Ann. Inst. Statist. Math.
Vol. 57, No. 4, 833–844 (2005)

D-OPTIMAL DESIGNS FOR WE IGHTED POLYNOMIAL REGRESSION—A FUNCTI( )NAL APPROACH

FU-CHUEN CHANG

Department of Applied Mathematics, National Sun Yat-sen University, Kaohsiung, Taiwan 804, R.O.C., e-mail: changfc@math.nsysu.edu.tw

(Received March 25, 2004; revised October 15, 2004)

Abstract. This paper is concerned with the problem of computing approximate D-optimal design for polynomial regression with analytic weight function on a interval $[m_0 - a, m_0 + a]$. It is shown that the structure of the optimal design depends on a and weight function. Moreover, the optimal support points and weights are analytic functions of a at $a = 0$. We make use of a Taylor expansion to provide a recursive procedure for calculating the D-optimal designs.

Key words and phrases: Approximate D-optimal design, Chebyshev system, D-efficiency, D-Equivalence Theorem, implicit function theorem, recursive algorithm, Taylor expansion, weighted polynomial regression.

1. Introduction

Consider the weighted polynomial regression models of degree d

$$\begin{aligned} y(x) &= \sum_{i=0}^{d} \beta_i x^i + \epsilon(x), \qquad x \in I \\ \mathrm{Var}(y(x)) &= \sigma^2/\omega(x) \end{aligned} \tag{1.1}$$

where $\omega(x) \geq 0$ denotes a nonnegative weight function on the design interval $I = [m_0 - a, m_0 + a]$, $a > 0$, and the control variable x is taken from I. These models are widely used in situations where the response is curvilinear, as even complex nonlinear relationships can be adequately modeled by polynomials over reasonably small range of the x's. The problem of determining optimal designs for weighted polynomial regression models has been investigated by several authors (e.g. Hoel (1958), Karlin and Studden (1966*a*), Huang *et al.* (1995), Chang and Lin (1997), Imhof *et al.* (1998), Dette *et al.* (1999), and Antille *et al.* (2003), among many others). All of these studies concentrate on deriving the closed forms of the optimal designs. However, the analytic results exist only for very special classes of weight functions and design intervals.

The differential equation and canonical moments are two main powerful tools for determining the closed forms of the D-optimal designs for weighted polynomial regression. The first approach is used in Karlin and Studden (1966*a*), Huang *et al.* (1995), Chang and Lin (1997), Imhof *et al.* (1998), Dette *et al.* (1999), and Antille *et al.* (2003) among many others. The second approach is used in Studden (1982), Lau and Studden (1985), Dette (1990, 1992), and Fang (2002).

The pioneering work of Melas (1978) uses a functional approach to obtain Taylor expansion of the optimal designs for exponential regression. This powerful and interesting tool is also used by Melas (2000, 2001), Chang (2005) and Dette *et al.* (2004). In the recent two papers Dette *et al.* (2002*a*) and Dette *et al.* (2002*b*) proves that for the trigonometric regression models on a partial circle the approximate D-optimal design depends only on the length of the design interval and that the support points (and weights) are analytic functions of this parameter by combining Taylor expansion and differential equation. Furthermore, Dette *et al.* (2004) provides a recursive algorithm to determine the coefficients of Taylor expansion.

Chang (2005) shows that for the model (1.1) if $\omega'(x)/\omega(x)$ is a rational function and a is sufficiently small, then the problem of constructing D-optimal designs 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 are analytic functions at $a = 0$ and can be approximated by Taylor polynomials whose coefficients can be computed recursively. Then the interior optimal support points can be computed from the zeros of a polynomial which the coefficients can be calculated from a linear system.

The purpose of this paper is to extend the Taylor expansion approach of Dette *et al.* (2002*b*) and Chang (2005) to compute the D-optimal designs for polynomial regression with a broad class of analytic weight functions satisfying

$$\omega(x) = \alpha(x - m_0)^s + o((x - m_0)^s), \qquad \alpha > 0, \;\; s = 0, 2, \ldots, \tag{1.2}$$

as $x \to m_0$. This class of weight functions covers almost all of weight functions for polynomial regression considered in the literature. The Taylor polynomials of the optimal support points and weights will be calculated directly instead of computing Taylor polynomials of auxiliary unknown constants in differential approach of Chang (2005).

