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Abstract

We study the D-optimal design problem for the common weighted univariate polynomial regression model with efficiency function λ. We characterize the efficiency functions for which an explicit solution of the D-optimal design problem is available based on a differential equation for the logarithmic derivative of the efficiency function. In contrast to the common approach which starts with a given efficiency function and derives a differential equation for the supporting polynomial of the D-optimal design, we derive a differential equation for the efficiency function, such that an explicit solution of the D-optimal design problem is possible. The approach is illustrated for various convex design spaces and is depicted in several new examples. Also, this concept incorporates all classical efficiency functions discussed in the literature so far.

Keywords and Phrases: polynomial regression, heteroscedasticity, optimal design, Sturm-Liouville problem

1 Introduction

Consider the common univariate polynomial regression model

$$Y(x) = \alpha^T \mathbf{f}(x) + \frac{\epsilon}{\sqrt{\lambda(x)}}, \tag{1.1}$$

where $\mathbf{f}^T(x) = (1, x, x^2, \ldots, x^n)$ is the vector of regression functions, $\alpha^T = (\alpha_0, \ldots, \alpha_n)$ is the vector of unknown parameters and ϵ denotes a centered random variable with constant variance, say $\sigma^2 > 0$. The design space is denoted by $\mathcal{X} \subset \mathbb{R}$ and we assume that in principle for each value of the explanatory variable $x \in \mathcal{X}$ an observation $Y(x)$ can be made with mean $\alpha^T \mathbf{f}(x)$ and variance $\sigma^2/\lambda(x)$, where different observations are uncorrelated. Throughout this paper $\lambda : \mathcal{X} \to \mathbb{R}_0^+$ denotes a continuously differentiable function which is positive in the interior of $\mathcal{X}$. The function λ is called efficiency function in the design literature and is used to model heteroscedasticity in the data. We call an efficiency function λ *admissible* if it is positive on the interior of the design space $\mathcal{X}$ and if the induced design space

$$\mathcal{G} = \{\sqrt{\lambda(x)}\mathbf{f}(x) \mid x \in \mathcal{X}\} \subset \mathbb{R}^{n+1}$$

is bounded.

Optimal designs for the polynomial regression models have been studied by numerous authors in the literature. Most authors investigate D-optimal designs which minimize the volume of the confidence ellipsoid for the vector of unknown parameters. Smith [36] was among the first who studied optimal design problems for polynomial regression. Hoel [24] and Guest [22] investigated D- and G-optimal designs, respectively and showed that these designs are identical in the polynomial regression model. These results motivated Kiefer and Wolfowitz [30] to prove the famous equivalence theorem which establishes the equivalence between D- and G-optimal designs. This result is a very powerful tool to verify D-optimality of a given design. Karlin and Studden [28] investigated D-optimal designs for weighted polynomial regression. Other interesting results can be found in Antille et al. [1], Chang and Lin [10], Dette [12], Dette et al. [13, 15], Dette and Studden [16], Dette and Wong [18], Fang [20], Federov [21], He et al. [23], Hoel [24], Huang et al. [25], Imhoff et al. [26], Karlin and Studden [27], Kiefer [29], Lau and Studden [32], Oritz and Rodrigues [33], Pukelsheim [34] or Studden [37] among others.

It is the purpose of this paper to present a review and unified treatment of the D-optimal design problem in the weighted, univariate polynomial regression model (1.1) for a broad class of efficiency functions. After a brief introduction into the terminology of optimal design theory we study the situation of D-optimal designs in the weighted polynomial regression. We consider the case where the logarithmic derivative of the efficiency function is a rational function and show that in our setting the D-optimal designs always have $(n + 1)$ support points. For sufficient conditions such that the D-optimal design for a given efficiency function and design space $\mathcal{X}$ is supported at exactly $(n+1)$-points we refer to Karlin and Studden [27], Chap. X, Theorem 3.6.

In contrast to previous work which starts with a given efficiency function and derives a differential equation for the supporting polynomial of the D-optimal design, we solve the differential equation with respect to the efficiency function λ such that the D-optimal design can be explicitly identified. This allows us to give a rather complete description of all efficiency functions for which an analytic solution of the D-optimal design problem is possible. Roughly speaking, the methodology presented in this paper is applicable to weighted polynomial regression models with convex design space and any efficiency function for which the logarithmic derivative $\lambda'(x)/\lambda(x)$ is a rational function, where the degree of the polynomial in the numerator and denominator is at most 2 and 3, respectively. As a consequence, our results contain - on the one hand - all solutions of D-optimal design problems for weighed polynomial regression which have been considered in the literature so far. On the other hand, numerous new results for D-optimal designs in the weighted polynomial regression model can be derived from our methodology, where the efficiency functions have not been investigated up to now.

The remaining part of this paper is organized as follows. We start to elaborate the main requirements in Section 2. In the following Sections 3, 4 and 5 we investigate the influence of the design space $\mathcal{X}$ on D-optimal designs considering admissible efficiency functions. Throughout these sections we also illustrate how D-optimal designs for admissible efficiency functions can be derived using different techniques. Technical details and proofs of our results can be found in the Appendix.

2 D-optimal designs for weighted polynomial regression

Consider the model (1.1) with mean $E[Y(x)] = \alpha^T \mathbf{f}(x)$ and (heteroscedastic) variance

$$Var(Y(x)) = \frac{\sigma^2}{\lambda(x)} .$$

An approximate design is a probability measure ξ on the design space $\mathcal{X}$ with finite support (see e.g. Kiefer [29]). The support points of the design ξ give the locations where observations are taken, while the weights give the corresponding proportions of total observations to be taken at these points. For uncorrelated observations (obtained from an approximate design) the covariance matrix of the least squares estimator for the parameter vector α is approximately proportional to the matrix

$$M(\xi) = \int_{\mathcal{X}} \lambda(x)\mathbf{f}(x)\mathbf{f}^T(x)d\xi(x) \in \mathbb{R}^{n+1\times n+1} , \tag{2.1}$$

which is called Fisher information matrix in design literature (see Atkinson and Cook [3], Atkinson and Donev [4], Federov [21], Pukelsheim [34] or Silvey [35] among many others).

Throughout this paper we assume that the form of the efficiency function $\lambda(x)$ is known and that the parameters in the variance function are nuisance parameters, which are not of primary interest for the construction of optimal designs (see Silvey [35]). An approximate design ξ^* is called D-optimal for the weighted polynomial regression (1.1) of degree n, if it maximizes the determinant $|M(\xi)|^{1/(n+1)}$ over all approximate designs. Note that the D-optimal design does not depend on the scaling of the efficiency function λ, i.e. the D-optimal design for the weighted polynomial regression model with efficiency function λ and $c \cdot \lambda$, $c \in \mathbb{R}^+$ coincide. If a design, say ξ, is given, its D-optimality can be checked by the celebrated Kiefer and Wolfowitz equivalence theorem (see Kiefer and Wolfowitz [30]), which characterizes the D-optimality of ξ by the inequality

$$d(x,\xi) = \lambda(x)\mathbf{f}^T(x)M^{-1}(\xi)\mathbf{f}(x) \le n+1 \quad \text{for all } x \in \mathcal{X}. \tag{2.2}$$

Moreover, if the design ξ is D-optimal, there is equality in (2.2) at its support points.

As a fundamental assumption we suppose that the logarithmic derivative of the efficiency function $\lambda(x)$ is of the form

$$\frac{d}{dx}\log\lambda(x) = \frac{\lambda'(x)}{\lambda(x)} = \frac{P_{p_1}(x)}{Q_{p_2}(x)}, \tag{2.3}$$

where $P_{p_1}(x)$ and $Q_{p_2}(x)$ are two real valued polynomials of degree p_1 and p_2, respectively, with greatest common divisor $\gcd(P_{p_1}, Q_{p_2}) = 1$. We may also assume without loss of generality that one of the coefficients of the polynomials is normalized (meaning it equals 1). We note that all efficiency functions which have been considered in the literature so far fulfill assumption (2.3). Some classical and new efficiency functions satisfying this assumption can be found in Table 1.

Because of the assumption of a convex design space there are essentially three different types of designs spaces $\mathcal{X}$, namely

1) $\mathcal{X} = \mathbb{R}$ if $supp(\xi^*) \subset \mathbb{R}$

2) $\mathcal{X} = \mathbb{R}_0^+$ if $supp(\xi^*) \subset \mathbb{R}_0^+$

3) $\mathcal{X} = [0,b]$ if $supp(\xi^*) \subset [0,b]$

Here $supp(\xi^*)$ denotes the support points of the D-optimal design ξ^*. These design spaces are discussed in the sections 3, 4 and 5, respectively. Note that all other possible choices of design spaces on the real axis can be reduced to one of these three situations by means of linear transformation. The following result shows that for these design spaces, the D-optimal designs for the weighted polynomial regression model (1.1) with efficiency functions satisfying (2.3) with $p_1 \le 2$ and $p_2 \le 3$ are always supported at $n+1$ points. The proof is given in the Appendix.

Lemma 2.1. *Let λ be an efficiency function satisfying (2.3) with $p = \max\{p_1 - 1, p_2 - 2\} \le 1$ and assume that the design space is a convex subset of $\mathbb{R}$. Then the D-optimal design for the weighted polynomial regression model is unique and supported at $n+1$ points.*

It follows by a standard argument from optimal design theory (see e.g. Silvey [35]) that the D-optimal design ξ^* with $n+1$ support points has equal weights at its support points because the determinant of the Fisher information matrix can be represented as

$$|M(\xi^*)| = \Big(\frac{1}{n+1}\Big)^{n+1} \prod_{j=0}^{n} \lambda(x_j) \prod_{0 \le i < j \le n} (x_j - x_i)^2 \tag{2.4}$$

where $x_0 < x_1 < \ldots < x_n$ denote the support points of the design ξ^*. Combined with Lemma 2.1 this yields the following Corollary.

Corollary 2.2. *If the assumptions of Lemma 2.1 are satisfied, the unique D-optimal design for the weighted polynomial regression model has equal mass at its $n+1$ support points.*

The $n+1$ support points can in principle be determined by differentiating the function defined by (2.4) with respect to the points $x_0, \ldots, x_n$. However, some care is necessary using this argument for at least three reasons. First, the gradient of the function (2.4) with respect to the support points may vanish at several points, and it is not instantly clear which of these critical points correspond to the support points of the D-optimal design. Secondly, differentiating the function (2.4) yields to a system of nonlinear equations, which is not easy to handle. Third, if the design space is bounded, differentiating with respect to the extreme support points may not be reasonable. More precisely, the function (2.4) can always be differentiated with respect to points $x_1, \ldots, x_{n-1}$, which are located in the interior of the design space $\mathcal{X}$. On the other hand, the two extreme support points x_0 and x_n of the D-optimal design ξ^* may be located at the left or right boundary of the design space, provided that the boundary points exist. Consequently, we have to distinguish between different structures of the design space $\mathcal{X}$ and different shapes of the efficiency function λ simultaneously.

3 Design space $\mathcal{X} = \mathbb{R}$

In the case $\mathcal{X} = \mathbb{R}$ all support points are interior points of the design space and differentiating the logarithm of (2.4) with respect to the support points $x_j, j = 0, \ldots, n$ yields the system of equations

$$\frac{\partial}{\partial x_j} \log |M(\xi)| = \frac{\lambda'(x_j)}{\lambda(x_j)} + \sum_{i \ne j} \frac{2}{x_i - x_j} = 0, \quad j = 0, \ldots, n\,. \tag{3.1}$$

$\lambda(x)$	p_1	p_2	$\log(\lambda(x))' = \frac{P_{p_1}}{Q_{p_2}}$
c	0	0	0
$\exp(-cx)$	0	0	$\frac{-c}{1}$
$(x+z_1)^a$	0	1	$\frac{a}{x+z_1}$
$\exp\left(-(x-z_1)^2\right)$	1	0	$\frac{2z_1-2x}{1}$
$(x+z_1)^{a+cz_1}\exp(-cx)$	1	1	$\frac{a-cx}{x+z_1}$
$\exp\left(\alpha\, arctan\,(x+z_1)\right)$	0	2	$\frac{a}{1+(x+z_1)^2}$
$\left(\frac{x+z_1}{x+z_2}\right)^{\frac{1}{z_2-z_1}}$	0	2	$\frac{1}{(x+z_1)(x+z_2)}$
$\exp\left(-\frac{\alpha}{x+z_1}\right)$	0	2	$\frac{\alpha}{(x+z_1)^2}$
$\left(1+(x-z_1)^2\right)^{a+1}\exp\left(2c\, arctan\,(x+z_1)\right)$	1	2	$\frac{2(c+(1+a)(x+z_1))}{1+(x+z_1)^2}$
$(x+z_1)^{\alpha_2}\exp\left(-\frac{\alpha_1}{x+z_1}\right)$	1	2	$\frac{\alpha_1+\alpha_2(x+z_1)}{(x+z_1)^2}$
$(x+z_1)^{a+1}(x+z_2)^{c+1}$	1	2	$\frac{c(x+z_1)+a(x+z_2)}{(x+z_1)(x+z_2)}$
$(x+z_1)^{\alpha_1}\exp\left(dx-\frac{\alpha_2}{x+z_1}\right)$	2	2	$\frac{\alpha_2(-1+x+z_1)+d(x+z_1)^2}{(x+z_1)^2}$
$\exp\left(ax+c\cdot\arctan\left(\frac{x+z_1}{\sqrt{e}}\right)\right)\left(e+(x+z_1)^2\right)^d$	2	2	$\frac{c\sqrt{e}+2d(x+z_1)+a\left(e+(x+z_1)^2\right)}{e+(x+z_1)^2}$
$(x+z_1)^a\,(x+z_2)^c\exp(dx)$	2	2	$\frac{a(x+z_1)+(x+z_2)(c+d(x+z_1))}{(x+z_1)(x+z_2)}$
$(x+z_1)^{\alpha_1}\exp\left(\alpha_2\cdot\arctan\,(x+z_2)\right)\left(1+(x+z_2)^2\right)^{\alpha_3}$	2	3	$\frac{\alpha_1(1+x^2+2xz_2+z_2^2)+(x+z_1)(\alpha_2+2\alpha 3(x+z_2))}{(x+z1)(1+(x+z_2)^2)}$
$(x+z_1)^{\alpha_1}\exp\left(\frac{\alpha_2 x}{(x+z_1)^2}\right)$	2	3	$\frac{\alpha_1(x+z_1)^2-\alpha_2(x-z1)}{(x+z_1)^3}$
$(x+z_1)^{\alpha_1}(x+z_2)^{\alpha_2}(x+z_3)^{\alpha_3}$	2	3	$\frac{\alpha_1(x+z_2)(x+z_3)+(x+z1)(\alpha_3(x+z_2)+\alpha_2(x+z_3))}{(x+z_1)(x+z_2)(x+z_3)}$
$(x+z_1)^{\alpha_1}(x+z_2)^{\alpha_2}\exp\left(-\frac{\alpha_3}{x+z_2}\right)$	2	3	$\frac{\alpha_3(x+z_1)+(x+z_2)(\alpha_2(x+z_1)+\alpha_1(x+z_2))}{(x+z_1)(x+z_2)^2}$

Table 1: *Table of admissible efficiency functions and their logarithmic derivatives discussed in this paper*

Let

$$f(x) = \prod_{j=0}^{n} (x - x_j) = \sum_{k=0}^{n+1} s_k x^k \tag{3.2}$$

denote the polynomial f which has its roots at the support of the design ξ ($s_k \in \mathbb{R}$, $k = 0, \ldots, n+1$). Since (see Pukelsheim [34], Chapter 9.5)

$$\sum_{i \neq j} \frac{2}{x_i - x_j} = \frac{f''(x_j)}{f'(x_j)} \, ,$$

the system of nonlinear equations (3.1) is then equivalent to

$$\frac{\partial}{\partial x_j} \log |M(\xi)| = \frac{\lambda'(x_j)}{\lambda(x_j)} + \frac{f''(x_j)}{f'(x_j)} = 0, \qquad j = 0, \ldots, n \, .$$

Observing the assumption (2.3) we obtain

$$P_{p_1}(x_j) f'(x_j) + Q_{p_2}(x_j) f''(x_j) = 0, \qquad j = 0, \ldots, n \, .$$

The function $P_{p_1}(x)f'(x) + Q_{p_2}(x)f''(x)$ is a polynomial of degree $\max\{n + p_1, n - 1 + p_2\}$ with roots $x_0, \ldots, x_n$. With (3.2) it therefore follows for all $x \in \mathbb{R}$

$$P_{p_1}(x) f'(x) + Q_{p_2}(x) f''(x) = \alpha R_p(x) f(x) \, . \tag{3.3}$$

Here $R_p(x)$ denotes a polynomial of degree

$$p = \max\{p_1 - 1, p_2 - 2\} \geq 0 \tag{3.4}$$

with leading coefficient 1 and α is a unique constant defined by comparing the leading coefficients on both sides.

