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AN ALGEBRAIC CONSTRUCTION OF MINIMALLY-SUPPORTED D-OPTIMAL DESIGNS FOR WEIGHTED POLYNOMIAL REGRESSION

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Abstract: In this paper we investigate $(d+1)$-point D-optimal designs for dth degree polynomial regression with weight function $\omega(x) \geq 0$ on the interval $[a,b]$. We propose an algebraic approach and provide a numerical method for the construction of optimal designs. Thus if $\omega'(x)/\omega(x)$ is a rational function and the information of whether the optimal support contains the boundary points a and b is available, the problem of constructing $(d+1)$-point D-optimal designs can be transformed into a differential equation problem. One is led to a matrix that includes a finite number of auxiliary unknown constants, and the differentiation can be solved from a system of polynomial equations in those constants. Moreover, the $(d+1)$-point D-optimal interior support points are the zeros of a polynomial whose coefficients can be computed from a linear system.

Key words and phrases: Approximate D-optimal design, differential equation, matrix, minimally-supported, rational function, weighted polynomial regression.

1. Introduction

This paper is concerned with the weighted polynomial regression model of degree d

$$\begin{aligned} E[Y|x] &= \beta^T f(x), \\ \mathrm{Var}(Y|x) &= \frac{\sigma^2}{\omega(x)}, \end{aligned} \tag{1.1}$$

where $\beta = (\beta_0, \ldots, \beta_d)^T$ denotes the vector of unknown parameters, $f(x) = (1, x, \ldots, x^d)^T$ the vector of monomials up to order d, σ^2 a fixed unknown parameter, $\omega(x) \geq 0$ a weight function on the design interval $I = [a,b] \subseteq \mathbb{R}$. For each $x \in I$, a random variable Y with mean $\beta^T f(x)$ and variance $\sigma^2/\omega(x) > 0$ can be observed. The model (1.1) is widely used in situations where the response is curvilinear, because complex nonlinear relationships can be adequately modeled by polynomials over reasonably small range of the x's, and the variance of an observation depends on the explanatory variable in the hypothesized model, as is the case with some econometric models. For example, if the response variable is household expenditure and one explanatory variable is household income, then the variance of the observations may be a function of household income.

An approximate design ξ is a probability measure on I with finite support. The Fisher information matrix of a design ξ for the parameters β can be expressed as

$$M(\xi) = \int_I \omega(x) f(x) f^T(x)\, d\xi(x).$$

A design ξ^* is called D-optimal for β if ξ^* maximizes the determinant of the information matrix $M(\xi)$ among the set of all designs on I. Note that a D-optimal design minimizes the volume of the ellipsoid of concentration for β. Additional background reading on approximate design theory can be found in Fedorov (1972), Silvey (1980), Atkinson and Donev (1992) and Pukelsheim (1993).

Weighted polynomial regression models have played a central role in the development of optimal design theory. Smith (1918) was the first to study optimal design problems for polynomial regression. Guest (1958) and Hoel (1958) obtained the G- and D-optimal designs for polynomial regression. The pioneering work of Kiefer and Wolfowitz (1960) established the famous D-Equivalence Theorem, a powerful tool to verify whether an approximate design is D-optimal. Karlin and Studden (1966) were the first to investigate the D-optimal designs for weighted polynomial regression. The problem of determining D-optimal designs for weighted polynomial regression models has also been extensively investigated by several authors (see Huang, Chang and Wong (1995), Chang and Lin (1997), Imhof, Krafft and Schaefer (1998), Dette, Haines and Imhof (1999), Fang (2002), Antille, Dette and Weinberg (2003) and Chang (2005), among many others).

The theory of differential equations is a powerful tool for determining the D-optimal designs for weighted polynomial regression. It makes use of the Stieltjes-Schur approach to maximizing a discriminant via an appropriate differential equation, and leads directly to a solution of the D-optimal design problem (see, for example, Szegö (1975, p.140).

This approach was first used by Guest (1958) to determine the G-optimal designs for polynomial regression models. In the following period numerous authors employed the technique to derive D-optimal designs for (1.1) with specific weight functions (see Karlin and Studden (1966), Huang, Chang and Wong (1995), Chang and Lin (1997), Imhof, Krafft and Schaefer (1998), Dette, Haines and Imhof (1999) and Antille, Dette and Weinberg (2003), among many others).

Chang (2005) proves that for the model (1.1) if $\omega'(x)/\omega(x)$ is a rational function and the length of design interval $b-a$ is sufficiently small, then D-optimal designs are equally supported at $d+1$ points, and that the problem of constructing D-optimal support points can be transformed into a differential equation problem leading us to a certain matrix including a finite number of auxiliary unknown constants. Those auxiliary unknown constants can be approximated by Taylor polynomials whose coefficients can be computed recursively. Then the interior support points of the optimal design coincide with the zeros of a polynomial whose coefficients can be obtained from a linear system. These computations can be done very efficiently. The disadvantage of this approach is that in general, it is not applicable when $b-a$ is not close to zero.

The number of the approximate D-optimal support points for the model (1.1) must be at least $d+1$; when optimal designs are found from the class of designs supported on $d+1$ points, they are called minimally-supported D-optimal designs. These designs are optimal within the class of $(d+1)$-point designs and may or may not be optimal within the class of all designs, depending on the weight functions and the design interval. Most of the D-optimal designs for the model (1.1) in the literature are minimally supported, for example, see Theorem 2.3.2 of Fedorov (1972) and Lemma 2.1 of Chang (2005). In such a case, $(d+1)$-point D-optimal designs are also the approximate D-optimal designs. Furthermore, the D-optimality of a $(d+1)$-point design can be checked by D-Equivalence Theorem (Kiefer and Wolfowitz (1960)). The theorem states that a design ξ^* is D-optimal for β if and only if

$$d(x,\xi^*) = \omega(x)f^T(x)M^{-1}(\xi^*)f(x) \leq d+1 \tag{1.2}$$

for all $x \in I$, henceforth abbreviated as the DET. Here equality holds if x belongs to the support of ξ^*.