This paper is organized in the following way. In Section 2, the structure of the D-optimal designs as a approaches to 0 is given. We also derive the D-optimal designs for polynomial regression with weight function $\omega(x) = |x|^s$ which will be used in Taylor expansion of D-optimal support points and weights as the constant terms. In Section 3, we show that if $\omega(x)$ is analytic at $a = 0$, then the D-optimal support points and weights are analytic functions of a. A recursive formula is given for computing Taylor polynomials of D-optimal support points and weights. Finally, in Section 4 three examples are used to illustrate the Taylor expansion method established in Section 3. Concluding comments are given in Section 5. The proofs of two main lemmas in Section 2 are deferred to Appendixes A and B.

2. Preliminary results

An approximate design ξ is a probability measure with finite support on the design interval I. The information matrix of a design ξ for the parameter $\beta = (\beta_0, \beta_1, \ldots, \beta_d)^T$ is defined by

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

where $f(x) = (1, x, \ldots, x^d)^T$ denotes the vector of regression functions. A design ξ^* is called approximate D-optimal for β if ξ^* maximizes the determinant of the information matrix $M(\xi)$ among the set of all approximate designs on I. For more about the theory of optimal designs see Fedorov (1972), Silvey (1980) and Pukelsheim (1993).

First we consider the structure of the D-optimal designs for polynomial regression $f(x)$ with $\omega(x)$ on $[m_0 - a, m_0 + a]$ where $\omega(x) = \alpha(x - m_0)^s + o((x - m_0)^s)$, $\alpha > 0$ and $s = 0, 2, \dots$ as $a \to 0$. Consider the linear transformation $x = m_0 + at$ which maps t in $[-1, 1]$ to x in $[m_0 - a, m_0 + a]$. It is easy to see that $f(x) = Lf(t)$ where $L = (\binom{i}{j} m_0^{i-j} a^j)_{i,j=0}^d$ is a $(d+1) \times (d+1)$ lower triangular matrix. Then the information matrix of a design ξ supported at $\{x_i\}_{i=1}^m$ is given by

$$\begin{aligned} M(\xi) &= \sum_{i=1}^m \omega(x_i)\xi(x_i)f(x_i)f^T(x_i) \\ &= L\left(\sum_{i=1}^m \omega(m_0 + at_i)\xi(m_0 + at_i)f(t_i)f^T(t_i)\right)L^T. \end{aligned}$$

Since $\omega(x) \approx \alpha(x - m_0)^s = \alpha a^s t^s$ as $a \to 0$, it follows that the structure of approximate D-optimal design for $f(x)$ with weight function $\omega(x)$ on $[m_0 - a, m_0 + a]$ is the same as that of D-optimal design for $f(t)$ with t^s on $[-1, 1]$ as $a \to 0$.

The following two lemmas characterize the D-optimal designs for polynomial regression with weight function $|x|^s$ on $[-1, 1]$. The proofs are tedious and deferred to Appendixes A and B.

LEMMA 2.1. *For the polynomial regression model $f(x)$ with $\omega(x) = |x|^s$, $s \geq 0$, on $[-1, 1]$, the D-optimal design is supported on*

(a) *symmetric $d + 1$ points including both end-points ± 1 if $s = 0$ or $s > 0$ and d is odd,*

(b) *symmetric $d + 2$ points including both end-points ± 1 if $s > 0$ and d is even.*

Combining Lemma 2.1 and the discussions at the beginning of this section, we conclude that there exists an $\bar{a}$ such that if $0 < a \leq \bar{a}$, then the D-optimal design for weighted polynomial regression on $[m_0 - a, m_0 + a]$ is unique and has the form

$$\xi = \begin{cases} \begin{Bmatrix} x_0 & x_1 & \cdots & x_d \\ 1/(d+1) & 1/(d+1) & \cdots & 1/(d+1) \end{Bmatrix} \\ \quad \text{if} \quad s = 0 \text{ or } s > 0 \text{ and } d \text{ is odd,} \\ \begin{Bmatrix} x_0 & x_1 & \cdots & x_{d+1} \\ w_0 & w_1 & \cdots & w_{d+1} \end{Bmatrix} \\ \quad \text{if} \quad s > 0 \text{ and } d \text{ is even,} \end{cases} \tag{2.1}$$

where $m_0 - a = x_0 < x_1 < \cdots < x_d(x_{d+1}) = m_0 + a$ and $\sum w_i = 1, w_i > 0$.