Note that the assumptions on the efficiency functions yield some conditions for the polynomial in the denominator of (2.3) which will be important in the following discussion. For example, if $p_1 > p_2$ the ratio of the two polynomials can be rewritten

$$\frac{P_{p_1}(x)}{Q_{p_2}(x)} = \tilde{P}_{p_1 - p_2}(x) + \frac{\hat{P}(x)}{Q_{p_2}(x)},$$

where the degree of $\hat{P}(x)$ is smaller than the degree of $Q_{p_2}(x)$. In this case, all coefficients of even powers of the polynomial $\hat{P}(x)$ have to vanish and the coefficients corresponding to odd powers must have negative signs. This follows from integrating (2.3) and the fact that the induced design space $\mathcal{G}$ has to be bounded. It turns out that it is also important to differ between the different types of roots of the polynomial $Q_{p_2}(x)$. For example, if $p_2 = 2$, Q_2 can have no roots, one root of multiplicity 2, or two different roots. This classification will be important in the following analysis. Surprisingly, this classification is not necessary for the polynomial $P_{p_1}(x)$.

3.1 p=0: "classical" orthogonal polynomials

A very fundamental observation is that (3.3) defines a differential equation of second order for the polynomial f which can be solved explicitly only for $p = 0$. This particular case has attracted broad interest and has been studied intensively in literature (see e.g. Federov [21], Karlin and Studden [27] and Antille et al. [1] among many others). In the following we show that there exist precisely 2 types of valid efficiency functions for the weighted polynomial regression model (1.1) on the design space $\mathcal{X} = \mathbb{R}$ and $p = 0$ (this implies either $p_1 = 1$ or $p_2 = 2$), for which the D-optimal design can be determined explicitly via the differential equation (3.3). The analysis is done in a strict sequential way and discusses all of the possible combinations of degrees of the polynomials $P_{p_1}(x)$ and $Q_{p_2}(x)$ depending on the value of p as defined in (3.4). For this, we first analyze the possible shapes of the polynomials $P_{p_1}(x)$ and $Q_{p_2}(x)$ satisfying $p = 0$. The condition $p = \max\{p_1 - 1, p_2 - 2\} = 0$ yields four cases for the degrees of the polynomials $P_{p_1}(x)$ and $Q_{p_2}(x)$, which are listed in Table 2 and are discussed in the following.

	$\mathbf{p_1}$	$\mathbf{p_2}$	$\mathbf{p}$
a)	1	2	0
b)	1	0	0
c)	1	1	0
d)	0	2	0

Table 2: *Possible degrees of the polynomials $P_{p_1}(x)$ and $Q_{p_2}(x)$ on the design space $\mathcal{X} = \mathbb{R}$ for $p = \max\{p_1 - 1, p_2 - 2\} = 0$*

a) If both polynomials in (3.3) are present with their highest possible degrees - that is $\boldsymbol{p_1 = 1}$ and $\boldsymbol{p_2 = 2}$ - and $Q_2(x)$ has no real root, one may state the differential equation (2.3) as

$$(\log \lambda(x))' = 2\frac{c + (a+1)(x - z_1)}{1 + (x - z_1)^2} .$$

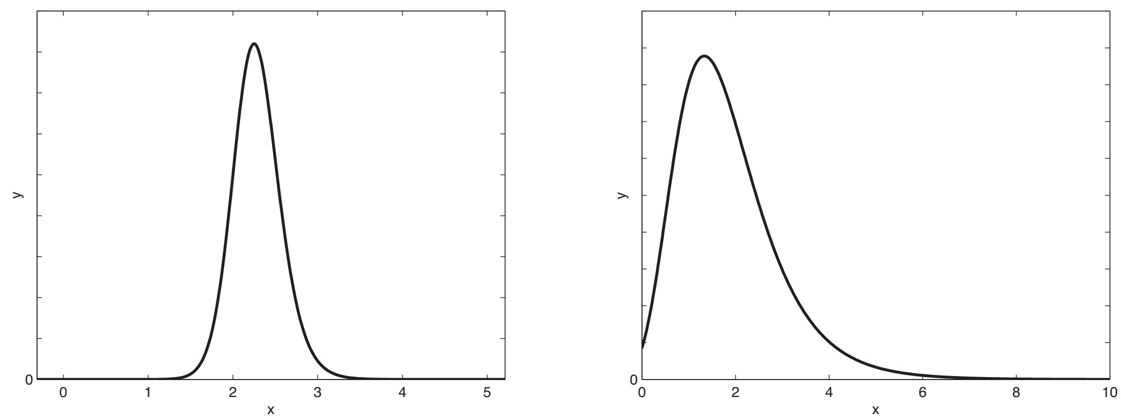
Integrating yields the solution

$$\lambda(x) = (1 + (x - z_1)^2)^{a+1} \exp\big(2c \arctan(x - z_1)\big) \tag{3.5}$$

with $z_1 \in \mathbb{R}$, $a < -n-1$ and $c \in \mathbb{R}$. Antille et al. [1] considered this efficiency function for the case $z_1 = 0$. For arbitrary z_1, the unique polynomial solution $f(x)$ of the differential equation (3.3) is given by the Jacobi polynomial

$$P_{n+1}^{(a+ic,a-ic)}(i(x - z_1)) , \tag{3.6}$$

which has $(n+1)$ real roots (see Szegö [38]). The D-optimal design for the weighted polynomial regression model with efficiency (3.5) has equal mass at these points. It is also worthwhile to mention that the condition $a < -n-1$ yields to a bounded design space $\mathcal{G}$ which guarantees the existence of the D-optimal design on $\mathcal{X} = \mathbb{R}$. An admissible efficiency function of the type (3.5) is shown in the left part of Figure 1. For the cubic regression model ($n = 3$), the D-optimal design for efficiency function (a) has equal weights at the points $1.6912, 2.13, 2.5645$ and 3.2143.



(a) $\lambda(x) = (1+(x-2)^2)^{-8} \exp\big(-4 \arctan(x-2)\big)$ (b) $\lambda(x) = (x+2)^{-15} \exp\big(-\frac{50}{x+2}\big)$

Figure 1: *Plot of efficiency function (3.5) and (3.7)*

Next we consider the case where $Q_2(x)$ has a root of multiplicity two at the point $-z_1$. Setting $Q_2(x) = (x+z_1)^2$ and $P_1(x) = \alpha_1 + \alpha_2(x+z_1)$ yields

$$(\log \lambda(x))' = \frac{\alpha_1 + \alpha_2(x+z_1)}{(x+z_1)^2}$$

and results in the efficiency function

$$\lambda(x) = (x+z_1)^{\alpha_2} \exp\left(-\frac{\alpha_1}{x+z_1}\right) . \tag{3.7}$$

To avoid a pole or root at the point $-z_1$ (recall that λ has to be bounded and strictly positive) we must set $\alpha_2 = 0$ which contradicts the assumption $p_1 = 1$. Thus, the efficiency function defined by (3.7) is not admissible on the design space $\mathcal{X} = \mathbb{R}$. We will show in the following sections that it is admissible on other design spaces.

If $Q_2(x)$ has two different roots, say $-z_1$ and $-z_2$, and $p_1 = 1$, we derive by the same technique as before

$$(\log \lambda(x))' = \frac{-\alpha_1(x+z_1) + \alpha_2(z_2 - x))}{(x+z_1)(z_2-x)}$$

and

$$\lambda(x) = (x+z_1)^{\alpha_1}(z_2-x)^{\alpha_2}\,, \tag{3.8}$$

which is not admissible because it has either roots or poles at the points $-z_1$ and $-z_2$, or the induced design space $\mathcal{G}$ is not bounded.

b) If $\boldsymbol{p_1 = 1}$ **and** $\boldsymbol{p_2 = 0}$, we obtain by integrating (2.3) with $P_1(x) = -2\alpha_1(\alpha_1 x + z_1)$ and $Q_0(x) = 1$ the solution

$$\lambda(x) = \exp\Big(-(\alpha_1 x + z_1)^2\Big) \tag{3.9}$$

with $\alpha_1 > 0$ and $z_1 \in \mathbb{R}$. The polynomial solution of the differential equation (3.3) with efficiency function (3.9) is given by the $(n+1)$th (scaled) Hermite polynomial

$$H_{n+1}(\alpha_1 x + z_1)\,. \tag{3.10}$$

The D-optimal design for the weighted polynomial regression model (1.1) with efficiency function (3.9) has equal mass at the roots of this polynomial (see e.g. Federov [21], Theorem 2.3.3 or Karlin and Studden [27], Theorem 3.5). For the cubic regression model $(n = 3)$, the D-optimal design for efficiency function (3.9) with $\alpha_1 = 0.5, z_1 = 0$ has equal weights at the points $-3.30136, -1.0493, 1.0493$ and 3.30136.

c) If $\boldsymbol{p_2 = 1}$ **and** $\boldsymbol{p_1 = 1}$ we obtain by integrating (2.3) with $P_1(x) = -c(x+z_1)+a$ and $Q_1(x) = (x+z_1)$ the efficiency function

$$\lambda(x) = (x+z_1)^{\alpha}\exp(-cx) \tag{3.11}$$

for some constants $\alpha, c \in \mathbb{R}$. In this case the induced design space $\mathcal{G}$ is not bounded for any choice $c \neq 0$. On the other hand, if $c = 0$, the polynomial degree of $P(x)$ in (2.3) changes. Thus, this efficiency function is not admissible on $\mathcal{X} = \mathbb{R}$.

d) A similar argument holds in the case $\boldsymbol{p_1 = 0}$ and $\boldsymbol{p_2 = 2}$ with $Q_2(x)$ having no real roots. Integrating (2.3) with $P_0(x) = -a$ and $Q_2(x) = 1 + (x + z_1)^2$ yields the efficiency function

$$\lambda(x) = \exp\bigl(a \arctan(x + z_1)\bigr) , \tag{3.12}$$

while a polynomial $Q_2(x)$ with two different real roots, say $-z_1$ and $-z_2$, yields

$$\lambda(x) = \Bigl(\frac{x + z_1}{x + z_2}\Bigr)^{\frac{1}{z_2 - z_1}} . \tag{3.13}$$

If $Q_2(x)$ has a real root at $-z_1$ of multiplicity 2, integration of (2.3) gives

$$\lambda(x) = \exp\Bigl(\frac{\alpha}{x + z_1}\Bigr) \tag{3.14}$$

for some $\alpha \in \mathbb{R}$. In all three cases the efficiency functions are not admissible because the induced design space $\mathcal{G}$ is not bounded.

Note that there may exist linear transformations of these efficiency functions, which might also yield polynomials satisfying (2.3) with $p = 0$. Subject to these transformations, there exist only two admissible efficiency functions on the design space $\mathcal{X} = \mathbb{R}$ which fulfill assumption (2.3) with $p = 0$ for which the D-optimal design problem in regression model (1.1) can be solved explicitly: the efficiency functions defined by (3.5) and (3.9).

3.2 p=1: no solutions on $\mathcal{X} = \mathbb{R}$

In contrast to the case $p = 0$, much less is known about solutions of the differential equation (3.3) with $p \geq 1$ (see e.g. Chang [7], Chang and Jiang [8, 9], Chang and Lin [10], Huang et al. [25]). Note that one has to determine a polynomial solution f of the equation (3.3), which defines the support points of the D-optimal design by its roots. However, in the case $p \geq 1$ there may exist many solutions and it is not instantly clear which solution corresponds to the D-optimal design. In the following discussion we try to present a complete description of the structure of the efficiency functions for which a solution is possible. In particular we demonstrate that on the design space $\mathcal{X} = \mathbb{R}$ there does not exist any admissible efficiency function for which conditions (2.3) and (3.3) with $p = 1$ are satisfied. On the other hand, if the design space $\mathcal{X}$ is of the form $[0, \infty)$ or $[0, b]$, some of the efficiency functions described here will be admissible and these cases are investigated in Section 4 and 5. Therefore, the discussion in this section is also useful for the determination of D-optimal designs on the other design spaces.

Note that in the current case $p = \max(p_1 - 1, p_2 - 2) = 1$, the differential equation (3.3) takes the form

$$P_{p_1}(x) f'(x) + Q_{p_2}(x) f''(x) = \alpha\,(x - \gamma) \cdot f(x), \tag{3.15}$$

with unknown constant $\gamma \in \mathbb{R}$ and the constant α is defined by comparing the leading coefficients on both sides. From the last equation it follows that $P_{p_1}(x)$ and $Q_{p_2}(x)$ are polynomials of degree at most 2 and 3, respectively. We again have to distinguish between possible degrees, roots and multiplicities of roots of each of the polynomials $P_{p_1}(x)$ and $Q_{p_2}(x)$. These cases are listed in Table 3 and are carefully discussed in the following paragraph.

	$\mathbf{p_1}$	$\mathbf{p_2}$	$\mathbf{p}$
a)	2	2	1
b)	2	1	1
c)	2	0	1
d)	2	3	1
e)	{0,1}	3	1

Table 3: *Possible degrees of the polynomials $P_{p_1}(x)$ and $Q_{p_2}(x)$ on the design space $\mathcal{X} = \mathbb{R}$ for $p = \max\{p_1 - 1, p_2 - 2\} = 1$*

a) If $\boldsymbol{p_1 = 2}$ and $\boldsymbol{p_2 = 2}$ and the polynomial $Q_2(x)$ is positive, we may assume without loss of generality that $Q_2(x) = e + (z_1 + x)^2$ with $z_1 \in \mathbb{R}$ (note that the highest coefficient is normalized, i.e. equals 1). Integrating the logarithmic derivative (2.3) with $P_2(x) = a + cx + dx^2$ yields after some simplifications

$$\lambda(x) = \exp\Big(dx + \alpha_1 \arctan\big(\frac{x + z_1}{\sqrt{e}}\big)\Big)(e + (x + z_1)^2)^{\alpha_2} ,$$

which implies that $d = 0$ because the induced design space $\mathcal{G}$ has to be bounded (note that $\mathcal{X} = \mathbb{R}$). This contradicts the assumption $p = 1$ and thus the polynomial $Q_2(x)$ must have at least one real root. If $Q_2(x)$ has a root of multiplicity 2, say $-z_1$, then integrating (2.3) yields

$$\lambda(x) = (x + z_1)^{\alpha_1} \exp\Big(dx + \frac{\alpha_2}{x + z_1}\Big) . \tag{3.16}$$

Again, the assumption of a bounded induced design space $\mathcal{G}$ implies $d = 0$ which contradicts the assumption $p = 1$. If $Q_2(x)$ has two real roots, say $-z_1$ and $-z_2$, similar arguments give

$$\lambda(x) = (x + z_1)^{\alpha_1} (x + z_2)^{\alpha_2} \exp(dx) . \tag{3.17}$$

Once again, we must set $d = 0$ to ensure a bounded induced design space $\mathcal{G}$ which contradicts the assumption $p = 1$. Therefore the choice $p_1 = p_2 = 2$ does not yield an admissible efficiency function on the design space $\mathcal{X} = \mathbb{R}$.

b) If $Q_1(x)$ has exactly one real root, say $z_1 \in \mathbb{R}$, then $\boldsymbol{p_1 = 2}$ and $\boldsymbol{p_2 = 1}$ and this yields with $P_2(x) = (\alpha_1 + 2\alpha_2 x)(x + z_1) + \alpha_3$ and $Q_1(x) = (x + z_1)$ the efficiency

$$\lambda(x) = \exp\Big(\alpha_1 x + \alpha_2 x^2\Big)(x + z_1)^{\alpha_3} . \tag{3.18}$$

This efficiency is only admissible if $\alpha_3 = 0$ in order to avoid either a pole or a root of the efficiency λ at the point $-z_1$. A simple calculation shows that this is a contradiction to $\gcd(P_{p_1}, Q_{p_2}) = 1$ and thus λ is not an admissible efficiency function on the design space $\mathcal{X} = \mathbb{R}$.

c) If $\boldsymbol{p_1 = 2}$ and $\boldsymbol{p_2 = 0}$, i.e. $Q_0(x)$ is constant, integrating the logarithmic derivative (2.3) with $P_2(x) = \alpha_1 + x(2\alpha_2 + 3\alpha_3 x)$ yields

$$\lambda(x) = \exp\Big(\alpha_1 x + \alpha_2 x^2 + \alpha_3 x^3\Big) , \tag{3.19}$$

and the boundedness of the induced design space $\mathcal{G}$ yields $\alpha_3 = 0$. This is a contradiction to $p_1 = 2$ and thus this efficiency function is not admissible on the design space $\mathcal{X} = \mathbb{R}$.

d) The same reasoning applies to the case $\boldsymbol{p_1 = 2}$ and $\boldsymbol{p_2 = 3}$ where $Q_3(x)$ has exactly one real root. We assume $Q_3(x) = (x + z_1)\big(1 + (x + z_2)^2\big)$ with $z_1, z_2 \in \mathbb{R}$ and $P_2(x) = (x + z_1)(\alpha_2 + 2(x + z_2)) + \alpha_1(1 + (x + z_2)^2)$. Integrating the logarithmic derivative (2.3) gives

$$\lambda(x) = (x + z_1)^{\alpha_1} \exp\Big(\alpha_2 \arctan(x + z_2)\Big) (1 + (x + z_2)^2)^{\alpha_3} \tag{3.20}$$

for some constants $\alpha_1, \alpha_2, \alpha_3 \in \mathbb{R}$. Because $\lambda(x)$ is strictly positive on the design space $\mathcal{X} = \mathbb{R}$, it follows that $\alpha_1 = 0$. This choice reduces the degree of the polynomials $P_{p_1}(x)$ and $Q_{p_2}(x)$ in the the logarithmic derivative (2.3) to $p_1 = 1$ and $p_2 = 2$, contradicting the assumption $p = 1$. Thus, this efficiency function is not admissible on the design space $\mathcal{X} = \mathbb{R}$.

