t^4 + q_3^* t^3 + q_2^* t^2 + q_1^*$ and the interior support points t_2^*, t_3^* and weights w_2^*, w_3^*, w_4^* of the e_1-optimal design in a polynomial regession of degree 4 on the interval $[-1, b]$, where $b \in (0.6583, 1.5190)$. The center of the expansion is $b_2 = 1$.

	0	1	2	3	4	5
q_1^*	-0.0491	0.0082	10.6119	105.9225	739.2750	4342.6757
q_2^*	3.7749	-58.4185	77.2667	-3304.2811	10400.7601	-156116.3023
q_3^*	2.8499	-150.9503	420.0437	-9168.6057	80190.6009	-1124228.3000
q_4^*	0.0000	-93.4900	335.4455	-5936.4356	69157.4923	-972322.2982
t_2^*	-0.7208	-2.3080	40.7391	-679.9934	7305.5833	2431.3342
t_3^*	-0.1623	-1.8080	-6.1247	-3.8733	-109.1540	-1255.3129
w_2^*	0.0250	0.6896	8.8546	27.5008	226.0771	-824.2231
w_3^*	0.4935	-0.2604	-3.3989	-15.8341	-113.9147	653.8339
w_4^*	0.4750	-0.6896	-8.8546	-27.5008	-226.0771	824.2231

Table 4.3c First six coefficients of the Taylor expansions of the coefficients of the extremal polynomial $t + q_4^* t^4 + q_3^* t^3 + q_2^* t^2 + q_1^*$ and the interior support points t_2^*, t_3^* and weights w_2^*, w_3^*, w_4^* of the e_1-optimal design in a polynomial regession of degree 4 on the interval $[-1, b]$, where $b \in (0.0808, 0.1817)$. The center of the expansion is $b_3 \approx 0.1169$.