Now we are ready to derive the D-optimal designs for the model in Lemma 2.1. The results will be used in Taylor expansion of D-optimal designs in Section 3 as the constant terms. Chang (1998) derives the D-optimal designs on $[a, 1]$, $a \geq 0$, in terms of the smallest eigenvalue of a certain tridiagonal matrix. The following lemma gives the closed forms of the D-optimal designs in terms of Jacobi polynomial and an explicit formula for the determinant of information matrix of a design in (2.1).

LEMMA 2.2. *Consider the polynomial regression model $f(x)$ with $\omega(x) = |x|^s$, $s \geq 0$, on $[-1, 1]$.*

(a) *If* $s = 0$, *then the D-optimal design* μ_0^* *puts equal masses at the zeros of* $(1-x^2)P_d'(x) = (1/2)(d+1)(1-x^2)P_{d-1}^{(0,0)}(x)$ *where* $P_d(x)$ *is the d-th Legendre polynomial and* $P_n^{(\alpha,\beta)}(x)$ *denotes the n-th Jacobi polynomial orthogonal with respect to the measure* $(1-x)^\alpha(1+x)^\beta$ *on the interval* $[-1,1]$.

(b) *If* $s > 0$ *and d is odd, then the D-optimal design* μ_0^* *puts equal masses at the zeros of the polynomial* $(1-x^2)P_{(d-1)/2}^{(1,(s-1)/2)}(2x^2-1)$.

(c) *If* ξ *denotes a design of the form* (2.1), *then*

$$\det M(\xi) = \begin{cases} \frac{1}{(d+1)^{d+1}} \prod_{i=0}^{d} \omega(x_i) \prod_{0\le i<j\le d}(x_i - x_j)^2 \\ \quad \text{if} \quad s = 0 \text{ or } s > 0 \text{ and } d \text{ is odd}, \\ \sum_{0\le k_0<\cdots<k_d\le d+1} \prod_{i=0}^{d} \omega(x_{k_i})w_{k_i} \prod_{0\le i<j\le d}(x_{k_i} - x_{k_j})^2 \\ \quad \text{if} \quad s > 0 \text{ and } d \text{ is even}. \end{cases} \tag{2.2}$$

The D-optimal designs μ_0^* for $f(x)$ with $\omega(x) = |x|^s$ on $[-1,1]$ are listed in Table 1 for $d = 1,2,\ldots,5$ and $s = 0,2,\ldots,10$. There is no closed form available for the case $s > 0$ and d even. It can be computed by a modified Fedorovs exchange algorithm (Fedorov (1972), Chapter 3) for exact optimal designs. All of the designs are symmetric about the origin and include the two end-points. Moreover, the number of the optimal support points is $d+1$ if $s = 0$, or $s > 0$ and d odd, and $d+2$ otherwise. The optimal support points spread more closer to the two end-points and the optimal weights for d even do not vary too much as s increases.

Table 1. D-optimal design μ_0^* for $f(x)$ with $\omega(x) = |x|^s$ on $[-1,1]$.

$s\backslash d$	1	2		3		4			5		
0	±1	0	±1	±.447	±1	0	±.655	±1	±.285	±.765	±1
	1/2	1/3	1/3	1/4	1/4	1/5	1/5	1/5	1/6	1/6	1/6
2	±1	±.602	±1	±.655	±1	±.434	±.781	±1	±.469	±.830	±1
	1/2	.178	.322	1/4	1/4	.124	.178	.198	1/6	1/6	1/6
4	±1	±.726	±1	±.745	±1	±.560	±.835	±1	±.571	±.867	±1
	1/2	.179	.321	1/4	1/4	.127	.175	.198	1/6	1/6	1/6
6	±1	±.790	±1	±.798	±1	±.637	±.867	±1	±.639	±.890	±1
	1/2	.180	.320	1/4	1/4	.128	.174	.198	1/6	1/6	1/6
8	±1	±.829	±1	±.832	±1	±.691	±.889	±1	±.688	±.906	±1
	1/2	.180	.320	1/4	1/4	.129	.174	.197	1/6	1/6	1/6
10	±1	±.856	±1	±.856	±1	±.731	±.905	±1	±.724	±.919	±1
	1/2	.180	.320	1/4	1/4	.130	.173	.197	1/6	1/6	1/6