Using similar arguments it is easy to see that none of the following choices yield admissible efficiency functions for the design space $\mathcal{X} = \mathbb{R}$. Nevertheless, we will briefly state the resulting efficiency functions of the remaining cases, since they will be important later in Section 4 where different design spaces are considered. If the polynomial $Q_3(x)$ has a simple root of multiplicity 3 at $-z_1$, integration of (2.3) yields

$$\lambda(x) = (x + z_1)^{\alpha_1} \exp\Big(\frac{a_2 x}{(x + z_1)^2}\Big) . \tag{3.21}$$

If $Q_3(x)$ has three simple roots, say $-z_1, -z_2, -z_3$, the resulting efficiency function $\lambda(x)$ is

$$\lambda(x) = (x + z_1)^{\alpha_1} (x + z_2)^{\alpha_2} (x + z_3)^{\alpha_3} \tag{3.22}$$

The remaining case $Q_3(x)$ with a simple root at $-z_1$, and a root of multiplicity 2 at $-z_2$ yields after integration

$$\lambda(x) = (x+z_1)^{\alpha_1}(x+z_2)^{\alpha_2} \exp\Big(\frac{\alpha_3}{x+z_2}\Big) . \tag{3.23}$$

e) The same reasoning can be applied for the remaining cases $\boldsymbol{p_1 \in \{0,1\}}$ and $\boldsymbol{p_2 = 3}$ to show that none of the efficiency functions is admissible in this case. The details are omitted for the sake of brevity.

Summarizing the discussion of this section leads the conclusion that on the design space $\mathcal{X} = \mathbb{R}$ there does not exist any efficiency function fulfilling (2.3) with $p = 1$ in (3.3). In the following sections we will show that some of these efficiency functions are admissible on the design spaces $[0, \infty)$ and $[0, b]$.

4 Design space $\mathcal{X} = \mathbb{R}_0^+$

If the design space $\mathcal{X}$ is bounded from below, say $\mathcal{X} = \mathbb{R}_0^+$, a similar approach can be adopted, but some more care is necessary here. One may not be able to differentiate (2.4) with respect to the point x_0 if that point is located at the boundary of the design space, i.e. $x_0 = 0$. Therefore, we must distinguish between the cases of D-optimal designs ξ^* with smallest support point at $x_0 = 0$ and smallest support point $x_0 > 0$: these two cases will be investigated separately in Section 4.1 and Section 4.2. Before we discuss these in detail, we present two auxiliary results, which allow a partial classification of the different cases. The proofs can be found in the Appendix.

Lemma 4.1. *If the efficiency function λ fulfills $\arg\max_{x \in \mathbb{R}_0^+} \lambda(x) = 0$, the D-optimal design $\xi^*_{\mathbb{R}_0^+}$ for the regression model (1.1) on the design space $\mathcal{X} = \mathbb{R}_0^+$ has positive weight at the point $x = 0$.*

Lemma 4.2. *Let λ be an admissible efficiency function on $\mathcal{X} = \mathbb{R}$ satisfying (2.3), $p = \max\{p_1 - 1, p_2 - 2\} \leq 1$, and let supp($\xi^*_{\mathbb{R}}$) denote the support of the D-optimal design $\xi^*_{\mathbb{R}}$ on the design space $\mathcal{X} = \mathbb{R}$.*
If $\min(supp(\xi^*_{\mathbb{R}})) < 0$, the D-optimal design $\xi^*_{\mathbb{R}_0^+}$ on $\mathcal{X} = \mathbb{R}_0^+$ has $x_0 = 0$ as its smallest support point.

4.1 D-optimal designs with positive support points

We will first investigate the case where 0 is not a support point of the D-optimal design, that is $x_0 > 0$. One necessary - but not sufficient - condition is that the efficiency function $\lambda(x)$ on the design space $\mathcal{X} = \mathbb{R}_0^+$ has no global maximum at the point $x = 0$, that is $\arg\max_{x \in \mathbb{R}_0^+} \lambda(x) \neq 0$ (see Lemma 4.1). We have to analyze similar problems as considered in the previous subsections. Because we assume that $x_0 > 0$, we can use the same calculations as presented in Section 3.1 with the differential equation (3.3), where two differences caused by the restricted design space have to be taken into account:

- The admissibility of the efficiency function has now to be checked under the assumption $\mathcal{X} = \mathbb{R}_0^+$. As a consequence, some of the non admissible efficiency functions for the design space $\mathcal{X} = \mathbb{R}$ are now admissible.
- An admissible efficiency function for the design space $\mathcal{X} = \mathbb{R}$ is obviously also admissible in the case $\mathcal{X} = \mathbb{R}_0^+$. However, it is not clear if the corresponding D-optimal design is supported on $\mathbb{R}_0^+$. If this is not the case Lemma 4.2 shows that $x_0 = 0$ is a support point of the D-optimal design. This case is discussed in Section 4.2.

4.1.1 p=0: more "classical" orthogonal polynomials

The case $p = 0$ admits an explicit characterization of the D-optimal designs in terms of roots of classical orthogonal polynomials. Note that $p = \max\{p_1 - 1, p_2 - 2\} = 0$ in (3.3) implies $p_1 = 1$ or $p_2 = 2$.

In the following paragraph we discuss the cases for $p = 0$ on the design space $\mathcal{X} = \mathbb{R}_0^+$. All possible combinations for the degrees of the polynomials $P_{p_1}(x)$ and $Q_{p_2}(x)$ for $p = 0$ are listed in Table 2 and have already been discussed in Section 3.1. To see the influence of the design space $\mathcal{X}$ on D-optimal designs for certain efficiency functions, we would like to point out that the two efficiency functions (3.7) and (3.11) are both not admissible on the design space $\mathcal{X} = \mathbb{R}$. The situation is different on the design space $\mathcal{X} = \mathbb{R}_0^+$.

a) If $\boldsymbol{p_1 = 1}$ **and** $\boldsymbol{p_2 = 2}$ and the polynomial $Q_2(x)$ has no real roots, the corresponding efficiency function has been derived in Section 3.1 and is shown in (3.5). The solution of the differential equation (3.3) is given by the Jacobi polynomial stated in (3.6). If j_{n+1} denotes the largest root of the Jacobi polynomial $P_{n+1}^{(a+ic,a-ic)}(ix)$, and $z_1 > j_{n+1}$, then it follows that the D-optimal design for the weighted polynomial regression model is located in $\mathcal{X} = [0, \infty)$ and puts equal mass at the roots of the Jacobi polynomial defined in (3.6). The choice $z_1 \leq j_{n+1}$ is considered in Section4.2.2 because in this case Lemma 4.2 implies $x_0 = 0$. An admissible efficiency function of the type (3.5) with the parameter $z_1 = 2, a = -9, c = -2$ is shown in the left part of in Figure 1. Note that for the cubic regression model the D-optimal design has equal weights at the points $1.6912, 2.13, 2.5645, 3.2143$ and is D-optimal on the design space $\mathcal{X} = \mathbb{R}_0^+$ and $\mathcal{X} = \mathbb{R}$.

If $Q_2(x)$ has a root of multiplicity 2 - that is $Q_2(x) = (x + z_1)^2$ - the solution of the differential equation (2.3) has been derived in (3.7). Because the induced design space has to be bounded it follows that $\alpha_2 < -2n$. Moreover, we also obtain that $z_1 \geq 0$ and $\alpha_1 > -\alpha_2 z_1$ because otherwise the efficiency λ would have a maximum at the point 0 contradicting Lemma 4.1 and the assumption $x_0 > 0$. The polynomial solution of the differential equation (3.3) is derived using the generalized Rodrigues' formula (see Cryer [11], Erdélyi et al. [19]) and is given by the generalized Bessel polynomial (see Krall and Frink [31])

$$Y_{n+1}\left(x - z_1, \alpha_2, \alpha_1\right) = \sum_{k=0}^{n+1} \begin{pmatrix} n+1 \\ k \end{pmatrix} (n + k + \alpha_2 + 1)^{(k)} \left(\frac{x - z_1}{\alpha_1}\right)^k, \tag{4.1}$$

where $z^{(0)} := 1$ and $z^{(k)} := z(z-1)\dots(z-k+1)$ if $k \geq 1$. The support points of the D-optimal design for the corresponding weighted polynomial regression model (1.1) on the design space $\mathcal{X} = \mathbb{R}_0^+$ are given by the roots of the polynomial (4.1) (see Antille et al. [1]). For example in the cubic regression model the efficiency function

$$\lambda(x) = (x+2)^{-15} \exp\left(-\frac{50}{x+2}\right)$$

fulfills the above condition and the resulting D-optimal design has equal weights at the points $0.39854, 1.6521, 3.779$ and 8.3926. A plot of this efficiency function is depicted in the right part of Figure 1.

If $Q_2(x)$ has two different roots, the solution of the differential equation (2.3) has been derived in (3.8). This efficiency is admissible on the design space $\mathcal{X} = \mathbb{R}_0^+$ if α_2 is even, $\alpha_1 + \alpha_2 < -2n$, $z_1 > 0$ and $z_2 < 0$. In this case the efficiency function $\lambda(x)$ is decreasing in $\mathcal{X} = \mathbb{R}_0^+$ which gives $\arg\max_{x \in \mathcal{X}} \lambda(x) = 0$. By Lemma 4.1 we have for the smallest support point of the D-optimal design $x_0 = 0$, which is discussed in Section 4.2.2 with a different technique.

b) Next consider the case $\boldsymbol{p_1 = 1}$ and $\boldsymbol{p_2 = 0}$, where we obtain the efficiency defined in (3.9). We may chose $\alpha_1 \neq 0$, but to assure that the support of the design is contained in $\mathcal{X} = \mathbb{R}_0^+$, the parameter z_1 has to be smaller than the smallest root of the Hermite polynomial $H_{n+1}(x)$ because otherwise Lemma 4.2 implies that $x_0 = 0$ (this case is discussed in Section 4.2.2). Under this assumption the resulting D-optimal design for the weighted polynomial regression model on the design space $\mathcal{X} = [0, \infty)$ has equal weights at the roots of the $(n+1)$th Hermite polynomial

$$H_{n+1}(\alpha_1 x + z_1)\,,$$

see e.g. Federov [21], Theorem 2.3.3 or Karlin and Studden [27], Theorem 3.5. For example, we consider the cubic regression model with efficiency function $\lambda(x) = \exp(-(x - z_1)^2)$

$(\alpha_1 = 1)$. The smallest root of $H_4(x)$ is $h_1 = -1.65068$ and if we set $z_1 = -3$, the efficiency function $\lambda(x) = \exp(-(x-3)^2)$ fulfills the above condition. The D-optimal design for the weighted polynomial regression model on the design space $\mathcal{X} = [0, \infty)$ has equal weights at the points $1.34932, 2.47535, 3.52465$ and 4.65068.

c) Assume $\boldsymbol{p_1 = 1}$ and $\boldsymbol{p_2 = 1}$ and that $Q_1(x)$ has a root at the point $-z_1$. This case has been analyzed in (3.11). To obtain a bounded induced design space $\mathcal{G}$, the parameters have to fulfill $z_1 > 0$ and $c > 0$. Furthermore, $\alpha > cz_1$, because otherwise the efficiency λ would have a maximum at the point 0, which would yield $x_0 = 0$ as a support point as seen in Lemma 4.1 . It is well known that the polynomial solution of the differential equation (3.3) is given by the Laguerre polynomial

$$L_{n+1}^{(\alpha-1)}\Big(c(x+z_1)\Big)\,, \tag{4.2}$$

see i.e. Karlin and Studden [27], Theorem 3.4 or Federov [21], Theorem 2.3.3. Consequently, if z_1 is smaller than the smallest root of $L_{n+1}^{(\alpha-1)}(cx)$, say l_1, then the D-optimal design is supported at the roots of this polynomial. For the cubic regression model on the design space $\mathcal{X} = \mathbb{R}_0^+$ with efficiency function $\lambda(x) = (x+2)^{15}\exp(-2x)$ $(z_1 = 2, \alpha = 15$ and $c = 2)$, we have $l_1 = 4.488$ and the D-optimal design has equal weights at the points $2.488, 5.03455, 8.14108$ and 12.3364.

d) For the case $\boldsymbol{p_1 = 0}$ and $\boldsymbol{p_2 = 2}$ we have to distinguish between the different multiplicities of the roots of the polynomial $Q_2(x)$ again. All possible options have been derived in Section 3.1, see (3.12), (3.13) and (3.14). Similar arguments as given in Section 3.1 show that these efficiency functions are also not admissible on the design space $\mathcal{X} = \mathbb{R}_0^+$.

4.1.2 p=1: "eigenvalue problems"

Note that in this case $p = \max(p_1 - 1, p_2 - 2) = 1$, and we end up with the differential equation (3.15) with unknown constant $\gamma \in \mathbb{R}$. Since the differential equation is the same as for the design space $\mathcal{X} = \mathbb{R}$, all possible candidates of efficiency functions λ have been derived in Section 3.2 already, where we showed that on the design space $\mathcal{X} = \mathbb{R}$ there does not exist an admissible efficiency function if $p = 1$. However, some of these efficiency functions are admissible on the restricted design space $\mathcal{X} = \mathbb{R}_0^+$ and will be discussed in this section. The possible degrees of the polynomials $P_{p_1}(x)$ and $Q_{p_2}(x)$ for $p = 1$ are listed in Table 3.