The purpose of this paper is to extend the differential equation approach of Chang (2005) for (1.1), with $\omega'(x)/\omega(x)$ a rational function on I, to determine the $(d+1)$-point D-optimal design for β. In contrast to Chang (2005), who finds numerical D-optimal designs by using Taylor approximation, we adopt an algebraic method to solve polynomial equations for the auxiliary unknown constants used in Chang (2005). Our choice of the class of weight function is useful since it is quite flexible and includes many well-known weight functions in design literature (Fedorov (1972)).

This paper is organized in the following way. In Section 2, the differential equation for the $(d+1)$-point D-optimal support points for (1.1) is derived. An algebraic method for solving polynomial equations to compute the D-optimal support points is given in Section 3. In Section 4, several examples are presented. Finally, proofs of lemmas in Sections 2 are deferred to the Appendix.

2. The Differential Equation

There are two requirements for using the Stieltjes-Schur approach (Chang (2005)). The first is that the weight function must satisfy

$$\frac{\omega'(x)}{\omega(x)} = \frac{p(x)}{q(x)} = \frac{p_m x^m + p_{m-1}x^{m-1} + \cdots + p_0}{q_n x^n + q_{n-1}x^{n-1} + \cdots + q_0} \tag{2.1}$$

is a rational function on I, where the greatest common divisor of $p(x)$ and $q(x)$ is 1, and $q(x) \neq 0$ for all $x \in I$. Chang (2005) then shows that $\omega(x)$ has the form

$$\left(\prod_i |r_i(x)|^{\alpha_i}\right) e^{r(x)+\sum_i \beta_i \tan^{-1}\gamma_i(x+\delta_i)}, \tag{2.2}$$

where $r_i(x)$ is either a monic linear or quadratic real polynomial, $r(x)$ is a rational function and $\alpha_i, \beta_i, \gamma_i, \delta_i$ are real.

One also requires the knowledge of whether the boundary points a and b are optimal support points. This information for (1.1) exists for many commonly used weight functions, by an argument using DET. For example, the optimal support contains the two boundary points if $\omega(x) = (1 + x^2)^{-n}$ and $n = 0, 1, \ldots, d-1, I = [a, b]$ or $d > n, n(n-1)\cdots(n-d) > 0, I = [-b, b]$ (see Dette, Haines and Imhof (1999)).

Let ξ_{d+1} denote a design supported at x_i with weight $w_i > 0$, $i = 0, \ldots, d$, $\sum_{i=0}^{d} w_i = 1$. Then $\det M(\xi_{d+1}) = (\prod_{i=0}^{d} w_i)(\prod_{i=0}^{d} \omega(x_i) \prod_{0\le i<j\le d}(x_i - x_j)^2)$ by a direct application of the Vandermonde determinant formula. Thus the maximum of $\det M(\xi_{d+1})$ occurs only if $\prod_{i=0}^{d} w_i$ attains its maximum of $1/(d+1)^{d+1}$ when $w_0 = \cdots = w_d = 1/(d+1)$. Then the approximate $(d+1)$-point D-optimal design for (1.1) has the form

$$\xi_{d+1} = \left\{ \begin{array}{cccc} x_0 & x_1 & \cdots & x_d \\ \frac{1}{(d+1)} & \frac{1}{(d+1)} & \cdots & \frac{1}{(d+1)} \end{array} \right\},$$

where $a \le x_0 < \cdots < x_d \le b$ (see Pukelsheim (1993), Corollary 8.12). The following lemma characterizes some situations that the information on $x_0 = a$ or $x_0 > a$ and $x_d = b$ or $x_d < b$ is available. The proof is deferred to an Appendix.

Lemma 2.1. *Consider the $(d+1)$-point D-optimal design ξ^*_{d+1} for dth degree polynomial regression with weight function $\omega(x)$ on $[a, b]$. Then*

(i) *if $\omega(a) = 0$, then $x_0 > a$, and if $\omega(b) = 0$, then $x_d < b$;*

(ii) *if a is a global maximum point of $\omega(x)$ on $[a, b]$, then $x_0 = a$, and if b a global maximum point of $\omega(x)$ on $[a, b]$, then $x_d = b$;*

(iii) *if* $g(a) > 0$, *then* $x_0 > a$, *and if* $g(b) < 0$, *then* $x_d < b$, *where* $g(x) = p(x)/q(x) + s''(x)/s'(x)$ *with* $s(x) = \prod_{i=0}^{d}(x - x_i)$.

For example, if $\omega(x) = x/(1+x)$ and $I = [0, b], b > 0$, then Lemma 2.1 shows $x_0 > 0$ and $x_d = b$. This weight function is considered by Imhof, Krafft and Schaefer (1998). Note that the conditions of (i) and (ii) are more easier verified and applicable than those of (iii).

Let $u(x) = \prod_{a<x_i<b}(x - x_i) = \sum_{i=0}^{\ell} u_i x^i$, $u_\ell = 1$, denote a monic polynomial of degree ℓ which has the ℓ interior support points of design ξ^*_{d+1} as its zeros. Then

$$\ell = \begin{cases} d-1 & \text{if } x_0 = a \text{ and } x_d = b, \\ d & \text{if } x_0 = a \text{ and } x_d < b, \text{ or } x_0 > a \text{ and } x_d = b, \\ d+1 & \text{if } x_0 > a \text{ and } x_d < b. \end{cases}$$

Let $\delta_z(x) = x - z$ if $z \in \{x_0, x_d\}$, $\delta_z(x) = 0$ otherwise. Then the following result characterizes the supporting polynomial $u(x)$ via a second order differential equation. For this, let $deg(h)$ denote the degree of a polynomial h.

Lemma 2.2. *Consider the* $(d + 1)$*-point* D*-optimal design* ξ^*_{d+1} *for* d*th degree polynomial regression with weight function* $\omega(x)$ *on* $[a, b]$. *Then the following second-order nonhomogeneous linear differential equation with polynomial coefficients holds with*

$$L(x) = \delta_a(x)\delta_b(x)q(x)u''(x) + \left[\delta_a(x)\delta_b(x)p(x) + 2(\delta_a(x)\delta_b(x))'q(x)\right] u'(x). \quad (2.3)$$

One has the second-order nonhomogeneous linear equation,

$$L(x) = v(x)u(x), \quad (2.4)$$

where $v(x) = v_k x^k + v_{k-1}x^{k-1} + \cdots + v_0$, $k = \max(m-1, n-2) + deg(\delta_a(x)\delta_b(x))$, $v_0, v_1, \ldots, v_{k-1}$ *are unknown real constants, and* v_k *is the leading coefficient of* $L(x)$.