3. Taylor expansion for D-optimal designs

To relate the D-optimal support points and weights to the Taylor expansion we now consider the standardized design $\mu(t) = \xi(x)$ where $x = m_0 + at$. Note that $t_0 = -1$, $t_d = 1$ and $w_d = 1 - \sum_{i=0}^{d-1} w_i$ if $s = 0$ or $s > 0$ and d odd; $t_{d+1} = 1$ and $w_{d+1} = 1 - \sum_{i=0}^{d} w_i$ if $s > 0$ and d even. Then the D-optimal design problem reduces to determine the maximum of

$$(3.1)\qquad \det M(\xi) = \begin{cases} \frac{a^{(d+1)(s+d)}}{(d+1)^{d+1}} \prod_{i=0}^{d} \frac{\omega(m_0+at_i)}{a^s} \prod_{0\le i<j\le d}(t_i - t_j)^2 \\ \quad \text{if} \quad s = 0 \text{ or } s > 0 \text{ and } d \text{ is odd,} \\ a^{(d+1)(s+d)} \sum_{0\le k_0<\cdots<k_d\le d+1} \prod_{i=0}^{d} \frac{\omega(m_0+at_{k_i})}{a^s} w_{k_i} \\ \quad \times \prod_{0\le i<j\le d}(t_{k_i} - t_{k_j})^2 \\ \quad \text{if} \quad s > 0 \text{ and } d \text{ is even,} \end{cases}$$

where $x_i = m_0 + at_i$, $i = 1, \ldots, d-1$, by Lemma 2.2(c). If $s = 0$ or $s > 0$ and d is odd, then the determinant can be written as

$$(3.2)\qquad \det M(\xi) = 4\frac{a^{(d+1)(s+d)}}{(d+1)^{d+1}} \frac{\omega(m_0 - a)}{a^s} \frac{\omega(m_0 + a)}{a^s} \phi(\tau \mid a)$$

where $\phi(\tau \mid a) = \prod_{i=1}^{d-1} \frac{\omega(m_0+at_i)}{a^s} \prod_{1\le i<j\le d-1}(t_i - t_j)^2$ and $\tau = (t_1, \ldots, t_{d-1})^T$. On the other hand, if $s > 0$ and d is even, then it can be expressed as

$$(3.3)\qquad \det M(\xi) = a^{(d+1)(s+d)}\phi(\tau \mid a)$$

where $\phi(\tau \mid a) = \sum_{0\le k_0<\cdots<k_d\le d+1}(\prod_{i=0}^{d} \frac{\omega(m_0+at_{k_i})}{a^s} w_{k_i} \prod_{0\le i<j\le d}(t_{k_i} - t_{k_j})^2)$ and, $t_0 = -1$, $t_{d+1} = 1$, $\tau = (t_1, \ldots, t_d, w_0, \ldots, w_d)^T$. Thus the problem of finding $\max_\xi M(\xi)$ is equivalent to that of finding $\max_\tau \phi(\tau \mid a)$.

Next we study the maximum of the function $\phi(\tau \mid a)$. For a fixed a close to 0, the function $\phi(\tau \mid a)$ has a unique maximum in

$$T = \begin{cases} \{(t_1, \ldots, t_{d-1}) | -1 < t_1 < \cdots < t_{d-1} < 1\} \quad \text{if} \quad s = 0 \text{ or } s > 0 \text{ and } d \text{ odd,} \\ \{(t_1, \ldots, t_d, w_0, \ldots, w_d) | -1 < t_1 < \cdots < t_d < 1, 0 < w_i < 1, 0 < \sum_{i=0}^{d} w_i < 1\} \\ \quad \text{if} \quad s > 0 \text{ and } d \text{ even,} \end{cases}$$

which will be denoted by $\tau^*(a) = (\tau_1^*(a), \ldots, \tau_k^*(a))^T$ where k is the dimension of τ. Note that the maximum point $\tau^*(a)$ of $\phi(\tau \mid a)$ is a vector function of a. It is clear that if the partial derivative of $\omega(m_0 + at)$ with respect to t exists for $t \in (-1, 1)$, then $\tau^*(a)$ can be obtained as the unique solution of the k simultaneous equations by taking partial derivatives of $\phi(\tau \mid a)$ with respect to τ

$$(3.4)\qquad g(\tau \mid a) = \frac{\partial}{\partial \tau}\phi(\tau \mid a) = \mathbf{0} \in \Re^k.$$

Moreover, if $\omega(m_0 + at)$ is an analytic function at $t = 0$ and the Jacobian of $\phi(\tau \mid a)$ with respect to τ is given by

$$(3.5)\qquad H(\tau \mid a) = \left(\frac{\partial^2}{\partial \tau_i \partial \tau_j}\phi(\tau \mid a)\right)_{i,j=1}^{k}$$

is a nonsingular matrix at $a = 0$, then from the implicit function theorem (see Khuri (2002), Theorem 7.6.2), $\tau^*(a)$ are analytical functions of a on the interval $(-R, R)$ where R is the radius of convergence and a function of $\omega(x)$ and d. This implies that the Taylor series of τ^* at the origin exists. If $a < R$, then

$$(3.6)\qquad \tau^*(a) = \sum_{i=0}^{\infty} \tau_{(i)}^* a^i$$

where $\tau^*_{(0)} = \tau^*(0) = \lim_{a\to 0}\tau^*(a)$ can be found from Lemma 2.2 and Table 1.