To solve any of the new cases for $p = 1$ listed in Table 3 we adopt an interesting approach of Huang et al. [25] and Chang and Lin [10] who identified the support points of the

D-optimal designs as the roots of a polynomial with coefficients obtained from the entries of an eigenvector of a special band matrix A. For this purpose we use the notation $f(x) = \sum_{k=0}^{n+1} s_k x^k$ for the supporting polynomial of the D-optimal design and rewrite the differential equation (3.15) for the design space $\mathcal{X} = \mathbb{R}_0^+$ as

$$\begin{aligned}\big(a + cx + dx^2\big) \sum_{k=1}^{n+1} k \cdot s_k x^{k-1} + \big(e + fx + gx^2 + hx^3\big) \sum_{k=2}^{n+1} (k-1)k \cdot s_k x^{k-2} \\ = (n+1)(d+hn)\,(x-\gamma) \cdot \sum_{k=0}^{n+1} s_k x^k\,,\end{aligned}$$

where we have used the representation

$$\begin{aligned}P_{p_1}(x) &= a + cx + dx^2 \\ Q_{p_2}(x) &= e + fx + gx^2 + hx^3\end{aligned}$$

with some constants $a, c, d, e, f, g, h \in \mathbb{R}$. Note that the value of α in (3.15) is determined by a comparison of the leading coefficient, i.e. $\alpha = (n+1)(d+hn)$. Comparing the coefficients of x^k, $k = 0, \dots, n+1$, we derive by straightforward (but tedious) calculations the equation

$$A \cdot \mathbf{s} = \gamma \mathbf{s}\,,$$

where the vector $\mathbf{s} = (s_0, \dots, s_{n+1})^T$ is given by the coefficients of the polynomial $f(x)$, and the matrix A is defined as

$$A = \begin{pmatrix} \tau_0(0) & \tau_{+1}(0) & \tau_{+2}(0) & 0 & \cdots & 0 \\ \tau_{-1}(1) & \tau_0(1) & \tau_{+1}(1) & \tau_{+2}(1) & \cdots & 0 \\ 0 & \tau_{-1}(2) & \tau_0(2) & \tau_{+1}(2) & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & \tau_{-1}(n) & \tau_0(n) & \tau_{+1}(n) \\ 0 & 0 & \cdots & 0 & \tau_{-1}(n+1) & \tau_0(n+1) \end{pmatrix} \in \mathbb{R}^{(n+2)\times(n+2)}. \quad (4.3)$$

The corresponding entries of the matrix A for the design space $\mathcal{X} = \mathbb{R}_0^+$ are

$$\begin{aligned}\tau_{-1}(k) &= -\Big(\frac{(k-1)\,(h(k-2)+d)}{(n+1)(d+hn)} - 1\Big) \\ \tau_0(k) &= -\frac{k\,(c+g(k-1))}{(n+1)(d+hn)} \\ \tau_{+1}(k) &= -\frac{(k+1)\,(a+fk)}{(n+1)(d+hn)} \\ \tau_{+2}(k) &= -\frac{e(k+1)(k+2)}{(n+1)(d+hn)}\,.\end{aligned} \quad (4.4)$$

Throughout this paper the matrix A plays an essential role in analyzing the case $p = 1$ and we assume

Assumption 4.1. *The dimension of the eigenspace for each eigenvalue γ_j, $j = 1, \dots, r$ of the matrix A defined in (4.3) is one. Hence, each of the eigenvector $\mathbf{s}_j$ corresponding to the eigenvalue γ_j, $j = 1, \dots, r$ is unique (up to scalar multiplication).*

The following Theorem identifies the roots of the polynomial $f(x)$ with coefficients of the eigenvector corresponding to the smallest eigenvalue of the band matrix A defined in (4.3) as the D-optimal design. The proof is complicated and therefore deferred to the Appendix.

Theorem 4.3. *The D-optimal design for the weighted polynomial regression model (1.1) on the design space $\mathcal{X} = \mathbb{R}_0^+$ for an admissible efficiency function λ satisfying*

$$(\log \lambda(x))' = \frac{a + cx + dx^2}{e + fx + gx^2 + hx^3}$$

has equal mass at $(n+1)$ support points. If Assumption 4.1 is satisfied and the smallest support point of the D-optimal design is positive, then these points are given by the roots of the polynomial $f(x) = \sum_{j=0}^{n+1} s_j x^j$, where the vector of coefficients $\mathbf{s}^T = (s_0, \dots, s_{n+1})$ is the eigenvector corresponding to the smallest eigenvalue of the $(n+2) \times (n+2)$ band matrix A defined in (4.3). The entries $\tau_{-1}(k)$, $\tau_0(k)$, $\tau_{+1}(k)$ and $\tau_{+2}(k)$ depend on the the efficiency function λ and are given in (4.4).

Remark 4.4. It should be mentioned that Assumption 4.1 is satisfied in most cases. In fact we are not aware of any case where it is not satisfied. To explain this observation we denote by I_{n+2} the identity matrix of dimension $(n+2)$ and briefly justify why

$$rank(A - \gamma_j I_{n+2}) = n + 1$$

is usually satisfied for all eigenvalues γ_j, $j = 1, \dots, r$. If $\tau_{-1}(k) \neq 0$, $k = 1, \dots, n+1$ we are able to eliminate $(\tau_0(0) - \gamma_j)$ by $\tau_{-1}(1)$ applying row elimination to the matrix $(A - \gamma_j I)$. Then we eliminate elements above $\tau_{-1}(2)$ of the resulting matrix by $\tau_{-1}(2)$, and continuing in this way we end up with the equivalent matrix

$$\begin{pmatrix} 0 & 0 & \dots & 0 & 0 \\ \tau_{-1}(1) & 0 & \ddots & \vdots & * \\ 0 & \tau_{-1}(2) & \ddots & 0 & \vdots \\ \vdots & \vdots & \ddots & 0 & * \\ 0 & 0 & \dots & \tau_{-1}(n+1) & \tau_0(n+1) \end{pmatrix}$$

which shows that $rank(A - \gamma_j I_{n+2}) = n + 1$.

On the other hand, if $\tau_{-1}(k) = 0$ for some k it follows that $\tau_{-1}(k)$ as defined in (5.2) (and in all other cases considered in this paper) is strictly monotone in k. Thus, at most one of the elements $\tau_{-1}(k)$ equals 0 and the matrix A splits in two blocks with the same structure as A. With the same arguments we obtain that the rank of the matrix $A - \gamma_j I_{n+2}$ is at least n and at most $n+1$. Therefore in this case it is possible that the rank of the matrix $A - \gamma_j I_{n+2}$ is n and this property depends on the structure of the elements of the matrix A

Remark 4.5. Note that the additional root γ in the differential equation (3.15) is always real, i.e. $\gamma \in \mathbb{R}$, since Lemma A.2 in the Appendix identifies γ as an eigenvalue of a Sturm-Liouville system (see e.g. Arfken and Weber [2], Chapter 10 or Birkhoff and Rota [6], Chapter 10).

Remark 4.6. It should be pointed out here that in general - although the polynomial solution corresponding to the eigenvector of the minimal eigenvalue can always be calculated - the resulting design is not necessarily the D-optimal design on the design space $\mathcal{X} = \mathbb{R}_0^+$, because Theorem 4.3 does not guarantee that the roots of the calculated polynomial are located in the given design space $\mathcal{X} = \mathbb{R}_0^+$. This problem mainly affects efficiency functions which have a root in $\mathbb{R}^-$. However, it can be shown (see Birkhoff and Rota [6], Chapter 10) that the support points of the design calculated by the method indicated in Theorem 4.3 are always located in the interval $(-z_1, +\infty)$, where z_1 is the largest root of the efficiency function λ. If the smallest support point of the D-optimal design on the design space $\bar{\mathcal{X}} = (-z_1, +\infty)$ is negative, Lemma 4.2 states that $x_0 = 0$ on $\mathcal{X} = \mathbb{R}_0^+$. With this knowledge, the polynomial R_p would be of degree $p = 2$, which yields a differential equation not solvable with the presented approach. Recent research provides a functional algebraic construction of D-optimal designs for the case $p \geq 2$ on design spaces of the type $\mathcal{X} = [a, b]$ where $b - a$ is close to 0, see Chang [7], Chang and Jiang [9], Dette et al. [17].

In the following, we derive all possible efficiency functions which can be obtained by our approach for $p = 1$. These are listed in Table 3. Since the discussion and imposed conditions are somewhat intricate, we only elaborate one efficiency function in detail. For all other cases listed in Table 3, we only state the necessary properties for the efficiency function to be admissible. The detailed verification is left to the reader.

a) The case which will be discussed in more detail is given by $\boldsymbol{p_1 = 2}$ **and** $\boldsymbol{p_2 = 2}$, and it is additionally assumed that the polynomial $Q_2(x)$ has a root of multiplicity 2, say z_1. The corresponding efficiency function has been derived in (3.16), that is

$$\lambda(x) = (x + z_1)^{\alpha_1} \exp\Big(dx + \frac{\alpha_2}{x + z_1}\Big) . \tag{4.5}$$

The assumption of a bounded induced design space $\mathcal{G}$ implies $d < 0$ and the assumptions on the efficiency function on the design space $\mathcal{X} = \mathbb{R}_0^+$ yield $z_1 \geq 0$. To simplify the discussion we set $d = -1$ without loss of generality. Let $\alpha_1 \in \mathbb{R}$; the efficiency function λ

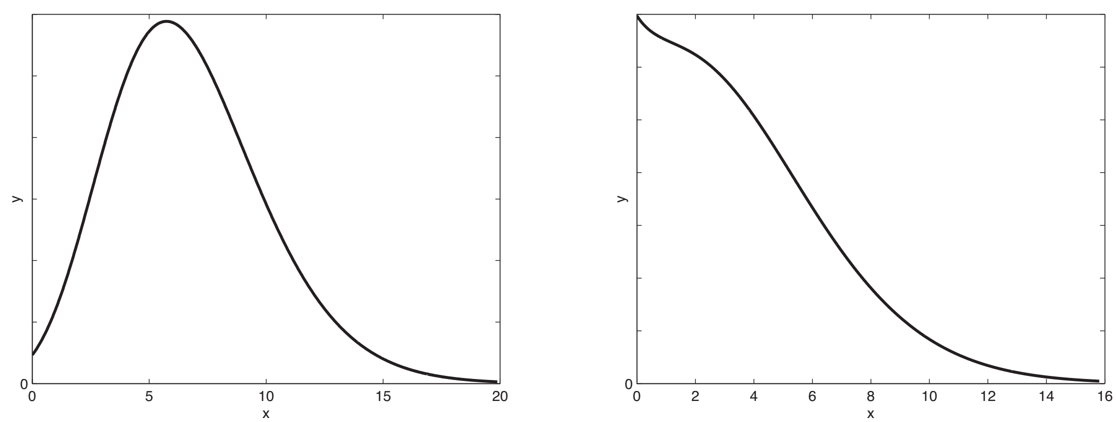
has two possible extrema at

$$r^{\pm} = \frac{1}{2}(\alpha_1 - 2z_1 \pm \sqrt{\alpha_1^2 - 4\alpha_2}).$$

If the discriminant is not real or equals zero, the basic shape of λ is controlled by the exponential term in (4.5) which implies $\arg max_{x\in\mathcal{X}}\lambda(x) = 0$ and by Lemma 4.1 $x_0 = 0$. Consequently, because this case is excluded here, the discriminant has to be positive and a simple calculation shows that r^- always corresponds to a minimum, and r^+ always to a maximum. Furthermore, to avoid $\arg max_{x\in\mathcal{X}}\lambda(x) = 0$ a necessary condition is that the maximum r^+ is attained in $\mathbb{R}_0^+$. A straightforward calculation yields the equivalent condition

$$\alpha_2 < -\frac{1}{4}(\alpha_1 - 2z_1)^2 - \alpha_1 \tag{4.6}$$

which also implies $r^- < 0$. This assures $\arg max_{x\in\mathcal{X}}\lambda(x) > 0$, and the efficiency function λ is admissible if the conditions (4.6), $d = -1, z_1 > 0$ and $\alpha_1 \in \mathbb{R}$ are satisfied. Only minor modifications are necessary to derive the result for arbitrary $d < 0$.



(a) $\lambda(x) = (x+3)^{10}\exp(-x + \frac{11}{x+3})$

(b) $\lambda(x) = (x+4)^{10}\exp(-x + \frac{26}{x+4})$

Figure 2: *Plots of efficiency function (4.5)*

Two possible shapes of the efficiency function (4.5) are listed in Figure 2. Even though both efficiency functions are admissible on the design space $\mathcal{X} = \mathbb{R}_0^+$, only the efficiency function (a) satisfies condition (4.6). For the efficiency function (b) the D-optimal design has $x_0 = 0$ as a support point. The polynomials of the logarithmic derivative of the efficiency function (a) are given by

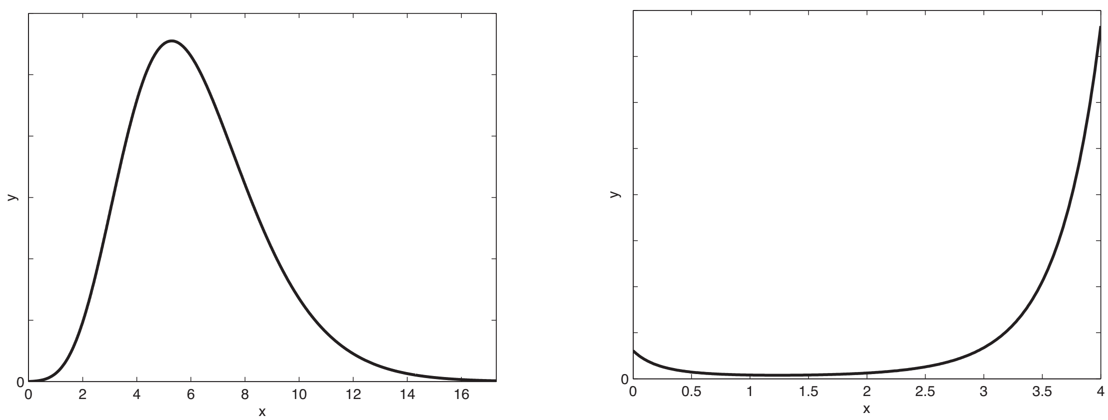
$$P_2(x) = 10 + 4x - x^2$$
$$Q_2(x) = 9 + 6x + x^2 = (3+x)^2\ .$$

The D-optimal design for the cubic regression model with efficiency function (a) is now derived by applying Theorem 4.3. It has equal weights at the points $1.0143, 5.19204, 10.4839$ and 17.8842.

If the polynomial $Q_2(x)$ is positive integrating the logarithmic derivative (2.3) gives

$$\lambda(x) = \exp\Big(dx + \alpha_1 \arctan\big(\frac{x+z_1}{\sqrt{e}}\big)\Big)(e + (x+z_1)^2)^{\alpha_2} . \tag{4.7}$$

The corresponding induced design space $\mathcal{G}$ is bounded if $d < 0$ and the non-negativity of the efficiency function implies $e > 0$. The remaining variables may be chosen arbitrary in $\mathbb{R}\backslash 0$ as long as the condition $\arg max_{x\in\mathcal{X}}\lambda(x) \neq 0$ is fulfilled. Two typical efficiency



(a) $\lambda(x) = \exp\Big(-x+25\arctan\big(x+2\big)\Big)(1+(x+2)^2)^2$ (b) $\lambda(x) = \exp\Big(5x+-25\arctan\big(x+2\big)\Big)(1+(x+2)^2)^{-5}$

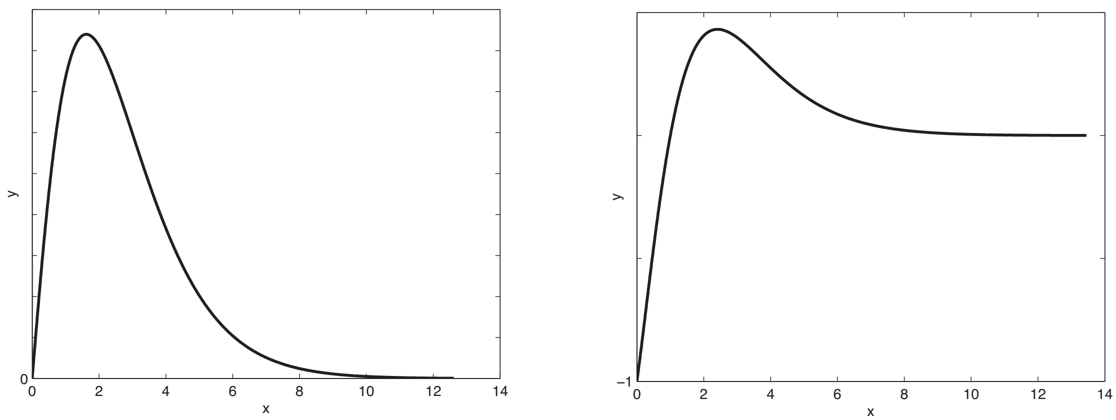
Figure 3: *Plots of efficiency function (4.7)*

functions of the type (4.7) are plotted in Figure 3. Only the efficiency function (a) is admissible on the design space $\mathcal{X} = \mathbb{R}_0^+$, since the induced design space $\mathcal{G}$ corresponding to efficiency function (b) is not bounded. For the cubic regression model, the D-optimal design for efficiency function (a) has equal mass at the points $2.3458, 5.2517, 9.2767$ and 15.2925.

If $Q_2(x)$ has two different real roots, we derive the efficiency function (3.17), that is

$$\lambda(x) = (x+z_1)^{\alpha_1}(x+z_2)^{\alpha_2}\exp(dx) . \tag{4.8}$$

The assumption of a bounded induced design space $\mathcal{G}$ implies $d < 0$ and $z_2 > z_1 > 0$. We may chose $\alpha_2 \in \mathbb{R}$ arbitrarily, but for the choice of the value of α_1 we have to assure that $\arg max_{x\in\mathcal{X}}\lambda(x) \neq 0$. Two typical efficiency functions of the type (4.8) are plotted in Figure 4. Note that the efficiency function (b) is not admissible on the design space $\mathcal{X} = \mathbb{R}_0^+$ since it is partly negative. For the cubic regression model, the D-optimal design for efficiency function (a) has equal weights at the points $0.486102, 2.26174, 5.40687$ and 10.6237.