3. Algebraic Method

In this section we present an algebraic method to solve for the zeros of $u(x)$, a polynomial solution of (2.4). Substituting $u(x) = \sum_{i=0}^{\ell} u_i x^i$ into (2.4) and comparing the coefficients on both sides, we obtain an equation in matrix-vector form

$$(1, x, \ldots, x^{k+\ell-1})Au = 0, \quad (3.1)$$

where $A = (a_{ij}) = D - V, u = (u_0, u_1, \ldots, u_\ell)^T$, and

$$D = \begin{pmatrix}
0 & d_{0,1} & d_{0,2} & 0 & \cdots & \cdots & \cdots & 0 \\
0 & d_{1,1} & d_{1,2} & d_{1,3} & \ddots & & & \vdots \\
0 & d_{2,1} & d_{2,2} & d_{2,3} & \ddots & \ddots & & \vdots \\
\vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\
\vdots & \vdots & & & \ddots & d_{\ell-3,\ell-2} & d_{\ell-3,\ell-1} & 0 \\
\vdots & \vdots & & & & \ddots & d_{\ell-2,\ell-1} & d_{\ell-2,\ell} \\
\vdots & \vdots & & & & & \ddots & d_{\ell-1,\ell} \\
\vdots & \vdots & & & & & & \vdots \\
0 & d_{k,1} & & & & & & \vdots \\
0 & d_{k+1,1} & d_{k+1,2} & & & & & \vdots \\
0 & 0 & d_{k+2,2} & d_{k+2,3} & & & & \vdots \\
\vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\
\vdots & \vdots & & \ddots & \ddots & d_{k+\ell-3,\ell-2} & d_{k+\ell-3,\ell-1} & d_{k+\ell-3,\ell} \\
\vdots & \vdots & & & \ddots & d_{k+\ell-2,\ell-2} & d_{k+\ell-2,\ell-1} & d_{k+\ell-2,\ell} \\
0 & 0 & \cdots & \cdots & \cdots & 0 & d_{k+\ell-1,\ell-1} & d_{k+\ell-1,\ell}
\end{pmatrix}_{(k+\ell)\times(\ell+1)} \tag{3.2}$$

is a band matrix with bandwidth $k+3, d_{i,j}$ is the coefficient of $x^i u_j$ in $L(x)$, and V is a lower band matrix which has the bandwidth $k+1$ and constant values along negative-sloping diagonals of the form

$$V = \begin{pmatrix}
v_0 & 0 & \cdots\cdots & 0 \\
v_1 & v_0 & \ddots & 0 \\
\vdots & \ddots & \ddots\ddots & \vdots \\
v_{k-1} & & \ddots\ddots & 0 \\
v_k & v_{k-1} & \ddots & v_0 \\
0 & v_k & \ddots & v_1 \\
\vdots & \ddots & \ddots\ddots & \vdots \\
0 & \cdots\; 0 & v_k & v_{k-1}
\end{pmatrix}_{(k+\ell)\times(\ell+1)} . \tag{3.3}$$

Note that the first column of D is a zero vector since u_0 does not appear in $L(x)$.

The ijth entry of D can be expressed as

$$d_{i,j} = \begin{cases} j[(j-1)(q_{i-j} - (a+b)q_{i-j+1} + abq_{i-j+2}) + p_{i-j-1} - (a+b)p_{i-j} \\ \quad +abp_{i-j+1} + 4q_{i-j} - 2(a+b)q_{i-j+1}] \\ \qquad\qquad\qquad\qquad \text{if } \delta_a(x) = x-a \text{ and } \delta_b(x) = x-b, \\ j[(j-1)(q_{i-j+1} - aq_{i-j+2}) + p_{i-j} - ap_{i-j+1} + 2q_{i-j+1}] \\ \qquad\qquad\qquad\qquad \text{if } \delta_a(x) = x-a \text{ and } \delta_b(x) = 1, \\ j[(j-1)(q_{i-j+1} - bq_{i-j+2}) + p_{i-j} - bp_{i-j+1} + 2q_{i-j+1}] \\ \qquad\qquad\qquad\qquad \text{if } \delta_a(x) = 1 \text{ and } \delta_b(x) = x-b, \\ j[(j-1)q_{i-j+2} + p_{i-j+1}] \quad \text{if } \delta_a(x) = 1 \text{ and } \delta_b(x) = 1, \end{cases} \tag{3.4}$$

where $p_i = 0$ if $i \notin \{0, \ldots, m\}$ and $q_i = 0$ if $i \notin \{0, \ldots, n\}$.

Now the D-optimal design problem is reduced to determining the $k + \ell$ unknown constants $v = (v_0, \ldots, v_{k-1})^T$ and $\{u_0, \ldots, u_{\ell-1}\}$ such that

$$Au = (0, \ldots, 0)^T, \tag{3.5}$$

by (2.4) and (3.1). This implies that u is orthogonal to the row space of A. Note that the entries of A are functions of v only. Moreover, the number of rows of A is greater than or equal to the number of columns of A. The solution of D-optimal design can be done in three steps. At the first step, we compute v if $k \geq 1$; the second step is to find u; the third step determines the zeros of $u(x)$. If v is available, then it is clear that u can be calculated by a backward-substitution process since A is a special band matrix. The most difficult task is to solve for v.