To determine the coefficients $\tau^*_{(i)}$ in this expansion, we will make use of the following recursive formula, which has been found explicitly in Theorem 3.4 of Dette *et al.* (2004):

$$\tau^*_{(n+1)} = -\frac{1}{(n+1)!}H^{-1}(\tau^*(0) \mid 0)\frac{d^{n+1}}{da^{n+1}}g(\tau^*_{<n>}(a) \mid a)\Bigg|_{a=0} \tag{3.7}$$

where

$$\tau^*_{<n>}(a) = \sum_{i=0}^{n} \tau^*_{(i)}a^i$$

denotes the n-th degree Taylor polynomials of $\tau^*(a)$ at $a = 0$. The preceding recursive formula of $\tau^*_{(n+1)}$ provides an easy and simple way to calculate the Taylor polynomials of $\tau^*(a)$.

4. Examples

In this section we will present three examples to illustrate the Taylor expansion method for computing the D-optimal designs given in Section 3.

Example 4.1. In the first example we consider the quadratic polynomial regression model with $\omega(x) = 2 + x$ on the interval $[-a, a]$. If a is close to 0, then the D-optimal design has the form of

$$\xi^* = \left\{\begin{matrix} -a & at_1^* & a \\ 1/3 & 1/3 & 1/3 \end{matrix}\right\}$$

by Lemma 2.1. From (3.7) the 10th-degree Taylor polynomial of $t_1^*(a)$ at $a = 0$ is given by

$$t_{1,10}(a) = .125a - .00977a^3 + .00153a^5 - .000298023a^7 + .0000651926a^9.$$

Let

$$\hat{\xi} = \left\{\begin{matrix} -a & at_{1,10}(a) & a \\ 1/3 & 1/3 & 1/3 \end{matrix}\right\}$$

denote the numerical approximation of ξ^*. Numerical result shows that if $a \le 1.473$, then $\hat{\xi}$ is nearly D-optimal in the sense of the D-Equivalence criterion (see Fedorov (1972)) satisfying

$$\max_{x\in[-a,a]} d(x, \hat{\xi}) - (d+1) \le 10^{-5} \tag{4.1}$$

where $d(x, \hat{\xi}) = \omega(x)f^T(x)M^{-1}(\hat{\xi})f(x)$. For example, if $a = 1$, then the nearly D-optimal design is given by

$$\hat{\xi} = \left\{\begin{matrix} -1 & .117 & 1 \\ 1/3 & 1/3 & 1/3 \end{matrix}\right\}.$$

Throughout this paper we use the criterion (4.1) to compute the nearly D-optimal designs.

In this case the analytic formula of t_1^* can be obtained by solving the maximizer of the function $\det M(\xi^*) = -4a^6(-4 + a^2)(2 + at_1^*)(-1 + (t_1^*)^2)^2/27$ directly. Simple algebra yields that $t_1^* = (-4 + \sqrt{16 + 5a^2})/(5a)$. The 10th-degree Taylor polynomial of t_1^* at $a = 0$ is given by

$$.125a - .00976563a^3 + .00152588a^5 - .000298023a^7 + .0000651926a^9$$

which coincides with $t_{1,10}(a)$ except the rounding error.

Figure 1 shows the graph of the difference of the nearly and truly optimal support point $e(a) = a(t_{1,10} - t_1^*)$ for $0 < a < 1.5$. It reveals that $e(a)$ is a strictly convex, positive and increasing function in a and $e(.1) = 7.177 \times 10^{-17}$, $e(.5) = 3.515 \times 10^{-9}$, $e(1) = 1.228 \times 10^{-5}$, $e(1.5) = 1.283 \times 10^{-3}$. It follows that both the nearly and truly optimal design points are very close to each other. Note that if $1.48 < a < 2$, then the optimal support contains the right end-point a and one positive and one negative interior points.