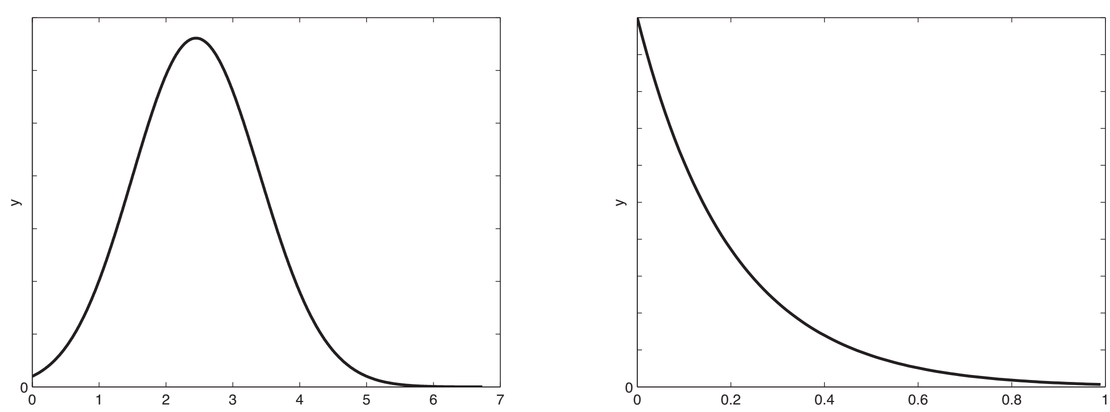
(a) $\lambda(x) = x(x+1)\exp(-x)$ (b) $\lambda(x) = (x+1)(x-1)\exp(-x)$

Figure 4: *Plots of efficiency function (4.8)*

b) If $\boldsymbol{p_1 = 2}$ and $\boldsymbol{p_2 = 1}$ and the polynomial $Q_1(x)$ has exactly one real root, say $-z_1$, we derive by integrating equation (2.3) the efficiency function (3.18), i.e.

$$\lambda(x) = \exp\Big(\alpha_1 x + \alpha_2 x^2\Big)(x + z_1)^{\alpha_3}\,. \tag{4.9}$$

The assumption of a bounded induced design space yields $\alpha_2 < 0$ and $z_1 > 0$. No conditions are necessary for $\alpha_1 \in \mathbb{R}$ but α_3 has to be chosen such that the resulting D-optimal design positive support points.



(a) $\lambda(x) = \exp(2x - 0.5x^2)(x+2)^2$ (b) $\lambda(x) = \exp(-2x + -x^2)(x+1)^{-3}$

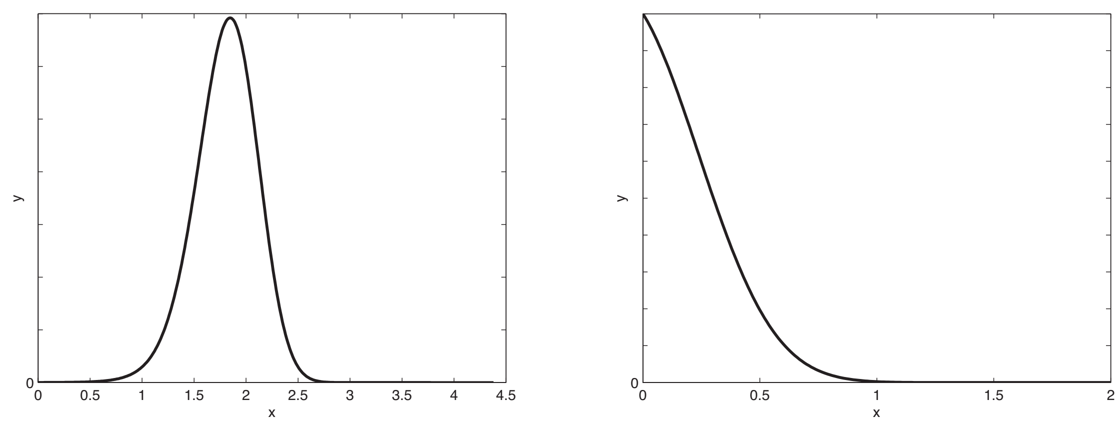
Figure 5: *Plots of efficiency function (4.9)*

Two efficiency functions of the type (4.9) are plotted in Figure 5. Both efficiency functions are admissible on the design space $\mathcal{X} = \mathbb{R}_0^+$. For the cubic regression model, the D-optimal design for efficiency function (a) has equal weights at the points $0.486102, 2.26174, 5.40687$ and 10.6237. For the efficiency function (b) the D-optimal design for the weighted polynomial regression has a support point at $x_0 = 0$ because of Lemma 4.1.

c) If $\boldsymbol{p_1 = 2}$ and $\boldsymbol{p_2 = 0}$ and $Q_0(x)$ is constant, integrating the logarithmic derivative (2.3) yields the efficiency function (3.19), that is

$$\lambda(x) = \exp\Big(\alpha_1 x + \alpha_2 x^2 + \alpha_3 x^3\Big) . \tag{4.10}$$

This function is admissible if $\alpha_3 < 0$. The other variable α_1 may be chosen arbitrarily in $\mathbb{R}$, whereas the constant α_2 is restricted by the condition that the smallest support point of the resulting D-optimal design is not given by $x_0 = 0$. A necessary condition for this property is $\arg max_{x\in\mathcal{X}} \lambda(x) \neq 0$ (see Lemma 4.1).



(a) $\lambda(x) = \exp(2x + 5x^2 - 2x^3)$ (b) $\lambda(x) = \exp(-x - 4x^2 - x^3)$

Figure 6: *Plots of efficiency function (4.10)*

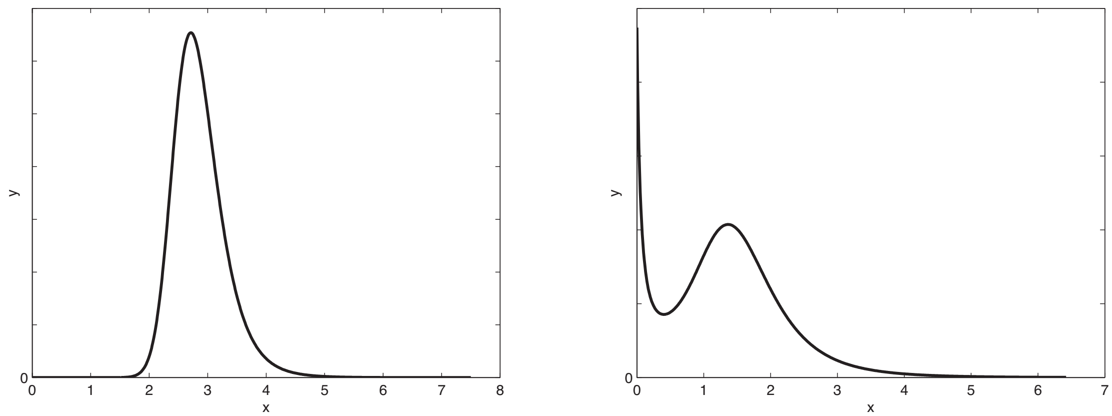
Two typical efficiency functions of the type (4.9) are plotted in Figure 6. For the cubic regression model, the D-optimal design for efficiency function (a) has equal mass at the points $0.8455, 1.4972, 1.9585$ and 2.3839. The efficiency function (b) would yield to a D-optimal design with $x_0 = 0$ as a support point.

d) The possible efficiency functions for the choice $\boldsymbol{p_1 = 2}$ and $\boldsymbol{p_2 = 3}$ as a solution of the differential equation (2.3) have been derived in Section 3.2, see the equations (3.20), (3.21), (3.22), and (3.23). If $Q_3(x)$ has a single real root at $-z_1$, i.e.

$Q_3(x) = (x + z_1)(1 + (x + z_2)^2$, we obtain the efficiency (3.20), that is

$$\lambda(x) = (x + z_1)^{\alpha_1} \exp\Big(\alpha_2 \arctan(x + z_2)\Big) \,(1 + (x + z_2)^2)^{\alpha_3} \,. \tag{4.11}$$

This function is admissible for $\alpha_2 \in \mathbb{R}$, $z_1 \geq 0$, $z_2 \in \mathbb{R}$ and $\alpha_1 + 2\alpha_3 < -2n$. Further conditions on the parameter α_1 are needed such that $x_0 = 0$ is not the smallest support point of the resulting D-optimal design. The detailed (but straightforward) discussion is left to the reader. Two typical efficiency functions of the type (4.11) are shown in



(a) $\lambda(x) = x^{-1} \exp(4 \arctan(x-2))(1+(x-2)^2)^{-5}$ (b) $\lambda(x) = (x{+}0.1)^{-2} \exp(3 \arctan(x{-}1))(1{+}(x{-}1)^2)^{-2}$

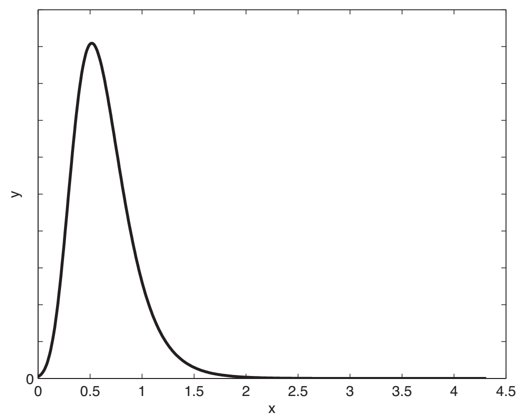
Figure 7: *Plots of efficiency function (4.11)*

Figure 7. For the cubic regression model, the D-optimal design for efficiency function (a) has equal mass at the points $2.2131, 2.7696, 3.5869$ and 5.5037. On the other hand, the D-optimal design for the polynomial regression model (1.1) with efficiency function (b) has a support point at $x_0 = 0$ because of Lemma 4.1.

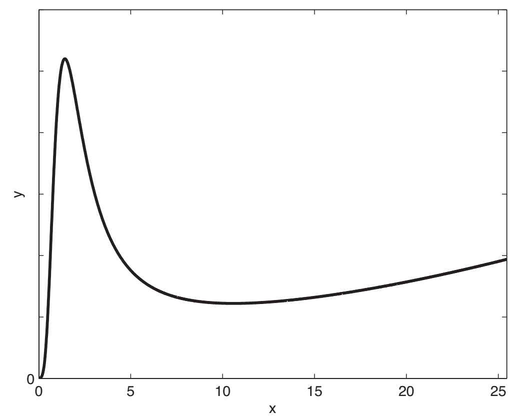
If $Q_3(x)$ has a real root of multiplicity 3, say $-z_1$, we derive the efficiency (3.21), i.e.

$$\lambda(x) = (x + z_1)^{\alpha_1} \exp\Big(\frac{a_2 x}{(x + z_1)^2}\Big) \,, \tag{4.12}$$

which is admissible for $z_1 > 0$, $\alpha_1 < -2n$ and $\alpha_2 > -\alpha_1 z_1$. Two typical efficiency functions of the type (4.12) are plotted in Figure 8. The efficiency function (a) is admissible on the design space $\mathcal{X} = \mathbb{R}_0^+$ and for the cubic regression model, the D-optimal design has equal mass at the points $0.23369, 0.57781, 1.1218$ and 2.3172. The efficiency function (b) is not admissible.



(a) $\lambda(x) = (x+1)^{-8}\exp(\frac{38x}{(x+1)^2})$



(b) $\lambda(x) = (x+1)^{2}\exp(\frac{28x}{(x+1)^2})$

Figure 8: *Plots of efficiency function (4.12)*

The efficiency function

$$\lambda(x) = (x+z_1)^{\alpha_1}(x+z_2)^{\alpha_2}(x+z_3)^{\alpha_3} \tag{4.13}$$

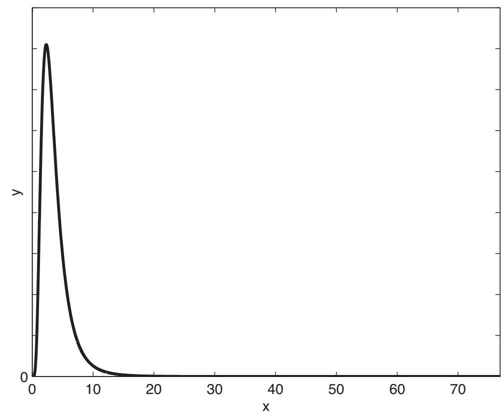
is derived if $Q_3(x)$ has three different real roots, say $-z_1, -z_2, -z_3$ (see the discussion before equation (3.22)). The assumption of a bounded induced design space yields $0 \le z_3 < z_2 < z_1$, $\alpha_3 + \alpha_2 + \alpha_1 < -2n$. However, some care is necessary, because there exist combinations of the parameters $\alpha_i, i = 1,2,3$ such that the D-optimal design is supported at the point $x_0 = 0$.

Two admissible efficiency functions of the type (4.13) are plotted in Figure 9. For the cubic regression model, the D-optimal design for efficiency function (a) has equal mass at the points $1.51837, 4.21625, 12.8156$ and 74.9104. Note that the largest support point of the D-optimal design is placed at a location with a very low efficiency, which contradicts intuition. The D-optimal design for the polynomial regression (1.1) with efficiency function (b) has positive weight at $x_0 = 0$ because of Lemma 4.1.

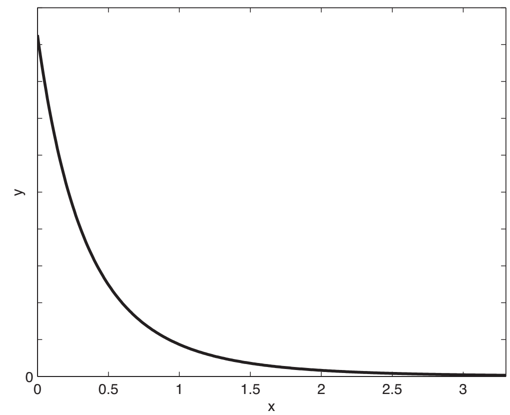
Finally, if the polynomial $Q_3(x)$ has a simple root at $-z_1$, and a root of multiplicity 2 at $-z_2$, the efficiency is given by

$$\lambda(x) = (x+z_1)^{\alpha_1}(x+z_2)^{\alpha_2}\exp\Big(\frac{\alpha_3}{x+z_2}\Big) \tag{4.14}$$

(see the discussion before equation (3.22)). This is an admissible efficiency function if $\alpha_1 + \alpha_2 < -2n$, $\alpha_3 \in \mathbb{R}$ and $z_1 > z_2 > 0$. Again, there exist combinations of the parameters such that the D-optimal design is supported at $x_0 = 0$. The details are omitted for the sake of brevity.



(a) $\lambda(x) = x^7(x+2)^{-9}(x+3)^{-5}$



(b) $\lambda(x) = (x+1)^{-1}(x+2)^{-2}(x+3)^{-3}$

Figure 9: *Plots of efficiency function (4.13)*

Two admissible efficiency functions of the type (4.14) are plotted in Figure 10. For the cubic regression model, the D-optimal design for efficiency function (a) has equal mass at the points $0.3956, 0.8256, 1.9952$ and 7.3477. The efficiency function (b) would have support at the point $x_0 = 0$ because of Lemma 4.1.

e) The resulting efficiency functions for $\boldsymbol{p_1 \in \{0,1\}}$ and $\boldsymbol{p_2 = 3}$ yield more restricted versions of the above efficiency functions. We only illustrate this for the case where $Q_3(x)$ has exactly one real root and $p_1 = 1$. Integrating (2.3) gives

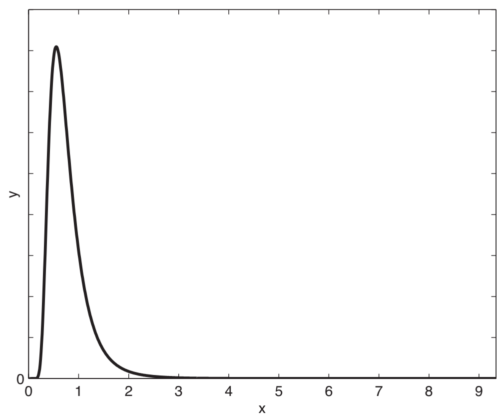
$$\lambda(x) = \exp\Big(\frac{a_1(z_1 - z_2) + a_2(1 - z_1 z_2 + z_2^2)}{1 + (z_1 - z_2)^2} \arctan(x + z_2)\Big)\Big(\frac{x + z_1}{\sqrt{(1 + (x + z_2)^2)}}\Big)^{\frac{a_1 - a_2 z_1}{1 + (z_1 - z_2)^2}}$$

The basic shape of this efficiency resembles the efficiency function (4.12) and a similar discussion yields conditions such that this function is admissible.