Here is an algebraic method to compute v for $k \geq 1$. If there exists a real solution for u in (3.5), then the following $\binom{k+\ell}{\ell+1}$ polynomial equations in k variables, $v_0, \ldots, v_{k-1}$,

$$\det A(i_1, \ldots, i_{\ell+1}) = 0, \qquad 1 \leq i_1 < \cdots < i_{\ell+1} \leq k + \ell, \tag{3.6}$$

must have real solutions, where

$$A(i_1, \ldots, i_{\ell+1}) = \begin{pmatrix} a_{i_1 1} & a_{i_1 2} & \cdots & a_{i_1(\ell+1)} \\ a_{i_2 1} & a_{i_2 2} & \cdots & a_{i_2(\ell+1)} \\ \vdots & \vdots & \ddots & \vdots \\ a_{i_{\ell+1} 1} & a_{i_{\ell+1} 2} & \cdots & a_{i_{\ell+1}(\ell+1)} \end{pmatrix}$$

denotes a square matrix composed of the $i_1, \ldots, i_{\ell+1}$th rows of A. Then v can be easily determined by standard numerical software, for example the function NSolve in Mathematica (Wolfram (2003)). For the system of polynomial equations, one constructs a Gröbner basis for $\det A(i_1, \ldots, i_{\ell+1})$, $1 \leq i_1 < \cdots < i_{\ell+1} \leq$

$k+\ell$, to find the solutions (Geddes, Czapor and Labahn (1992, Chap. 10)). The complexity of computing v depends on both k and ℓ.

Now we can derive the approximate $(d+1)$-point D-optimal designs as follows. Suppose there exist r real solutions of v in (3.6), say $V_i, i=1,\ldots,r$. Then substitute each V_i into (3.5) and find the solution of u by a backward-substitution process, say U_i. For each U_i determine the zeros of $u(x)$, say Z_i. Then select those Z_i's which have all points lying between a and b, say $S_j, j=1,\ldots,s$. If the endpoint a or b is a D-optimal point, then add it to each S_j. Let ξ_j denote a $(d+1)$-point design with equal mass on S_j. Then the design among ξ_j whose information matrix has the largest determinant is the $(d+1)$-point D-optimal design. The following algorithm generates the approximate $(d+1)$-point D-optimal designs for dth degree polynomial regression with weight function $\omega(x)$ on the interval $[a,b]$, where $\omega'(x)/\omega(x)=p(x)/q(x)$ is a rational function.

Algebraic Algorithm

INPUT regression function $f(x)$; endpoints a,b; weight function $\omega(x)$; knowledge of whether $x_0=a$ and $x_d=b$.

OUTPUT $(d+1)$-point D-optimal designs.

- **Step 1** Set $p/q=\omega'(x)/\omega(x)$, and compute k by Lemma 2.2 and A by (3.1).
- **Step 2** With $k\geq 1$, do Steps 3−8.
- **Step 3** Find all real solutions of v in (3.6), say V_i, $i=1,\ldots,r$.
- **Step 4** Substitute each V_i into (3.5) and find solution of u, say U_i.
- **Step 5** Substitute each U_i into $u(x)$ and find the zeros of $u(x)$, say Z_i.
- **Step 6** Select those Z_i's which have all points lying between a and b, say $S_j, j=1,\ldots,s$.
- **Step 7** Compute $\det M(\xi_j)$ where ξ_j is a $(d+1)$-point design with equal masses on S_j and boundary points (if necessary).
- **Step 8** Output $\xi_{(s)}$ where $\det M(\xi_{(s)})=\max_{1\leq j\leq s}\det M(\xi_j)$ and stop.
- **Step 9** Solve u at (3.5), then find the zeros S of $u(x)$.
- **Step 10** Output ξ where ξ is a $(d+1)$-point design with equal mass on S and endpoints (if necessary) and stop.

Lemma 2.1 only provides a partial solution on answering whether the endpoint a or b belong to the support of the $(d+1)$-point D-optimal designs. For those cases in which knowledge of whether $x_0=a$ and $x_d=b$ is unavailable, we can still use the same algorithm to find the optimal designs. Run the algorithm with (i) $x_0=a$ and $x_d=b$; (ii) $x_0=a$ and $x_d<b$; (iii) $x_0>a$ and $x_d=b$; (iv)

$x_0 > a$ and $x_d < b$. Then select a design from four outputs with the information matrix having largest determinant.

4. Examples

Take $\omega(x) = 1 + x^2$ on $I = [a, b]$. We construct the $(d+1)$-point D-optimal designs ξ^*_{d+1} for three cases: (i) $I = [-b, b]$, (ii) $I = [0, b]$ with $b > 0$, and (iii) $I = [5, 10]$. The designs ξ^*_{d+1} will be compared with the approximate D-optimal designs η^*_d as b varies. From Lemma 2.1 (ii), $x_d = -x_0 = b$ if $I = [-b, b]$, and $x_d = b$ if $I = [0, b]$ and $I = [5, 10]$.

This model with $I = [-b, b]$ is investigated by Dette, Haines and Imhof (1999) and Chang (2005). Dette, Haines and Imhof (1999), Lemma 2.1 (iii) shows that if d is odd, then the approximate D-optimal designs put equal masses at symmetric $d+1$ points including $\pm b$, and the closed-form for the optimal support points is unavailable. Chang (2005) studies the radius of convergence for Taylor polynomials of auxiliary parameters via a differential equation approach.

Case (i): $I = [-b, b], b > 0$.

First suppose $d = 1$. The preceding results yield that the unique two-point D-optimal design is $\xi^*_2 = \begin{Bmatrix} -b & b \\ 1/2 & 1/2 \end{Bmatrix}$. It is easy to see that the weighted variance function

$$d(x, \xi^*_2) = \omega(x) f^T(x) M^{-1}(\xi^*_2) f(x) = \frac{\left(1 + x^2\right)\left(b^2 + x^2\right)}{b^2 + b^4} \le 2, \qquad \text{for all } x \in I,$$

since $d(x, \xi^*_2)$ is a convex function with minimum $1/(1 + b^2)$ at $x = 0$, and maximum 2 at $x = \pm b$. Then the design ξ^*_2 is an approximate D-optimal η^*_1 by DET.