One of the quantities used to measure the efficiency of a design ξ is the D-efficiency given by

$$r(\xi) = \left(\frac{\det M(\xi)}{\det M(\xi^*)}\right)^{1/(d+1)}.$$

Figure 2 gives the plot of the D-efficiency function $r(\hat{\xi})$ for $0 < a < 1.5$. It shows that $r(\hat{\xi})$ is a strictly concave and decreasing function, and the design $\hat{\xi}$ has very high efficiency.

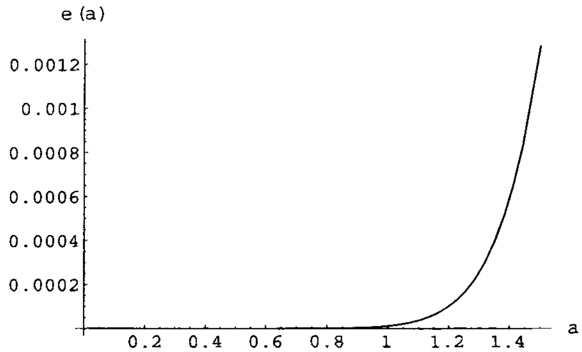

Fig. 1. Plot of $e(a)$ for $0 < a < 1.5$.

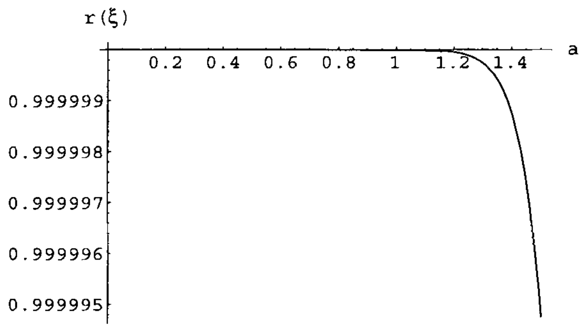

Fig. 2. The D-efficiency function $r(\hat{\xi})$ for $0 < a < 1.5$.

Example 4.2. Our second example considers $d = 2$ and $\omega(x) = x^2 + x^4$ on the interval $[-a, a]$. In this case $s = 2$ and d even, from Lemma 2.2 and the symmetry of weight function and design interval it can be argued that if a is close to 0, then the unique D-optimal design has the form

$$\xi^* = \begin{Bmatrix} -a & -at_1^* & at_1^* & a \\ 1/2 - w_1^* & w_1^* & w_1^* & 1/2 - w_1^* \end{Bmatrix}.$$

This case is more complicated since there are one support point and one weight need to be determined. Therefore we have to compute the two Taylor expansions for two variables in two equations at $a = 0$. From (3.7) the 10th-degree Taylor polynomials for t_1^* and w_1^* are given as

$$t_{1,10}(a) = .601706 + .0597043a^2 - .0109969a^4 - .0106096a^6 + .0138087a^8 - .0112085a^{10}$$
$$w_{1,10}(a) = .17792 - 0.00278443a^2 + .00512734a^4 - .00602918a^6 + .00631595a^8 - .0065627a^{10}.$$

All these polynomials are even. Let

$$\hat{\xi} = \begin{Bmatrix} -a & -at_{1,10}(a) & at_{1,10}(a) & a \\ 1/2 - w_{1,10}(a) & w_{1,10}(a) & w_{1,10}(a) & 1/2 - w_{1,10}(a) \end{Bmatrix}$$

denote the numerical approximation of ξ^*. Numerical result shows that if $a \le .451$, then $\hat{\xi}$ is nearly D-optimal. For example, if $a = .3$, then the nearly D-optimal design is given by

$$\hat{\xi} = \begin{Bmatrix} -.3 & -.182 & .182 & .3 \\ .322 & .178 & .178 & .322 \end{Bmatrix}.$$

Table 2. a_n for various weight functions.