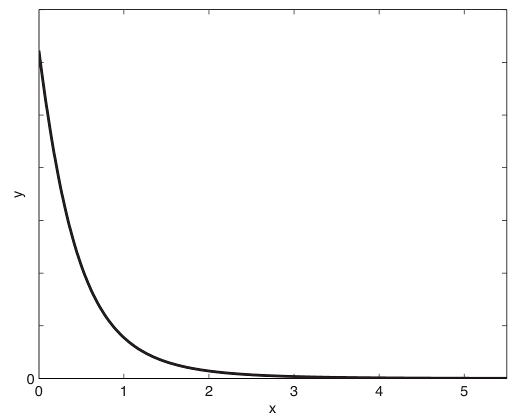
4.2 D-optimal designs supported at the boundary

If the D-optimal design has a support point at the boundary of $\mathcal{X} = [0, \infty)$, it is not possible to differentiate (2.4) with respect to the point $x_0 = 0$ and the arguments used in Section 3 have to be modified. A similar argument as in the previous section yields in this case the differential equation

$$x[P_{p_1}(x)f'(x) + Q_{p_2}(x)f''(x)] = \alpha R_p(x) \cdot f(x)\,, \qquad \forall x \in \mathbb{R}^+ \tag{4.15}$$



(a) $\lambda(x) = (x+1)^{-4} x^{-4} \exp(-\frac{3}{x})$



(b) $\lambda(x) = (x+2)^{-2}(x+1)^{-4} \exp(-\frac{3}{x+2})$

Figure 10: *Plots of efficiency function (4.14)*

for the supporting polynomial $f(x) = \prod_{j=0}^{n}(x - x_j)$ of the D-optimal design, where $R_p(x)$ is a polynomial of degree $p = \max\{p_1, p_2 - 1\}$. All possible combinations for the degree of the polynomials P_{p_1} and Q_{p_2} are listed in Table 4 for the case $p = 0$ and Table 5 for the case $p = 1$.

There are various reasons why the smallest support point equals 0, for example:

- If $\arg\max_{x\in[0,\infty)} \lambda(x) = 0$, Lemma 4.1 yields that the smallest support point of the D-optimal design is given by $x = 0$.
- If the D-optimal design on the design space $\mathcal{X} = \mathbb{R}$ has negative support, Lemma 4.2 yields that the smallest support point of the D-optimal design is given by $x = 0$.

Throughout this section we assume that $x_0 = 0$ is a support point of the D-optimal design and additionally that $\arg\max_{x\in[0,\infty)} \lambda(x) = 0$. It is worthwhile to mention that we may neglect possible shapes of efficiency functions by doing so, but due to the generality of our approach, no other option is available.

4.2.1 p=0: more explicit solutions

We start with the case $p = 0$, that is $\max\{p_1, p_2 - 1\} = 0$. The two possible choices for the different combinations of the degrees of the polynomials P_{p_1} and Q_{p_2} in Table 4 lead to D-optimal designs characterized by roots of classical orthogonal polynomials.

	$\mathbf{p_1}$	$\mathbf{p_2}$	$\mathbf{p}$
4.2.1 a)	0	0	0
4.2.1 b)	0	1	0

Table 4: *Possible degrees of the polynomials $P_{p_1}(x)$ and $Q_{p_2}(x)$ on the design space $\mathcal{X} = \mathbb{R}_0^+$ for $p = 0$ and $x_0 = 0$*

a) If $\boldsymbol{p_1 = 0}$ and $\boldsymbol{p_2 = 0}$, we obtain by integrating (2.3) the efficiency function

$$\lambda(x) = \exp(-ax) , \tag{4.16}$$

which is admissible for $a > 0$. The D-optimal design for the weighted polynomial regression model with efficiency function (4.16) has equal mass at the roots of the polynomial

$$xL_n^{(1)}(ax) ,$$

where $L_n^{(1)}(x)$ denotes the n-th Laguerre polynomial, see e.g. Federov [21], Theorem 2.3.3 or Karlin and Studden [27], Theorem 3.3. A classical example in the cubic regression model on the design space $\mathcal{X} = \mathbb{R}_0^+$ with this efficiency function is the choice $a = 1$, which yields $\lambda(x) = \exp(-x)$. The D-optimal design puts equal mass at the points $0, 0.93582, 3.3054$ and 7.7588.

b) In the case $\boldsymbol{p_1 = 0}$ and $\boldsymbol{p_2 = 1}$, it follows by integrating (2.3)

$$\lambda(x) = (x + z_1)^a, \tag{4.17}$$

where $-z_1$ is the root of the polynomial $Q_1(x)$. This efficiency function is admissible if $a < -2n$ and $z_1 > 0$. The D-optimal design for the weighted polynomial regression model has equal mass at the roots of the Jacobi polynomial

$$xP_n^{(1,a-1)}\left(\frac{2}{z_1}x + 1\right) ,$$

see Dette et al. [14]. For the cubic regression model on the design space $\mathcal{X} = \mathbb{R}_0^+$, the D-optimal design for the polynomial regression model with efficiency function $\lambda(x) = (x+3)^{-8}$ has equal mass at the points $0, 0.626136, 3$ and 14.3739.

4.2.2 p=1: more "eigenvalue problems"

For $p = 1$, we restate the differential equation (4.15) as

$$x \cdot [P_{p_1}(x)f'(x) + Q_{p_2}(x)f''(x)] = \alpha\,(x - \gamma) \cdot f(x), \qquad \forall x \in \mathcal{X} \tag{4.18}$$

	$\mathbf{p_1}$	$\mathbf{p_2}$	$\mathbf{p}$
a)	1	0	1
b)	1	1	1
c)	{0,1}	2	1

Table 5: *Possible degrees of the polynomials $P_{p_1}(x)$ and $Q_{p_2}(x)$ on the design space $\mathcal{X} = \mathbb{R}_0^+$ for $p = 1$ and $x_0 = 0$*

where $\gamma \in \mathbb{R}$ is the unknown root of $R_1(x)$, $p = \max(p_1, p_2 - 1) = 1$ and $f(x) = \sum_{k=0}^{n+1} s_k x^k$ is the unknown polynomial solution. The different combinations for the degrees of the polynomials $P_{p_1}(x)$ and $Q_{p_2}(x)$ are listed in Table 5. All cases have been discussed in Section 3.1 for the design space $\mathcal{X} = \mathbb{R}$ and $p = 0$ already. We will cross-reference the corresponding efficiency functions to stress the influence of the design space $\mathcal{X}$.

To derive D-optimal designs ξ^* for an admissible efficiency function $\lambda(x)$ with

$$(\log \lambda(x))' = \frac{a + cx}{d + ex + fx^2} \tag{4.19}$$

one may apply the following Theorem with

$$\begin{aligned}
\tau_{-1}(k) &= -\left(\frac{(k-1)\,(f(k-2)+c)}{(n+1)(c+fn)} - 1\right) \\
\tau_0(k) &= -\frac{k\,(a + e(k-1))}{(n+1)(c+fn)} \\
\tau_{+1}(k) &= -\frac{d(k+1)k}{(n+1)(c+fn)} \\
\tau_{+2}(k) &= 0\,.
\end{aligned} \tag{4.20}$$

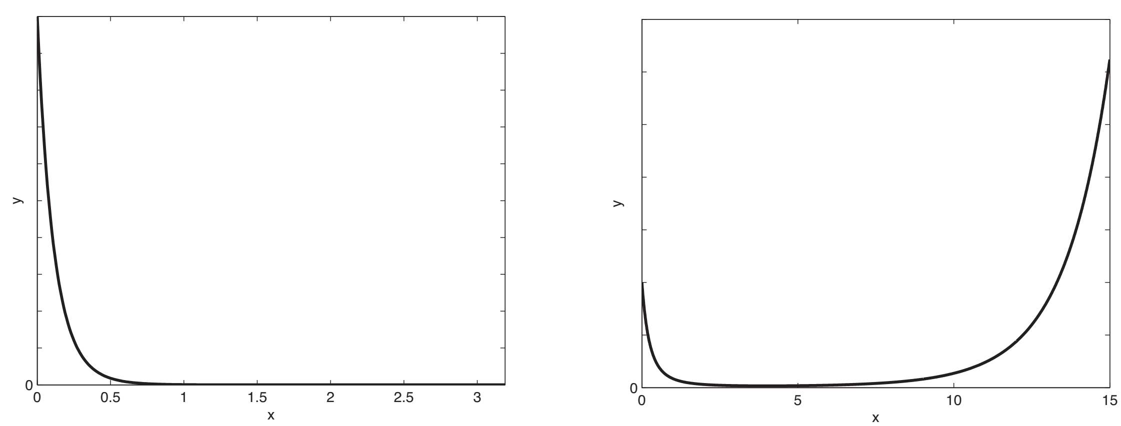
as entries of the band matrix A defined in (4.3).

Theorem 4.7. *The D-optimal design for the weighted polynomial regression model (1.1) on the design space $\mathcal{X} = \mathbb{R}_0^+$ for an admissible efficiency function λ satisfying (4.19) has equal mass at $(n+1)$ support points. If Assumption 4.1 is satisfied and the smallest support point of the D-optimal design is 0, then these points are given by the roots of the polynomial $f(x) = \sum_{j=0}^{n+1} s_j x^j$, where the vector of coefficients $\mathbf{s}^T = (s_0, \dots, s_{n+1})$ is the eigenvector corresponding to the smallest eigenvalue of the $(n+2)\times(n+2)$ band matrix A defined in (4.3). The entries $\tau_{-1}(k)$, $\tau_0(k)$, $\tau_{+1}(k)$ and $\tau_{+2}(k)$ depend on the the efficiency function λ and are given in (4.20).*

a) If $\boldsymbol{p_1 = 1}$ and $\boldsymbol{p_2 = 0}$, the corresponding efficiency function was derived in (3.9) and was admissible on the design space $\mathcal{X} = \mathbb{R}$ with $\alpha_1 > 0$ and $z_1 \in \mathbb{R}$. The support of the D-optimal design on the design space $\mathcal{X} = \mathbb{R}$ is located at the roots of the Hermite polynomial $H_{n+1}(\alpha_1 x - z_1)$, see (3.10). If z_1 is smaller than the largest root h_{n+1} of the $(n+1)$th Hermite polynomial $H_{n+1}(x)$ it follows from Lemma 4.2 that the D-optimal design on the design space $\mathcal{X} = \mathbb{R}_0^+$ is supported at $x_0 = 0$ and Theorem 4.7 can be used to determine the D-optimal design.

For example, if $\alpha_1 = 5, z_1 = 1$ we have for the cubic regression model $h_4 = 1.65068$, and thus the D-optimal design with efficiency function (a) can be derived by an application of Theorem 4.7 with $(\log \lambda(x))' = \frac{10-50x}{1}$. The resulting support points of the D-optimal design have equal mass at $0, 0.1524, 0.3419$ and 0.5569.

b) The case $\boldsymbol{p_1 = 1}$ and $\boldsymbol{p_2 = 1}$ yields the efficiency function (3.11). This function is admissible and the D-optimal design yields to a support point at $x_0 = 0$ if the parameters satisfy $z_1 > 0$, $c > 0$ and $\alpha \le cz_1$. Two efficiency functions of the type (3.11)



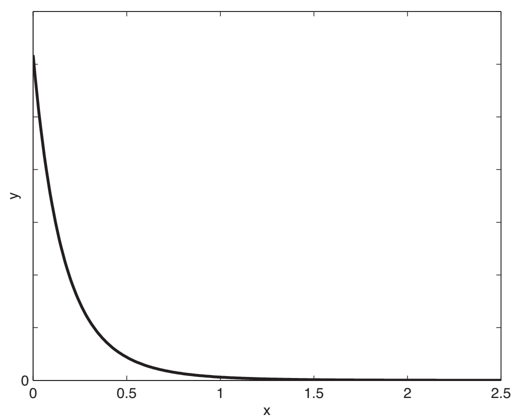
(a) $\lambda(x) = (x+1)^{-5}\exp(-x)$ (b) $\lambda(x) = (x+z_1)^{-5}\exp(x)$

Figure 11: *Plots of efficiency function (3.11)*

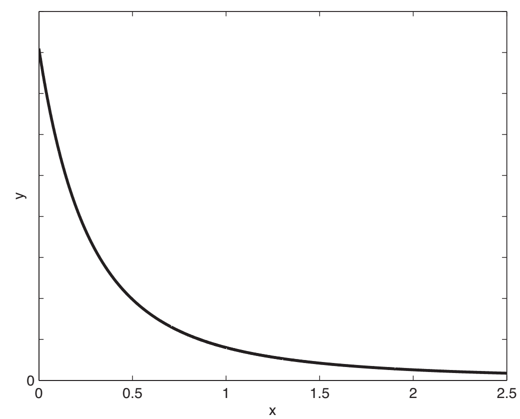
are plotted in Figure 11. The efficiency function (a) is admissible while for efficiency function (b) the induced design space $\mathcal{G}$ is not bounded. For the cubic regression model, the D-optimal design for efficiency function (a) is derived by an application of Theorem 4.7 and has equal mass at the points $0, 0.2465, 1.065$ and 3.2871.

c) For the choices $\boldsymbol{p_1 \in \{0, 1\}}$ and $\boldsymbol{p_2 = 2}$ we have to distinguish three cases corresponding to the possible real roots of the polynomial $Q_2(x)$ again. For the sake of brevity we restrict the discussion to the case $p_1 = 1$. It is worthwhile to mention that all of the following cases yield admissible efficiency functions on the design space $\mathcal{X} = \mathbb{R}_0^+$.

If $\boldsymbol{p_1 = 1}$ and $\boldsymbol{p_2 = 2}$, and if $Q_2(x)$ has two different real roots, say $-z_1$ and $-z_2$, we derive the efficiency function (3.8) again. This efficiency is admissible if the conditions $z_1 > 0, z_2 < 0$, α_2 even, $\alpha_1 + \alpha_2 < -2n$ and $-\alpha_2 z_1 + \alpha_1 z_2 > 0$ are satisfied. These choices also assure a maximum of $\lambda(x)$ at $x = 0$ and it follows from Lemma 4.1 that the D-optimal design has positive weight at $x = 0$.



(a) $\lambda(x) = (x+1)^{-5}(-3-x)^{-4}$



(b) $\lambda(x) = (x+1)^{-5}(-3-x)^{4}$

Figure 12: *Plots of efficiency function (3.8)*

Two efficiency functions of the type (3.8) are plotted in Figure 12. Even though both efficiencies functions look similar, only efficiency function (a) is admissible for the cubic regression model on the design space $\mathcal{X} = \mathbb{R}_0^+$; the induced design space $\mathcal{G}$ of efficiency function (b) is not bounded. The D-optimal design for the cubic regression model with efficiency function (a) derived by an application of Theorem 4.7 has equal mass at the points $0, 0.2609, 1.2287$ and 5.1883.

The case where $Q_2(x)$ has a real root of multiplicity 2, say $-z_1$, we derive the efficiency function (3.7). This function is admissible if $\alpha_2 < -2n$ and $z_1 \geq 0$. Moreover, the efficiency function has a maximum at $x = 0$ if $\alpha_1 \leq \alpha_2 z_1$.

Finally we consider consider the case where $Q_2(x)$ has no real roots. Here the efficiency is given in equation (3.5). Again, one may choose $a < -n-1$, $b \in \mathbb{R}$ arbitrarily, but z_1 must be smaller than the largest root of of the Jacobi polynomial $P_{n+1}^{(a+ic,a-ic)}(ix)$ to assure support at $x_0 = 0$.

5 A bounded design space $\mathcal{X} = [\mathbf{0}, \mathbf{b}]$

A bounded convex design space like $\mathcal{X} = [0, b]$ with $b > 0$ can be treated in a similar manner. As mentioned in Section 4, one may not be able to differentiate (2.4) with respect to the points x_0 or x_n if they are located at the boundary of the design space $\mathcal{X}$, i.e. $x_0 = 0$ or $x_n = b$. Hence, we have to distinguish three main cases.

- Neither the point 0 nor b is a support point of the D-optimal design.
- The point b is and the point 0 is not a support point of the D-optimal design.
- The points 0 and b are both support points of the D-optimal design.