In the quadratic regression model, the three-point D-optimal design has the form $\xi^*_3 = \begin{Bmatrix} -b & x_1 & b \\ 1/3 & 1/3 & 1/3 \end{Bmatrix}$. Then $p(x) = 2x$ and $q(x) = x^2 + 1$. The second-order differential equation in (2.4) reduces to $2x(3x^2 - b^2 + 2)u_1 = (6x^2 + v_1 x + v_0)(u_1 x + u_0)$, with $u_1 = 1$. We can rewrite the above equation in the matrix-vector form $(1, x, x^2) A (u_0, u_1)^T = 0$, where

$$A = \begin{pmatrix} -v_0 & 0 \\ -v_1 & 4 - 2b^2 - v_0 \\ -6 & -v_1 \end{pmatrix}.$$

The three polynomial equations for v_0 and v_1 in (3.6) are

$$\begin{aligned} v_0(v_0 + 2b^2 - 4) &= 0, \\ v_0 v_1 &= 0, \\ v_1^2 - 6(v_0 + 2b^2 - 4) &= 0. \end{aligned}$$

The system has one real solution $(v_0, v_1) = (4-2b^2, 0)$ if $0 < b \le \tau_2^{(2)}$, where $\tau_2^{(2)} = \sqrt{2}$, and three real solutions $(v_0, v_1) = (0, \pm\sqrt{12(b^2-2)}), (4-2b^2, 0)$ if $b > \sqrt{2}$. Then $u_0 = 0$ if $0 < b \le \sqrt{2}$, and $u_0 = \pm\sqrt{12(b^2-2)}/6, 0$ if $b > \sqrt{2}$. Thus it is straightforward to verify that there is a unique optimal design ξ_3^* with $x_1 = 0$ if $0 < b \le \sqrt{2}$, and two optimal designs ξ_3^* with $x_1 = \pm\sqrt{12(b^2-2)}/6$ if $b > \sqrt{2}$.

Numerical results show that ξ_3^* equals the unique approximate D-optimal design η_2^* if $b \le \tau_2^{(1)}$, where $\tau_2^{(1)} \approx 1.35014$. If $b > \tau_2^{(1)}$, then the design η_2^* is unique and has the form $\left\{ \begin{array}{cccc} -b & -x_2 & x_2 & b \\ 1/2-w & w & w & 1/2-w \end{array} \right\}$. This interesting relationship between ξ_3^* and η_2^* is supported by Figure 1 which is a plot of the weighted variance function $d(x, \xi_3^*)$ for some b.

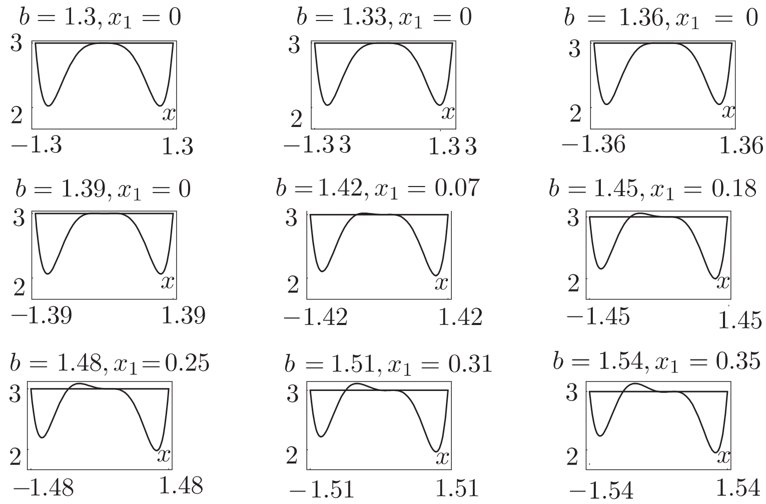

Figure 1. Weighted variance function $d(x, \xi_3^*)$ on $[-b, b]$ for $b = 1.30, 1.33, \ldots, 1.54$.

In general the optimal design ξ_{d+1}^* can be computed from the algebraic algorithm presented in Section 3. For the case d of odd, ξ_{d+1}^* is the same as η_d^* and has symmetric support points including boundary points $\pm b$. For the case of d even, the structure of ξ_{d+1}^* depends on b and is more complicated. Every ξ_{d+1}^* has symmetric support points including boundary points $\pm b$ and the origin 0 if $b \le \tau_d^{(2)}$, whereas ξ_{d+1}^* has asymmetric support points including boundary points $\pm b$ and excluding the origin if $b > \tau_d^{(2)}$. On the other hand, η_d^* is the same as ξ_{d+1}^* if $b \le \tau_d^{(1)}$, whereas η_d^* is a symmetric design with $d+2$ support points including boundary points $\pm b$ if $b > \tau_d^{(1)}$. Table 1 lists the critical values of $\tau_d^{(1)}$

and $\tau_d^{(2)}$ for even d. Note that $\tau_d^{(1)} < \tau_d^{(2)}$, and that $\tau_d^{(i)}$ increases as d increases for $i = 1, 2$.

Table 1. Critical values of $\tau_d^{(1)}$ and $\tau_d^{(2)}$.

d	2	4	6	8	10
$\tau_d^{(1)}$	1.350	2.108	2.788	3.429	4.045
$\tau_d^{(2)}$	$\sqrt{2}$	2.312	3.150	3.963	4.760

Let $d(x, \xi_{d+1}^*) = \omega(x) f^T(x) M^{-1}(\xi_{d+1}^*) f(x)$. The values of $\tau_d^{(1)}$ and $\tau_d^{(2)}$ are the solutions of the system of nonlinear equations

$$\begin{cases} \frac{d}{dx} d(x, \xi_{d+1}^*)\big|_{x=x_i} = 0, & \text{for } i = 1, 2, \ldots, d-1, \\ \frac{d^2}{dx^2} d(x, \xi_{d+1}^*)\Big|_{x=x_{d/2}} = 0, & \\ x_0 = -b, \quad x_d = b, & \end{cases}$$

and the constrained optimization problem

$$\begin{array}{lll} \text{Maximize} & b & \\ \text{subject to} & \frac{\partial}{\partial x_i} |M(\xi_{d+1}^*)| = 0, & \text{for } i = 1, 2, \ldots, d-1, \\ & x_{d/2} = 0, \quad x_0 = -b, \quad x_d = b, & \end{array}$$

respectively. The following well known formulae are very useful in reducing the preceding computational task

$$d(x, \xi_{d+1}^*) = (d+1)\omega(x) \sum_{i=0}^{d} \frac{1}{\omega(x_i)} \left(\prod_{j \neq i} \frac{x - x_j}{x_i - x_j} \right)^2, \qquad \text{and}$$

$$|M(\xi_{d+1}^*)| = \frac{1}{(d+1)^{d+1}} \left(\prod_{i=0}^{d} \omega(x_i) \right) \left(\prod_{0 \le i < j \le d} (x_i - x_j)^2 \right).$$