$\omega(x)$	n	$d = 2$	$d = 3$	$d = 4$
$x + 2$	5	1.240	1.284	1.352
	10	1.473	1.681	1.777
$x^2 + 1$	5	1.352	0.661	0.614
	10	1.352	1.080	0.914
e^{x+1}	5	1.220	1.649	1.994
	10	1.560	2.438	3.097
e^{x^2}	5	1.390	1.036	0.814
	10	1.390	1.366	1.665
$\frac{2}{1+x}$	5	0.723	0.595	0.556
	10	0.887	0.791	0.752
$\frac{2+x}{1+x^2}$	5	0.638	0.566	0.550
	10	0.813	0.859	0.827
$\cos x$	5	1.201	0.974	1.396
	10	1.202	1.342	1.419

Example 4.3. In this example we consider the problem of the radius R of convergence for the Taylor expansion of t_i^*'s and w_i^*'s at $a = 0$. In general, a closed form of R seems to be intractable. Even the task of computing the numerical values of R is formidable since the length of expressions involved in computing Taylor expansion growths quickly as n increases. Let a_n denote the maximum of a such that $t_{i,n}$'s and $w_{i,n}$'s give nearly D-optimal designs on $[-a, a]$. Then the function a_n can serve as an approximation of R and $\lim_{n\to\infty} a_n = R$. Table 2 lists a_n for various weight functions, $d = 2, 3, 4$, and $n = 5, 10$. For example, if $\omega(x) = 2x^2 + x + 1$ and $d = 2$, then a_n for $n = 5$ and 10 is .644 and .752, respectively. For any $\omega(x)$, R_5 is always less than R_{10}. If $\omega(0) \neq 0$, $\omega'(0) = 0$ and $d = 2$, then a_n is independent of n.

5. Conclusions

The main thrust of this article has been to provide a systematic procedure for computing the D-optimal designs for polynomial regression for a broad class of weight function on $[m_0 - a, m_0 + a]$ for any a in a neighborhood of 0 at a time. The only requirement is that weight function is analytic at m_0. The structure of the optimal designs is derived for a close to zero. Then we can use a recursive algorithm by Dette *et al.* (2004) to evaluate the Taylor polynomials of the optimal support points and optimal weights (if necessary) in a. This method is more efficient in determining the D-optimal designs for various a at a time.

All computations discussed in this article were performed on an IBM compatible PC using the numeric and symbolic computational software *Mathematica* 4.1 (Wolfram (1999)) and most of calculations with 16-digit precision.

Acknowledgements

This research was supported by the National Science Council of the Republic of China (Grant No. 92-2118-M-110-005-). The author is indebted to two referees for their constructive comments and suggestions on an earlier version of this paper.

Appendix A: Proof of Lemma 2.1

The following is the proof for the case (a). The proof for the case (b) is omitted since it can be proved similarly.

The assertion for the case $s = 0$ is well known in Fedorov (1972), Theorem 2.3.3 and is omitted here. Let ξ^* denote a D-optimal design. First we will show the symmetry of ξ^*. Consider the reflected design ξ^R of the design ξ^*, i.e. $\xi^R(x) = \xi^*(-x)$. Then it is easy to see that $\det M((\xi^* + \xi^R)/2) \geq (\det M(\xi^*))^{1/2}(\det M(\xi^R))^{1/2} = \det M(\xi^*)$ with equality holding if and only if ξ^* is a symmetric design since $\log(\det M(\xi))$ is a strictly concave function in ξ. The last equality follows from the fact that $\det M(\xi^R) = \det M(\xi^*)$. Thus ξ^* must be a symmetric design with the form

$$\left\{\begin{array}{cccccc} -x_k & \cdots & -x_1 & x_1 & \cdots & x_k \\ w_k/2 & \cdots & w_1/2 & w_1/2 & \cdots & w_k/2 \end{array}\right\}$$

where $0 < x_1 < \cdots < x_k \leq 1$ and $\sum_{i=1}^k w_k = 1$, $w_i > 0$.

Next we will show that $x_k = 1$. Suppose that $x_k < 1$ and let $\tau(x) = \xi^*(x_k x)$. Then it will imply that $\det M(\tau) = x_k^{-(d+s)(d+1)} \det M(\xi^*) > \det M(\xi^*)$ which would contradict the D-optimality of ξ^*.

Finally we will show that the number of the optimal support points is $d+1$ if d is odd. The Kiefer and Wolfowitz (1960) Equivalence Theorem (KWT) states that a design ξ^* is approximate D-optimal if and only if the directional derivative of $\log\det M(\xi^*)$ (see Silvey (1980), p. 20)