These three different cases are discussed in Section 5.1, 5.2 and 5.3, respectively. Note that the fourth case - where the point 0 is and the point b is not a support point of the D-optimal design - can be reduced to the opposite situation by an application of the linear transformation

$$y(x) = b - x$$

and the following result.

Lemma 5.1. *Let $x_0, \ldots, x_n$ denote the support points of the D-optimal design ξ^* for the regression model (1.1) on the design space $\mathcal{X}$. Consider the linear transformation*

$$y(x) = \alpha + \beta x, x \in \mathcal{X}$$

with $\alpha \in \mathbb{R}$ and $\beta \in \mathbb{R}\backslash 0$. Then the design putting equal weights on

$$\frac{x_0 - \alpha}{\beta}, \frac{x_1 - \alpha}{\beta}, \ldots, \frac{x_n - \alpha}{\beta}$$

is D-optimal for the efficiency $\lambda \circ y$ on the design space $y^{-1}(\mathcal{X})$.

A boundary point of the design space $\mathcal{X}$ is a support point of the D-optimal design if there exists a global maximum of the efficiency function $\lambda(x)$ at this point (see Lemma 4.1). As noted before this is only a sufficient but not a necessary condition. In other words there may exist efficiency functions which do not have a maximum at one of the boundary points, but the D-optimal design on the interval $\mathcal{X} = [0, b]$ is supported at $x = 0$ or $x = b$. On the other hand, if the efficiency function λ is admissible on $\mathcal{X} = \mathbb{R}_0^+$, and b is larger than the largest support point of the D-optimal design on $\mathcal{X} = \mathbb{R}_0^+$, then this design is also the D-optimal design on the interval $\mathcal{X} = [0, b]$. We can then use the methodology presented in the subsections of Section 4 to derive D-optimal designs.

Consequently, most of the possible efficiency functions are already covered in the discussion of Section 4.1 and 4.2. For the admissible efficiency functions presented in Section 4.1.1 we derive in Section 5.2.2 D-optimal designs with one support point at the boundary, and for the cases considered in Section 4.2.1 we derive in Section 5.3.2 D-optimal designs with two support points at the boundary of the design space $\mathcal{X} = [0, b]$.

5.1 No support points at the boundary

We first consider the case where neither $x = 0$ nor $x = b$ are support points of the resulting D-optimal design. Since all support points are assumed to be in the interior of the design space, the differential equation is given by (3.3), that is

$$P_{p_1}(x)f'(x) + Q_{p_2}(x)f''(x) = \alpha R_p(x)f(x), \qquad \forall x \in \mathcal{X}$$

where $p = \max(p_1 - 1, p_2 - 2)$. There are two major differences between admissible efficiency functions on the design space $\mathcal{X} = \mathbb{R}_0^+$ and $\mathcal{X} = [0, b]$.

- The efficiency function λ may have poles or may vanish in $\mathcal{X}^C = [0, b]^C$.
- It is not required that the efficiency function λ vanishes at infinity.

In the following discussion we restrict ourselves to the new cases arising from a bounded design space like $\mathcal{X} = [0, b]$.

5.1.1 p=0: more explicit polynomial solutions

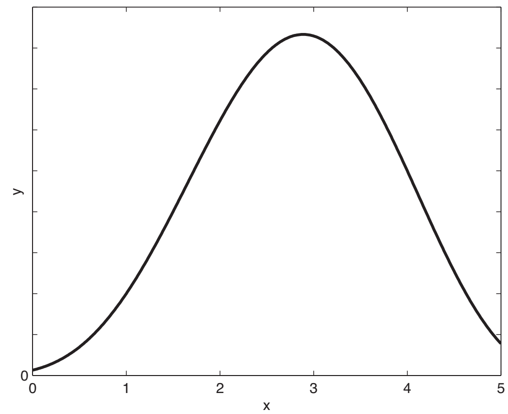
The possible degrees of the polynomials $P_{p_1}(x)$ and $Q_{p_2}(x)$ on the design space $\mathcal{X} = [0, b]$ for $p = 0$ are listed in Table 2. Again, the case $p = 0$ admits an explicit characterization of the D-optimal designs in terms of classical orthogonal polynomials.

a) If $\boldsymbol{p_1 = 1}$ and $\boldsymbol{p_2 = 2}$, possible shapes of efficiency functions $\lambda(x)$ have been discussed in (3.5), (3.7), (3.8). Recall that the D-optimal designs for (3.5) and (3.7) are determined by the roots of the Jacobi polynomial (3.6) and by the roots of the generalized Bessel polynomial (4.1), respectively. For the sake of brevity we only present details for the situation corresponding to (3.8), since the conditions for the other two cases arise naturally. For the special choice of $z_1 = 0$ and $z_2 = b$ in (3.8), we derive for $\alpha_1 > 0, \alpha_2 > 0$ the efficiency function

$$\lambda(x) = x^{\alpha_1}(b - x)^{\alpha_2} .$$

This efficiency function has been considered by numerous authors (e.g. Federov [21], Theorem 2.3.3 or Karlin and Studden [27], Theorem 3.2). It is well known that the D-optimal design is supported at the roots of the Jacobi polynomial $P_{n+1}^{(\alpha_1-1,\alpha_2-1)}\left(\frac{2x-b}{b}\right)$. For $z_1 < 0$ and $z_2 > b$ the D-optimal design has support at the roots of

$$P_{n+1}^{(\alpha_1-1,\alpha_2-1)}\left(2\frac{x - z_1}{z_2 - z_1} - 1\right),$$



(a) $\lambda(x) = (x+1)^3(6-x)^4$

Figure 13: *Plot of efficiency function (3.5)*

provided that the largest and smallest root of this polynomial are contained in the interval $[0, b]$. Note that choosing z_1 (or z_2) too small (or too large) leads to support points which are not located in the interior of the design space $\mathcal{X} = [0, b]$ anymore. For example, if we choose $z_1 = -1$ and $z_2 = 6$, an admissible efficiency function of the type (3.5) is plotted in Figure 13. For the cubic regression model on the design space $\mathcal{X} = [0, 5]$, the D-optimal design for efficiency function $\lambda(x) = (x+1)^3(6-x)^4$ has equal weights at the points $0.5452, 2.0089, 3.5190$ and 4.8602.

b) If $\boldsymbol{p_1 = 1}$ and $\boldsymbol{p_2 = 0}$, we obtain the efficiency function (3.9). For $\alpha_1 \neq 0$ and $z_1 \in \mathbb{R}$, the D-optimal design on the design space $\mathcal{X} = \mathbb{R}$ has equal weight at the roots of the Hermite polynomial $H_{n+1}(\alpha_1 x + z_1)$ (see e.g. Federov [21], Theorem 2.3.3 or Karlin and Studden [27], Theorem 3.5). If the roots of this polynomial are located inside the interval $[0, b]$, then the design is also D-optimal on the design space $\mathcal{X} = [0, b]$. Otherwise, Lemma 4.2 yields that at least one of the boundary points is a support point of the D-optimal design. This case is discussed in Section 5.2.2.

c) Next we consider the case $\boldsymbol{p_1 = 1}$ and $\boldsymbol{p_2 = 1}$. This case appeared first in (3.11), and the D-optimal design on the design space $\mathcal{X} = \mathbb{R}_0^+$ has equal mass at the roots of the Laguerre polynomial (4.2). The condition $z_1 > 0$, $c > 0$ and $\alpha > cz_1$ have also to be satisfied on the design space $\mathcal{X} = [0, b]$. Furthermore, the largest root of $L_{n+1}^{(\alpha-1)}(c(x+z_1))$ has to be smaller than b. The support points of the D-optimal design on the design space $\mathcal{X} = [0, b]$ are then located at the roots of this polynomial. Otherwise a boundary point of the design interval is among the support points of the optimal design.

d) The case $\boldsymbol{p_1 = 0}$ and $\boldsymbol{p_2 = 2}$ has been covered at (3.12), (3.13) and (3.14). The D-optimal designs for these efficiency function have always a support point either at $x = 0$ or $x = b$. This case is discussed in Section 5.2.2.

5.1.2 p=1: eigenvalue problems similar to Section 4.1.2

We now consider the case $p = 1$. The differential equation for this case is the same as for the design spaces $\mathcal{X} = \mathbb{R}$ and $\mathcal{X} = \mathbb{R}_0^+$ (with $x_0 > 0$) and is stated in equation (3.15) with $p = \max(p_1 - 1, p_2 - 2) = 1$. A necessary condition that the support points are located in the interior of the design space $\mathcal{X} = [0, b]$ is that the efficiency function λ does not have a maximum at either one of the boundary points. In general it seems to be difficult to specify simple conditions for the efficiency function λ such that a resulting D-optimal design is located in the interior of the design space $\mathcal{X} = [0, b]$ and a detailed discussion on this matter would be beyond the scope of this paper.

All of the possible shapes have been discussed before and are listed in Table 3. The only difference now is that we admit efficiency functions which have roots or are negative outside of the interval $[0, b]$. The generalization is straightforward and thus a detailed treatment is omitted. We also omit this case in the later discussion since the differential equation is essentially the same as in Section 4.1 and thus the analytical results are the same as well. Refer to Table 3 for possible combinations of the polynomial degrees of $P_{p_1}(x)$ and $Q_{p_2}(x)$, and to the values of τ given in (4.4) which are needed to use Theorem 4.3.

5.2 One support point at the boundary

If the right boundary point $x_n = b$ is a support point of the D-optimal design for the weighted polynomial regression model (1.1) on the design space $\mathcal{X} = [0, b]$, similar arguments as in the previous sections give the differential equation

$$(x - b)\left(P_{p_1}(x) f'(x) + Q_{p_2}(x) f''(x)\right) = \alpha R_p(x) f(x), \qquad \forall x \in \mathcal{X} \tag{5.1}$$

with $p = \max(p_1, p_2 - 1)$. The constant α is determined by comparing the leading coefficients. All possible efficiency functions have been discussed before but for different design spaces.

5.2.1 p=0:

Because the discussion for the case $p = 0$ is essentially the same as in Section 4.2.1, we omit the details. The possible polynomial degrees for $P_{p_1}(x)$ and $Q_{p_2}(x)$ on the design space $\mathcal{X} = [0, b]$ are listed in Table 4.

5.2.2 p=1: more eigenvalue problems

Similarly, the possible combination for the degrees of the polynomials $P_{p_1}(x)$ and $Q_{p_2}(x)$ have already been discussed in Section 4.2.2 and are listed in Table 5. The case $x_n = b$, which is assumed in this section, appears for example if the efficiency function λ either has a global maximum at b (see proof of Lemma 4.1), or - because of a similar argument as in the proof of Lemma 4.2 - there exists a D-optimal design on the design space $\mathcal{X} = (0, b+\delta], \delta > 0$ with support $x_n > b$.
For the first case the conditions on λ arise naturally. For the second case one may use results of Section 4.1.1 for $p = 0$ to check if the upper boundary point b of the design space $\mathcal{X} = [0, b]$ is smaller than the largest support point of the D-optimal design on $\mathcal{X} = \mathbb{R}_0^+$. Note that the only "new" admissible efficiency functions are given by (3.12), (3.13) and (3.14) with the condition that the efficiency λ attains its maximum at b for $x \in \mathcal{X} = [0, b]$.

To derive D-optimal designs for the case $p = 1$ on the design space $\mathcal{X} = [0, b]$ for admissible efficiency functions satisfying (4.19) one may apply the following theorem, where the entries for the band matrix A defined in (4.3) are given by

$$\begin{aligned}
\tau_{-1}(k) &= -\left(\frac{(k-1)\,(f(k-2)+c)}{(n+1)(c+fn)} - 1\right) \\
\tau_0(k) &= -\frac{k\,((a-bc)+(e-bf)\,(k-1))}{(n+1)(c+fn)} \\
\tau_{+1}(k) &= -\frac{(k+1)\,((d-be)\,k-ab)}{(n+1)(c+fn)} \\
\tau_{+2}(k) &= \frac{bd(k+1)(k+2)}{(n+1)(c+fn)}\,.
\end{aligned} \tag{5.2}$$

Theorem 5.2. *The D-optimal design for the weighted polynomial regression model (1.1) on the design space $\mathcal{X} = [0, b], b > 0$ for an admissible efficiency function λ satisfying (4.19) has equal mass at $(n+1)$ support points. If Assumption 4.1 is satisfied, the smallest support point of the D-optimal design is positive and the largest support point equals b, then these points are given by the roots of the polynomial $f(x) = \sum_{j=0}^{n+1} s_j x^j$, where the vector of coefficients $\mathbf{s}^T = (s_0, \ldots, s_{n+1})$ is the eigenvector corresponding to the smallest eigenvalue of the $(n+2) \times (n+2)$ band matrix A defined in (4.3). The entries $\tau_{-1}(k)$, $\tau_0(k)$, $\tau_{+1}(k)$ and $\tau_{+2}(k)$ depend on the the efficiency function λ and are given in (5.2).*

5.3 Two support points at the boundary

If both boundary points of the design space $\mathcal{X} = [0, b]$ are support points of the D-optimal design - i.e. $x_0 = 0$ and $x_n = b$ - the differential equation is given by

$$x \cdot (x-b)\,(P_{p_1}(x)f'(x) + Q_{p_2}(x)f''(x)) = \alpha R_p(x)f(x), \qquad \forall x \in \mathcal{X} \tag{5.3}$$

with $p = \max(p_1 + 1, p_2)$.

5.3.1 p=0: one more "classical" orthogonal polynomial

If $p = 0$ we have $\boldsymbol{p_1 = p_2 = 0}$ and we obtain the differential equation

$$x \cdot (x - b)\, f''(x) - n(n+1) f(x) = 0\,.$$

Solving (2.3) yields

$$\lambda(x) = 1$$

for some $c \in \mathbb{R}^+$. This efficiency function corresponds to homoscedastic data. The D-optimal design has support at the roots of

$$x(x-b)L'_n\left(\frac{2x-b}{b}\right),$$

where $L'_n(x)$ is the derivative of the nth Legendre polynomial (see e.g. Karlin and Studden [28], Theorem 3.1 or Pukelsheim [34], Chapter 9.5). For the homoscedastic cubic regression model on the design space $\mathcal{X} = [0, 5]$, the D-optimal design has equal mass at the points $0, 1.382, 3.618$ and 5.

5.3.2 p=1: more eigenvalue problems

The case $p = 1$ for the differential equation (5.3) only permits two cases for the polynomials $P_{p_1}(x)$ and $Q_{p_2}(x)$, namely $p_1 = p_2 = 0$ and $p_1 = 0, p_2 = 1$. To derive D-optimal designs for an admissible efficiency function $\lambda(x)$ with

$$(\log \lambda(x))' = \frac{a}{d + ex} \tag{5.4}$$

one may apply the following theorem, where the entries for the band matrix A defined in (4.3) are given by

$$\begin{aligned} \tau_{-1}(k) &= -\left(\frac{(k-1)\,(e(k-2)+a)}{(n+1)(a+en)} - 1\right) \\ \tau_0(k) &= -\frac{k\,((d-be)\,(k-1) - ba)}{(n+1)(a+en)} \\ \tau_{+1}(k) &= \frac{bd(k+1)k}{(n+1)(a+en)} \\ \tau_{+2}(k) &= 0\,. \end{aligned} \tag{5.5}$$

Theorem 5.3. *The D-optimal design for the weighted polynomial regression model (1.1) on the design space $\mathcal{X} = [0,b], b > 0$ for an admissible efficiency function λ satisfying (5.4) has equal mass at $(n+1)$ support points. If Assumption 4.1 is satisfied and $x_0 = 0$ and $x_n = b$ are both support points of the D-optimal design, then these points are given by the roots of the polynomial $f(x) = \sum_{j=0}^{n+1} s_j x^j$, where the vector of coefficients $\mathbf{s}^T = (s_0, \ldots, s_{n+1})$ is the eigenvector corresponding to the smallest eigenvalue of the $(n+2) \times (n+2)$ band matrix A defined in (4.3). The entries $\tau_{-1}(k)$, $\tau_0(k)$, $\tau_{+1}(k)$ and $\tau_{+2}(k)$ depend on the the efficiency function λ and are given in (5.5).*

We now discuss the two possible cases which have also been analyzed in Chang and Lin [10] but in a less general fashion. If $\boldsymbol{p_1 = 0}$ and $\boldsymbol{p_2 = 0}$, equation (2.3) takes the form $P_0(x)/Q_0(x) = -a$ and the corresponding efficiency function is listed in equation (4.16). To guarantee that the D-optimal design has a support point at $x_n = b$, the largest root of the Laguerre polynomial $L_n^{(1)}(ax)$ has to be larger than b. If we choose with $a = 1$ the efficiency function $\lambda(x) = \exp(-x)$, the largest root of $L_n^{(1)}(x)$ is 7.7588. On the design space $\mathcal{X} = [0,5]$, the D-optimal design is derived by an application of Theorem 5.3 and puts equal mass at the points $0, 0.7822, 2.6291$ and 5.