Given two designs ξ_1 and ξ_2, we can measure the D-efficiency of design ξ_1 with respect to design ξ_2 by

$$e_d = \left(\frac{\det M(\xi_1)}{\det M(\xi_2)} \right)^{\frac{1}{(d+1)}}$$

(Pukelsheim (1993)). The graph of the D-efficiency e_d^* of the design ξ_{d+1}^* with respect to the design η_d^* for $0 < b \le 10$ and $d = 2, 4, 6$, is given in Figure 2. It shows that e_d^* decreases as b increases for any d even. It decreases quickly at first, then converges to a limit. All efficiencies are greater than 0.978.

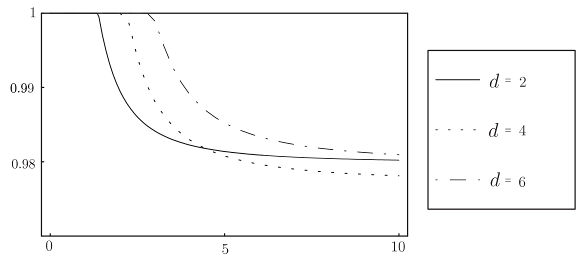

Figure 2. Graph of e_d^* for $0 < b < 10$ and $d = 2, 4, 6$.

Case (ii): $I = [0, b], b > 0$.

For $d = 1$, the unique two-point D-optimal design is $\xi_2^* = \begin{Bmatrix} 0 & b \\ 1/2 & 1/2 \end{Bmatrix}$ if $b \le \sigma_1^{(2)}$, and $\xi_2^* = \begin{Bmatrix} x_0 & b \\ 1/2 & 1/2 \end{Bmatrix}$ if $b > \sigma_1^{(2)}$, where $\sigma_1^{(2)} = \sqrt{(11+5\sqrt{5})/2} \approx 3.33019$. If $b > \sigma_1^{(2)}$, then the second-order differential equation in (2.4) can expressed as $2(2x^2 - bx + 1)u_1 = (4x + v_0)(u_1 x + u_0)$. We can rewrite this as $(1, x, x^2)A(u_0, u_1)^T = 0$, where

$$A = \begin{pmatrix} -v_0 & 2 \\ -4 & -2b - v_0 \end{pmatrix}.$$

There is only a polynomial equation $v_0^2 + 2bv_0 + 8 = 0$ in (3.6) which has two real solutions $v_0 = -b \pm \sqrt{b^2 - 8}$. Then it yields that $u_0 = -(v_0 + 2b)/4$. Thus it is straightforward to verify that there is a unique optimal design ξ_2^* with $x_1 = (b + \sqrt{b^2 - 8})/4$. Figure 2 is a plot of the weighted variance function $d(x, \xi_2^*)$.

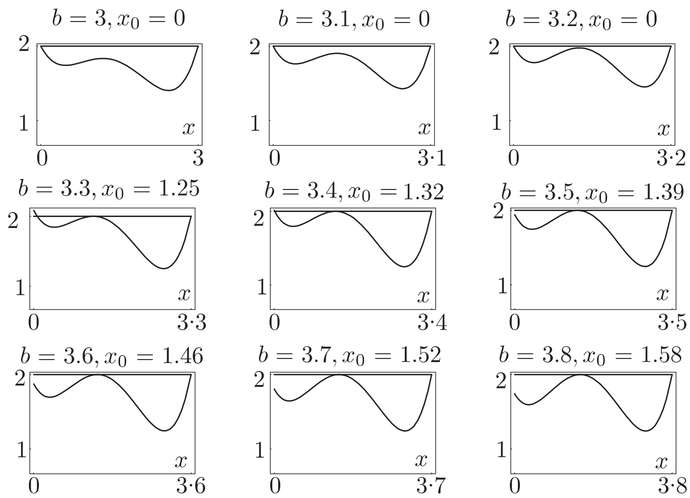

Figure 3. Weighted variance function $d(x, \xi_2^*)$ on $[0, b]$ for $b = 3.1, 3.2, \ldots, 3.8$.

Numerical results show that η_2^* is equally supported at boundary points 0 and b if $b \le \sigma_1^{(1)}$, where $\sigma_1^{(1)} \approx 3.2318$. The design η_2^* has the form $\left\{\begin{matrix} 0 & x_1 & b \\ w_0 & w_1 & 1-w_0-w_1 \end{matrix}\right\}$ if $\sigma_1^{(1)} < b < \sigma_1^{(3)}$, and $\left\{\begin{matrix} x_0 & b \\ 1/2 & 1/2 \end{matrix}\right\}$ if $b \ge \sigma_1^{(3)}$, where $\sigma_1^{(3)} \approx 3.41828$. Note that ξ_2^* equals η_1^* if $0 < b \le \sigma_1^{(1)}$ or $b \ge \sigma_1^{(3)}$.

In general the optimal support of ξ_{d+1}^* includes boundary points 0 and b if $0 < b \le \sigma_d^{(2)}$, and only right boundary point v if $b > \sigma_d^{(2)}$. The approximate D-optimal design η_d^* has the form

$$
\begin{cases}
\left\{\begin{matrix} 0 & x_1 & \cdots & b \\ \frac{1}{d+1} & \frac{1}{d+1} & \cdots & \frac{1}{d+1} \end{matrix}\right\} & \text{if } 0 < b \le \sigma_d^{(1)}, \\
\left\{\begin{matrix} 0 & x_1 & \cdots & x_d & b \\ w_0 & w_1 & \cdots & w_d & 1 - w_0 - \cdots - w_d \end{matrix}\right\} & \text{if } \sigma_d^{(1)} < b < \sigma_d^{(3)}, \\
\left\{\begin{matrix} x_0 & x_1 & \cdots & b \\ \frac{1}{d+1} & \frac{1}{d+1} & \cdots & \frac{1}{d+1} \end{matrix}\right\} & \text{if } b \ge \sigma_d^{(3)}.
\end{cases}
$$

Table 2 lists the critical values of $\sigma_d^{(1)}, \sigma_d^{(2)}$ and $\sigma_d^{(3)}$. The designs ξ_{d+1}^* coincide with η_d^* if $0 < b \le \sigma_d^{(1)}$ or $b \ge \sigma_d^{(3)}$. Note that $\sigma_d^{(1)} < \sigma_d^{(2)} < \sigma_d^{(3)}$, and $\sigma_d^{(2)}$ is closer to $\sigma_d^{(3)}$ than to $\sigma_d^{(1)}$. The value of $\sigma_d^{(i)}$ is an increasing function in d for $i = 1, 2, 3$.