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

is less than or equal to zero for all x in $[-a,a]$, with equality holding at the support point of ξ. The symmetry of ξ^* implies that $d(x,\xi^*)$ has the form

$$|x|^s Q_{2d}(x) - (d+1)$$

where $Q_{2d}(x)$ is an even function and a polynomial of degree $2d$. Let $y = x^2$. Then $e(y) = d(x,\xi^*)$ has the form

$$y^{s/2} U_d(y) - (d+1)$$

where $U_d(x)$ is a polynomial of degree d. The function $e(y)$ has at most $d+1$ zeros counting the multiplicity since $\{1, y^{s/2}, y^{s/2+1}, \ldots, y^{s/2+d}\}$ forms a Chebyshev system on $[0,1]$ (Karlin and Studden (1966*b*)). Therefore it follows that $k \le (d+2)/2$ since the function $e(y)$ has $k-1$ zeros at $y_i = x_i^2$, $i = 1, 2, \ldots, k-1$ with multiplicity 2 and one simple zero at $x_k = 1$. Then the assertion of the theorem follows from that the number of the support points of ξ^* is greater than or equal to $d+1$ since the optimal information matrix must be nonsingular.

Appendix B: Proof of Lemma 2.2

(a) It is well known that the D-optimal design for $f(x)$ with $\omega(x) = 1$ on $[-1,1]$ puts equal masses at the zeros of $(1-x^2)P_d'(x)$ (Fedorov (1972), Theorem 2.3.3(1)). The alternative representation of the polynomial $P_d'(x)$ is given by the formula (4.21.7) of Szegö (1975).

(b) From Lemma 2.1(a) the number of the optimal support points is equal to $d+1$, the number of the parameters. Therefore the optimal design has equal masses $1/(d+1)$. The optimal design has the form

$$\mu_0^* = \left\{ \begin{array}{cccccc} -x_k & \cdots & -x_1 & x_1 & \cdots & x_k \\ 1/(2k) & \cdots & 1/(2k) & 1/(2k) & \cdots & 1/(2k) \end{array} \right\} \tag{B.1}$$

where $k = (d+1)/2$ and $x_k = 1$. An application of the formula of Vandermonde determinant yields that

$$\begin{aligned} \det M(\mu_0^*) &= (\det F)\mathrm{diag}(\omega(-x_k)/(2k), \ldots, \omega(x_k)/(2k))(\det F^T) \\ &= (1/k)^{2k} \prod_{i=1}^{k-1}(1-x_i^2)^4 \prod_{1\le i<j\le k-1}(x_i^2 - x_j^2)^4 \prod_{i=1}^{k-1} x_i^{2(s+1)} \end{aligned}$$

where $F = (f(-x_k), \ldots, f(-x_1), f(x_1), \ldots, f(x_k))$. Let $y_i = x_i^2$, $i = 1, 2, \ldots, k-1$. We now study the function

$$g(y_1, \ldots, y_{k-1}) = \prod_{i=1}^{k-1}(1-y_i)^4 \prod_{1\le i<j\le k-1}(y_i - y_j)^4 \prod_{i=1}^{k-1} y_i^{s+1}. \tag{B.2}$$

Note that the function g is a strict concave function and consequently there is a unique maximum. Consider the partial derivative of $\log g(y_1, \ldots, y_{k-1})$ with respect to y_i

$$\frac{\partial \log g(y_1, \ldots, y_{k-1})}{\partial y_i} = \frac{4}{y_i - 1} + \sum_{j \neq i} \frac{4}{y_i - y_j} + \frac{s+1}{y_i} \tag{B.3}$$

$$= 0 \tag{B.4}$$

for $i = 1, \ldots, k-1$. Similar arguments as given in Theorem 2.3.3 of Fedorov (1972) show that the polynomial $u(y) = \prod_{i=1}^{k-1}(y - y_i)$ satisfies the differential equation

$$2y(y-1)u''(y) + (4y + (s+1)(y-1))u'(y) = (k-1)(2k+s+1)u(y). \tag{B.5}$$

Let $z = 2y - 1$ and $u(y) = v(z)$. After substituting $u'(y) = 2v'(z)$ and $u''(y) = 4v''(z)$ in (B.5) and simple algebra yields the following differential equation

$$(1 - z^2)v''(z) + (\beta - \alpha - (\alpha + \beta + 2)z)v'(z) + n(n + \alpha + \beta + 1)v(z) = 0, \tag{B.6}$$

where $\alpha = 1$, $\beta = (s-1)/2$ and $n = (d-1)/2$. From Theorem 4.2.2 of Szegö (1975) the equation (B.6) has a unique polynomial solution $P_n^{(\alpha,\beta)}(z)$. The assertion of the theorem is proved after substituting $z = 2x^2 - 1$ into $P_n^{(\alpha,\beta)}(z)$.

(c) The proof is straightforward by a direct application of the Binet-Cauchy and Vandermonde formulas.

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