The remaining case $\boldsymbol{p_1 = 0}$ and $\boldsymbol{p_2 = 1}$ has been discussed in (4.17). If the imposed conditions $a < 2n$ and $z_1 > 0$ remain active, the D-optimal design on the design space $\mathcal{X} = \mathbb{R}_0^+$ has support at the roots of the Jacobi polynomial $xP_n^{(1,a-1)}(\frac{2}{z_1}x+1)$. If the largest root of this polynomial is larger than b, then the D-optimal design on $\mathcal{X} = [0,b]$ puts weights at the boundary points 0 and b. To illustrate the results we consider the efficiency function $\lambda(x) = (x+3)^{-8}$, for which the largest root of that Jacobi polynomial is 14.3739. Thus, on the design space $\mathcal{X} = [0,5]$ the D-optimal design can be calculated with the aid of Theorem 5.3. The resulting design for the cubic regression model puts equal mass at the support points $0, 0.4977, 2.0515$ and 5.
We may now also chose $a \neq 0$ and $z_1 \in [0,b]^C$ arbitrarily. But for this choice it must be verified that the D-optimal design is supported at 0 and b. For example, the choice $a = z_1 = 4$ results in the efficiency function $\lambda(x) = (x+4)^4$. The D-optimal design for the weighted cubic regression model on the design space $\mathcal{X} = [0,5]$ is derived by an application of Theorem 5.3 and puts equal mass at the points $0, 2, 4$ and 5.

In either case, the D-optimal design can be calculated with Theorem 5.3.

A Appendix: Proofs

Proof of Lemma 2.1. We prove the case $p = \max\{p_1 - 1, p_2 - 2\} = 1$ and assume that all support points are located inside the design space $\mathcal{X}$. The remaining cases follow analogously.

We first show that the D-optimal design ξ^* is supported at $n+1$ points. The dispersion function (2.2) can be restated without loss of generality as

$$d(x, \xi) = \lambda(x) \cdot T_{2n}(x) \tag{A.1}$$

where in the following discussion $T_i(x)$ denotes a polynomial of degree i. We set the derivative of (A.1) equal zero and observe assumption (2.3), i.e.

$$Q_{p_2}(x) T_{2n-1}(x) + P_{p_1}(x) T_{2n}(x) = 0\,. \tag{A.2}$$

Because $\max\{p_1 - 1, p_2 - 2\} = 1$, the polynomial on the left hand side of equation (A.2) has at most $2n+2$ extreme points. Let ξ^* denote the D-optimal design and N the number of its support points. From standard arguments in design literature it follows that $N \geq n+1$ and we assume $N \geq n+2$. The dispersion function (2.2) has global maxima at the support points of the D-optimal design. This yields at least $n+2$ local maxima and $n+1$ local minima in between resulting in at least $2n+3$ critical points contradicting the polynomial degree of (A.2) (note that all support points are located in the interior of the design space). Thus, the assumption that the D-optimal design ξ^* has more than $n+1$ support points is false. There exists a D-optimal design, and since $N \geq n+1$ it follows that any D-optimal design has $N = n+1$ support points.

We now prove the uniqueness of the D-optimal design ξ^*. For this, we have to show that the D-optimal information matrix M^* is uniquely determined by a single design $\xi^* = \arg\max_\xi \det(M(\xi))$ where

$$M^* = M(\xi^*)$$

and M as defined in (2.1). From Silvey [35], Sec. 3.4 it follows that the set of design measures is convex, and the set of D-optimal design measures is also convex. Thus, if there exist two two different D-optimal designs, say ξ^* and ξ (both with information matrix M^*), then the design

$$\eta = \alpha\xi^* + (1-\alpha)\xi, \quad 0 \leq \alpha \leq 1$$

would also be D-optimal, again producing the same D-optimal information matrix M^*. From the first part of this proof it follows that a D-optimal design is supported at $n+1$ points, but the design η has at least $n+2$ support points for $0 < \alpha < 1$ because the two designs ξ^* and ξ are different. This is a contradiction and therefore the D-optimal design ξ^* is unique. □

Proof of Lemma 4.1. The determinant of the matrix $M(\xi)$ for a $(n+1)$ point design ξ is given by

$$|M(\xi)| = \left(\frac{1}{n+1}\right)^{n+1} \cdot \prod_{j=0}^{n} \lambda(x_j) \cdot \prod_{0 \leq i < j \leq n} (x_j - x_i)^2\,.$$

For D-optimality, this expression has to be maximized with respect to the support points x_j for $j = 0, \dots, n$. Maximizing $|M(\xi)|$ with respect to $x_0 \in \mathcal{X}$ for fixed $x_1, \dots, x_n$ readily yields the assertion. $\square$

Proof of Lemma 4.2. We only demonstrate the case $p = 0$. The case $p = 1$ is derived by the same arguments. Let λ be an admissible efficiency function on the design space $\mathcal{X} = \mathbb{R}$, and let $\xi^*_{\mathbb{R}}$ denote the D-optimal design having at least one negative support point. Thus, the D-optimal design $\xi^*_{\mathbb{R}_0^+}$ on the design space $\mathcal{X} = \mathbb{R}_0^+$ has to differ from the D-optimal design $\xi^*_{\mathbb{R}}$ on the design space $\mathcal{X} = \mathbb{R}$. We assume that the smallest support point of $\xi^*_{\mathbb{R}_0^+}$ is positive. The same reasoning as in the proof of Lemma 2.1 yields equation (A.2) where the degree of the corresponding polynomial is $(2n+1)$ because $p = \max\{p_1 - 1, p_2 - 2\} = 0$. Since there is equality in (2.2) at the $(n+1)$ support points of $\xi^*_{\mathbb{R}_0^+}$, there are $(n+1)$ local maxima and n local minima resulting in at least $(2n+1)$ critical points. Since the design $\xi^*_{\mathbb{R}_0^+}$ is not D-optimal on the design space $\mathcal{X} = \mathbb{R}$ (because $\min supp(\xi^*_{\mathbb{R}}) < 0$), the function d defined in (2.2) must exceed $(n+1)$ somewhere in $\mathbb{R}^-$. This requires another minimum, because the efficiency function λ has no roots or poles on $\mathbb{R}$, which contradicts the degree of the polynomial on the left hand side of (A.2). Thus, $x_0 = 0$ is always a support point of the design $\xi^*_{\mathbb{R}_0^+}$. $\square$

Proof of Lemma 5.1. The D-optimality criterion maximizes the determinant of the Fisher information matrix (2.1). In the case of $(n+1)$ support points, the weights are uniform, and the determinant can explicitly be stated as (2.4). A straightforward calculation yields the assertion. $\square$

Proof of Theorem 4.3, 4.7, 5.2 and 5.3. It follows instantly that the resulting D-optimal design is equally supported at $(n+1)$ support points because of Corollary 2.2. We only prove Theorem 5.2, where the design space is given by $\mathcal{X} = [0, b]$ with $x_0 > 0$ and $p = \max(p_1, p_2 - 1) = 1$. The arguments only need to be slightly modified for the remaining cases and are omitted for the sake of brevity.
Note that it can be shown that b is always an eigenvalue of the matrix A, whose corresponding polynomial (determined by the coefficients of the corresponding eigenvector) yields to a non-valid solution because equation (5.1) reduces with the choice $\gamma = b$ to equation (3.3) with $p = 0$. Thus, let γ_j, $j = 1, \dots, r$ denote the distinct eigenvalues of A excluding b. We split the proof into 4 parts.

Lemma A.1. *The upper bound b of the design space $\mathcal{X}$ is always a root of any polynomial f which is a solution of the differential equation (5.1).*

Lemma A.2. *All eigenvalues γ_j, $j = 1, \dots, r$ are real.*

Lemma A.3. *Let ξ^* denote the D-optimal design for the design space $\mathcal{X} = [0, b]$. Then, the slope of the function on the left hand side of (2.2) at the point $x_n = b$ is strictly positive i.e. $d'(b, \xi^*) > 0$.*

Lemma A.4. *The D-optimal design for the weighted polynomial regression model (1.1) has equal masses at the roots of the polynomial $\mathbf{f}^T\mathbf{s}_j$, where $\mathbf{s}_j$ is the eigenvector corresponding to the smallest eigenvalue $\gamma_j \neq b$, $j = 1, \dots, r$ of the matrix A defined in (4.3).*

□

Proof of Lemma A.1. It follows by a direct calculation that the vector $\mathbf{f}^T(b) = (1, b, b^2, \dots, b^{n+1})$ is a left eigenvector of the matrix A for the eigenvalue $\gamma = b$, i.e.

$$\mathbf{f}^T(b) \cdot A = b\mathbf{f}^T(b) .$$

Consequently, we observe that

$$f_j(b) = \mathbf{f}^T(b) \cdot \mathbf{s}_j = \frac{1}{b}\mathbf{f}^T(b) \cdot A \cdot \mathbf{s}_j = \frac{1}{b}\mathbf{f}^T(b) \cdot \gamma_j \cdot \mathbf{s}_j = \frac{\gamma_j}{b}\mathbf{f}^T(b) \cdot \mathbf{s}_j = \frac{\gamma_j}{b} \cdot f_j(b)$$

for any polynomial solution $f_j(x) = (1, x, \dots, x^{n+1}) \cdot \mathbf{s}_j$ corresponding to the eigenvector $\mathbf{s}_j$ and its eigenvalue $\gamma_j \neq b$, $j = 1, \dots, r$, which gives $f_j(b) = 0$ for all $j = 1, \dots, r$. □

Proof of Lemma A.2. We state equation (5.1) as a singular Sturm-Liouville equation with boundary condition $f(b) = 0$ and the requirement of a polynomial solution of degree $(n + 2)$. See e.g. Birkhoff and Rota [6], Chapter 10 for a more detailed discussion of this topic.

We start by restating equation (5.1) as

$$L[f] + (-\gamma)\rho(x)f = 0, \qquad x \in [0, b] \tag{A.3}$$

with

$$\begin{aligned}
L[f] &= \frac{d}{dx}\left[p(x)\frac{df}{dx}\right] + q(x)f(x) \\
p(x) &= \lambda(x) \\
\rho(x) &= |\alpha| \cdot \lambda(x) \;/\; \big(Q_{p_2}(x)(b - x)\big) \\
q(x) &= |\alpha| \cdot x \cdot \lambda(x) \;/\; \big(Q_{p_2}(x)(b - x)\big) .
\end{aligned}$$

Equation (A.3) is the general form of a Sturm-Liouville equation. Note that both $p(x)$ and $\rho(x)$ are real valued, positive functions on $(0, b)$ since the polynomial $Q_{p_2}(x)$ has no roots in $\mathcal{X} = (0, b)$, and because we can assume that $Q_{p2(x)}$ is positive in $\mathcal{X}$ without loss of generality. This set is singular because the functions $p(x)$ and $\rho(x)$ either vanish or are singular at the boundary points $x = 0$ and $x = b$. Nevertheless, several properties of a regular Sturm-Liouville system still apply here: the differential operator L is still self-adjoint for the solution set (see Birkhoff and Rota [6], Chapter 10 or Arfken and Weber [2], Chapter 9). Eigenvalues of self-adjoint operators are always real valued. □

Proof of Lemma A.3. Let ξ^* denote the D-optimal design for the design space $\mathcal{X} = [0, b]$ with positive smallest support point x_0. The derivation of the right hand side of (2.2) has been derived in the proof of Lemma 4.2 and is given by

$$d'(x, \xi^*) = \lambda(x) T_{2n-1}(x) + \lambda'(x) T_{2n}(x)$$

where $T_i(x)$ denotes a polynomial of degree i. This function vanishes for all interior support points $x_j, j = 0, \ldots, n-1$ (compare (A.2)). Furthermore, the derivative at b needs to be $d'(b, \xi^*) \neq 0$ because otherwise this design would also be optimal for the unbounded design space $\mathcal{X} = \mathbb{R}^+$. This can be seen by applying a similar counting argument as in the proof of Lemma 4.2. On the other hand, $d'(b, \xi^*)$ cannot be negative either: if $d'(b, \xi^*) < 0$ there must be an $\tilde{x} \in \mathcal{X}$, $\tilde{x} \in (0, b]$ with $d(\tilde{x}, \xi^*) > 1$. This contradicts the Kiefer-Wolfowitz theorem because the design ξ^* is D-optimal. □

Proof of Lemma A.4. We arrange the distinct eigenvalues which are different from b as $\gamma_1 < \ldots < \gamma_r$ and denote by n_j the number of roots of the corresponding polynomial solution $f_j(x) = (1, x, \ldots, x^{n+1}) \cdot \mathbf{s}_j^T$ falling into the design space $\mathcal{X} = (0, b]$. Using

$$\frac{d}{dx}\left[p(x)\frac{df}{dx}\right] + ((-\gamma)\rho(x) + q(x))\, f(x) = 0$$

as derived in the proof of Lemma A.2 allows us to apply the Sturm-Comparison-Theorem (see Birkhoff and Rota [6], Theorem 10.3 or Szegö [38], Theorem 1.82.1), which yields that the corresponding number of roots are decreasing, i.e.

$$n + 1 \geq n_1 \geq \ldots \geq n_r \,. \tag{A.4}$$

Note that all polynomials $f_j(b) = 0$, $j = 1, \ldots, r$ because of Lemma A.1.

In what follows we present a careful counting argument of the possible extrema of the function $d(x, \xi^*_{\mathbb{R}_0^+})$, where $\xi^*_{\mathbb{R}_0^+}$ denotes the D-optimal design on $\mathbb{R}_0^+$. The same arguing as used in the proof of Lemma 2.1 yields that the equation $d'(x, \xi^*_{\mathbb{R}_0^+}) = 0$ is equivalent to (A.2), which is in this case a polynomial of degree $(2n+1)$ because $p = \max\{p_1, p_2 - 1\} = 1$. Consequently, the function $d(x, \xi^*_{\mathbb{R}_0^+})$ has at most $(2n+1)$ local extrema.

Let us assume that there exist two different $(n+1)$ point designs, say ξ^* and ξ, with support within the design space $\mathcal{X} = [0, b]$ originating from two different eigenvalues. Since the D-optimality criterion is strictly concave, only one solution can be D-optimal. Otherwise, both designs would have to produce the same information matrix M (as defined in (2.1)) which is not possible in our setting, see the proof of Lemma 2.1. Without loss of generality, let ξ^* be the D-optimal solution. With the same arguments as in the proof of Lemma 2.1 we derive that the structure of an optimal design ξ^* follows a unique and somewhat fixed pattern: there exist $2n$ points in the interval $(0, b)$ solving the equation $d'(x, \xi^*_{\mathbb{R}_0^+}) = 0$, which corresponds to n maxima and n minima.

On the other hand, for the non-optimal design ξ with design points $x_0, \ldots, x_n$, there exists at least one $\tilde{x} \in [0, b]$ with $d(\tilde{x}, \xi) > (n+1)$. Note that the function $d'(x, \xi) = 0$ satisfies

$$d'(x_i, \xi) = 0, \quad i = 0, \ldots, n-1 \tag{A.5}$$

because the corresponding polynomial $\mathbf{f}^T \mathbf{s}_j$ is a solution of the differential equation (5.1). Let us first consider the case where the function on the left hand side of equation (2.2) crosses the line $y = (n+1)$ at two consecutive support points x_i, x_{i+1} and is larger than $n+1$ in the interval (x_i, x_{i+1}). This means that x_i and x_{i+1} are roots of the order larger than two because of equation (A.5). Counting the required roots of (A.2) yields n roots for the support points, n roots for local minima, and 2 additional roots for the second derivative at the points x_i, x_{i+1}. Thus, there are at least $(2n+2)$ roots of (A.2) inside the design space $\mathcal{X} = [0, b]$ (counting with their multiplicities). This contradicts the polynomial degree of $(2n+1)$ of (A.2). On the other hand, if we cross $y = n+1$ at a point $x \notin supp(\xi)$, then there is at least one additional maximum and minimum. A similar argument shows that this is not possible.

Therefore, because there exists a D-optimal designs, the inequality (A.4) is strict for the smallest eigenvalue, i.e $n + 1 = n_1 > n_2$, which yields the desired result. $\square$

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