Table 2. Critical values of $\sigma_d^{(1)}, \sigma_d^{(2)}$ and $\sigma_d^{(3)}$.

d	1	2	3	4	5
$\sigma_d^{(1)}$	3.232	6.888	11.695	17.685	24.864
$\sigma_d^{(2)}$	3.330	7.273	12.472	18.953	26.723
$\sigma_d^{(3)}$	3.418	7.604	13.132	20.029	28.298

The values of $\sigma_d^{(1)}, \sigma_d^{(2)}$ and $\sigma_d^{(3)}$ are the solutions of the system of nonlinear equations

$$
\begin{cases}
\frac{d}{dx} d(x, \xi_{d+1}^*)\big|_{x=x_i} = 0, & \text{for } i = 1, \ldots, d-1, \\
\frac{d}{dx} d(x, \xi_{d+1}^*)\big|_{x=x^*} = 0, & \\
d(x, \xi_{d+1}^*)\big|_{x=x^*} = d+1, & \\
x_0 = a, \quad x_d = b, &
\end{cases}
$$

the constrained optimization problem $\max_{x_0=0, x_d=b} |M(\xi_{d+1}^*)| = \max_{x_0>0, x_d=b} |M(\xi_{d+1}^*)|$, and

$$
\begin{cases}
\frac{d}{dx} d(x, \xi_{d+1}^*)\big|_{x=x_i} = 0, & \text{for } i = 0, \ldots, d-1, \\
d(x, \xi_{d+1}^*)\big|_{x=0} = d+1, & \\
x_d = b, &
\end{cases}
$$

respectively.

The graph of the D-efficiency function e_d^* of the design ξ_{d+1}^* with respect to the design η_d^* for $\sigma_d^{(1)} \leq b \leq \sigma_d^{(3)}$ and $d = 1, 2, 3$, is given in Figure 4.It shows that e_d^* decreases on $(\sigma_d^{(1)}, \sigma_d^{(2)})$ and increases on $(\sigma_d^{(2)}, \sigma_d^{(3)})$. All efficiencies are greater than 0.994.

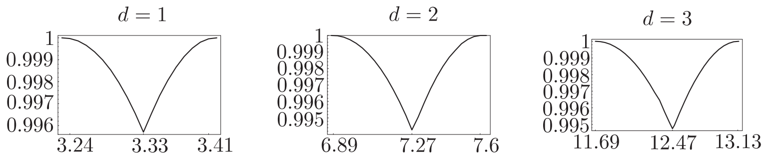

Figure 4. Graph of e_d^* for $\sigma_d^{(1)} \leq b \leq \sigma_d^{(3)}$ and $d = 1, 2, 3$.

Case (iii): $I = [5, 10]$.

If $d = 1$, the D-optimal design is equally supported at two boundary points 5 and 10 which can be shown by DET. Numerical results show that $x_0 = 5$ and $x_d = 10$. Table 3 lists the optimal support of ξ_{d+1}^*. All of them are also approximate D-optimal supports.

Table 3. D-optimal support of ξ_{d+1}^* on $[5, 10]$.

d	x_0	x_1	x_2	x_3	x_4	x_5
1	5	10				
2	5	7.881	10			
3	5	6.636	8.804	10		
4	5	6.010	7.703	9.235	10	
5	5	5.675	6.950	8.353	9.469	10

5. Remark

All computations discussed in this article were performed on an IBM compatible PC with Intel Pentium 4 CPU 3GHz and RAM 1GB, using the numeric and symbolic computational software *Mathematica* 5.0 (Wolfram (2003)). The CPU time to compute a ξ_{d+1}^* design for the model in Section 4 is within 5 seconds if $d \leq 10$ and within 25 seconds if $d \leq 20$.

Appendix

A.1. Proof of Lemma 2.1

Case (i): If $\omega(a) = 0$ and $x_0 = a$, then $M(\xi_{d+1}^*)$ is singular, since its rank is less than or equal to d. Thus ξ_{d+1}^* cannot be $(d+1)$-point D-optimal. The same argument holds for the case $\omega(b) = 0$.

Case (ii): Suppose that a is a global maximum point of $\omega(x)$ on $[a,b]$. Let $\Delta(x_0,\dots,x_d) = \det M(\xi^*_{d+1})$. Then $\Delta(x_0,\dots,x_d) = \prod_{i=0}^d \omega(x_i)\prod_{0\le i<j\le d}(x_i - x_j)^2/(d+1)^{d+1}$ by a direct application of the Vandermonde determinant formula. Note that if $x_0 > a$, then $\prod_{j=1}^d (x_0 - x_j)^2 < \prod_{j=1}^d (a-x_j)^2$. Combining this fact with $\omega(a) = \max_{x\in[a,b]}\omega(x)$ shows that $\Delta(x_0,\dots,x_d) < \Delta(a,x_1,\dots,x_d)$. Thus ξ^*_{d+1} cannot be $(d+1)$-point D-optimal. The proof for the other case is similar.

Case (iii): If $x_0 = a$, then $h(x) = \Delta(x,x_1,\dots,x_d)$ is decreasing on $[a,a+\epsilon]$ for some $\epsilon > 0$. It follows that

$$g(a) = \frac{d}{dx}\log h(x)\bigg|_{x=a} = \frac{\omega'(a)}{\omega(a)} + 2\left(\frac{1}{a-x_1} + \cdots + \frac{1}{a-x_d}\right) < 0.$$

Notice that $s''(a)/s'(a) = 2/(a-x_1)+\cdots+2/(a-x_d)$ and $\omega'(a)/\omega(a) = p(a)/q(a)$, and the result is proved. The proof for the other case is similar.

A.2. Proof of Lemma 2.2

The following is a proof for the case $\delta_a(x) = (x-a)$ and $\delta_b(x) = (x-b)$. The proofs for the other three cases are omitted. They can be proved similarly.

For the given case the design is of the form

$$\xi = \begin{Bmatrix} x_0 & x_1 & \cdots & x_d \\ 1/(d+1) & 1/(d+1) & \cdots & 1/(d+1) \end{Bmatrix},$$

where $a = x_0 < x_1 < \cdots < x_d = b$. The determinant of the information matrix of ξ can be expressed as $\det M(\xi) = (b-a)^2\omega(a)\omega(b)/(d+1)^{d+1}\phi(x_1,\dots,x_{d-1})$, where

$$\phi(x_1,\dots,x_{d-1}) = \prod_{i=1}^{d-1}\omega(x_i)\prod_{i=1}^{d-1}(x_i-a)^2(x_i-b)^2\prod_{1\le i<j\le d-1}(x_i-x_j)^2.$$

It is clear that maximizing $\det M(\xi)$ is equivalent to maximizing $\log\phi(x_1,\dots,x_{d-1})$. Then the following conditions must be satisfied

$$\begin{aligned}\frac{\partial\log\phi}{\partial x_i} &= \frac{\omega'(x_i)}{\omega(x_i)} + \left(\frac{2}{x_i-a} + \frac{2}{x_i-b}\right) + \sum_{j=1,j\ne i}^{d-1}\frac{2}{x_i-x_j} \\ &= 0,\end{aligned}$$

for $i = 1,\dots,d-1$. It is easy to verify that

$$\frac{u''(x_i)}{u'(x_i)} = \sum_{j=1,j\ne i}^{d-1}\frac{2}{x_i-x_j},$$

(see Fedorov (1972), Section 2.3). Then

$$\frac{\omega'(x)}{\omega(x)} + \frac{2(2x-a-b)}{(x-a)(x-b)} + \frac{u''(x)}{u'(x)} = 0 \tag{A.1}$$

for $x = x_1, \ldots, x_{d-1}$.

Substituting $\omega'(x)/\omega(x) = p(x)/q(x)$ into (A.1) and multiplying the equation by the common denominator, we obtain $L(x) = 0$ for $x = x_1, \ldots, x_{d-1}$, where

$$\begin{aligned} L(x) = &(x-a)(x-b)q(x)u''(x) + ((x-a)(x-b)p(x) \\ &+2(2x-a-b)q(x))u'(x), \end{aligned} \tag{A.2}$$

is a second order differential function. Note that $L(x)$ is a polynomial of degree $k+d-1$ and vanishes at $x = x_1, \ldots, x_{d-1}$, where $k = \max(m+1, n)$. This implies that $u(x)$ is a factor of $L(x)$. Thus there exists an auxiliary polynomial $v(x) = v_k x^k + v_{k-1}x^{k-1} + \cdots + v_0$ such that $L(x) = v(x)u(x)$, where v_k equals the leading coefficient of $L(x)$ and $v_0, \ldots, v_{k-1}$ are k unknown constants. Moreover, all of $v_0, \ldots, v_k$ must be real since both $L(x)$ and $u(x)$ are real polynomials.

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References

Antille, G., Dette, H. and Weinberg, A. (2003). A note on optimal designs in weighted polynomial regression for the classical efficiency functions. *J. Statist. Plann. Inference* **113**, 285-292.

Atkinson, A. C. and Donev, A. N. (1992). *Optimum Experimental Designs.* Oxford University Press, New York.

Chang, F.-C. (2005). *D*-optimal designs for weighted polynomial regression – a functional-algebraic approach. *Statist. Sinica* **15**, 153-163.

Chang, F.-C. and Lin, G.-C. (1997). *D*-optimal designs for weighted polynomial regression. *J. Statist. Plann. Inference* **62**, 317-331.

Dette, H., Haines, L. M. and Imhof, L. (1999). Optimal designs for rational models and weighted polynomial regression. *Ann. Statist.* **27**, 1272-1293.

Fang, Z. (2002). *D*-optimal designs for polynomial regression models through origin. *Statist. and Probab. Letters* **57**, 343-351.

Fedorov, V. V. (1972). *Theory of Optimal Experiments.* Translated and edited by Studden, W.J. and Klimko, E.M. Academic Press, New York.

Geddes, K. O., Czapor, S. R. and Labahn, G. (1992). *Algorithms for Computer Algebra.* Kluwer Academic Publishers, Boston.

Guest, P. G. (1958). The spacing of observations in polynomial regression. *Ann. Math. Statist.* **29**, 294-299.

Hoel, P. G. (1958). Efficiency problems in polynomial estimation. *Ann. Math. Statist.* **29**, 1134-1145.

Huang, M.-N. L., Chang, F.-C. and Wong, W.-K. (1995). D-optimal designs for polynomial regression without an intercept. *Statist. Sinica* **5**, 441-458.

Imhof, L., Krafft, O. and Schaefer, M. (1998). D-optimal designs for polynomial regression with weight function $x/(1+x)$. *Statist. Sinica* **8**, 1271-1274.

Karlin, S. and Studden, W. J. (1966). Optimal experimental designs. *Ann. Math. Statist.* **37**, 783-815.

Kiefer, J. C. and Wolfowitz, J. (1960). The equivalence of two extremum problems. *Canad. J. Math.* **12**, 363-366.

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

Silvey, S. D. (1980). *Optimal Design*. Chapman & Hall, London.

Smith, K. (1918). On the standard deviations of adjusted and interpolated values of an observed polynomial function and its constants and the guidance they give towards a proper choice of the distribution of observations. *Biometrika* **12**, 1-85.

Szegö, G. (1975). *Orthogonal Polynomials*. 4th edition. American Mathematical Society Colloquium Publications **23**. Providence, Rhode Island.

Wolfram, S. (2003). *The Mathematica Book*. 5th edition. Wolfram Media, Champaign, IL.

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