Statistica Sinica **15**(2005), 153-163

D-OPTIMAL DESIGNS FOR WEIGHTED POLYNOMIAL REGRESSION – A FUNCTIONAL-ALGEBRAIC APPROACH

Fu-Chuen Chang

National Sun Yat-sen University

Abstract: This paper is concerned with the problem of computing the approximate D-optimal design for polynomial regression with weight function $\omega(x) > 0$ on the design interval $I = [m_0 - a, m_0 + a]$. It is shown that if $\omega'(x)/\omega(x)$ is a rational function on I and a is close to zero, 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, which can be approximated by a Taylor expansion. We provide a recursive algorithm to compute Taylor expansion of these constants. Moreover, the D-optimal interior support points are the zeros of a polynomial which has coefficients that can be computed from a linear system.

Key words and phrases: Approximate D-optimal design, implicit function theorem, matrix, rational function, recursive algorithm, Taylor series, weighted polynomial regression.

1. Introduction

Consider the weighted polynomial regression model of degree d:

$$E[y(x)] = \sum_{i=0}^{d} \beta_i x^i, \qquad x \in I = [m_0 - a, m_0 + a],$$
$$\mathrm{Var}(y(x)) = \sigma^2/\omega(x), \tag{1.1}$$

where $\omega(x)$ denotes a positive weight function on the design interval I and the control variable x is taken from I. An approximate design ξ is a probability measure on I. The Fisher information matrix of a design ξ for the parameters $\beta = (\beta_0, \ldots, \beta_d)^T$ can be expressed as

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

where $f(x) = (1, x, \ldots, x^d)^T$ denotes the vector of monomials up to order d. 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. For more about the theory of optimal designs see Fedorov (1972), Silvey (1980) and Pukelsheim (1993).

The model (1.1) is 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 extensively investigated (e.g., Hoel (1958), Karlin and Studden (1966), Huang, Chang and Wong (1995), Chang and Lin (1997), Imhof, Krafft and Schaefer (1998), Chang (1998), Dette, Haines and Imhof (1999), Fang (2002) and Antille, Dette and Weinberg (2003), among many others).

The theory of differential equations is a powerful tool for determining the D-optimal designs for weighted polynomial regression. This approach was used in 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 others. However, the closed forms of the D-optimal designs for weighted polynomial regression exist only for very limited weight functions and restricted design spaces.

The pioneering work of Melas (1978) used a functional approach–Taylor expansion to determine the optimal design for exponential regression. This powerful and interesting tool was also used by Melas (2000, 2001) and Dette, Melas and Pepelyshev (2002, 2004). In a recent paper Dette, Melas and Biedermann (2002) combined it with an algebraic approach, transforming the original problem into a differential equation problem leading to an eigensystem of a certain matrix, to determine the D-optimal support points for trigonometric regression models on a partial circle. In this paper we extend the Dette, Melas and Biedermann (2002) approach to determine the D-optimal design for the parameters in (1.1) with a general class of weight functions $\omega(x)$ satisfying

$$\frac{\omega'(x)}{\omega(x)} = \frac{p(x)}{q(x)} \qquad \text{is a rational function,} \tag{1.2}$$

where both $p(x)$ and $q(x)$ are polynomials, the greatest common divisor of $p(x)$ and $q(x)$ is 1, and $q(x) \neq 0$ for all $x \in I$. Without loss of generality we consider the case $m_0 = 0$ only, i.e., the design space is on the symmetric interval $[-a, a]$, since the D-optimal design for (1.1) can be obtained from that for (1.1) with $\omega(m_0 + x)$ and $I = [-a, a]$ by a linear transformation.

This paper is organized in the following way. In Section 2, the differential equation for the D-optimal support points for the model (1.1) is derived. In addition, the form of $\omega(x)$ satisfying (1.2) is also established. An algorithm using a Taylor expansion to compute the D-optimal support points is given in Section 3. Finally, in Section 4, two illustrative examples are presented. All of the computations here were performed on an IBM compatible PC using the numeric and symbolic computational software *Mathematica* 5.0 (Wolfram (2003)).

2. The differential equation

First we establish the structure of the D-optimal designs on $[-a, a]$ when a is close to 0, and an explicit formula for the determinant of information matrix of designs, in the following lemma.

Lemma 2.1.

(a) *If $\omega(x)$ is a continuous function and $\omega(0) > 0$, then there exists a constant $\bar{a} > 0$ such that the D-optimal design for polynomial regression model on $[-a, a]$, $0 < a \leq \bar{a}$, is unique and has the form*

$$\xi = \begin{pmatrix} x_0 & x_1 & \cdots & x_d \\ 1/(d+1) & 1/(d+1) & \cdots & 1/(d+1) \end{pmatrix}, \tag{2.1}$$

where $-a = x_0 < x_1 < \cdots < x_d = a$.

(b) *If ξ denotes a design of the form* (2.1), *then* $\det M(\xi) = 4a^2\omega(-a)\omega(a)$ $\phi(x_1, \ldots, x_{d-1}, a^2)/(d+1)^{d+1}$, *where*

$$\phi(x_1, \ldots, x_{d-1}, a^2) = \prod_{i=1}^{d-1} \omega(x_i) \prod_{i=1}^{d-1} (x_i^2 - a^2)^2 \prod_{1 \leq i < j \leq d-1} (x_i - x_j)^2. \tag{2.2}$$

Proof. (a) Let $x = at$. Since $\omega(0) > 0$, it is easy to see that the problem of determining the structure of the approximate D-optimal design for $f(x)$ with $\omega(x)$ on $[-a, a]$ is equivalent to that of finding D-optimal designs for $f(t)$ with $\omega(t) = 1$ on $[-1, 1]$ as a tends 0. It is well-known (Fedorov (1972), Theorem 2.3.3) that the D-optimal design for $f(t)$ with $\omega(t) = 1$ on $[-1, 1]$ consists of two end points and $d-1$ interior points of the interval $[-1, 1]$. Therefore there exists an $\bar{a} > 0$ such that if $0 < a \leq \bar{a}$, then the D-optimal design is unique and has the form (2.1).

(b) The proof is straightforward by a direct application of Theorem 2.3.1 (Fedorov (1972)) and the determinant of the Vandermonde matrix.

It is clear that maximizing $\det M(\xi)$ is equivalent to maximizing $\log \phi(x_1, \ldots, x_{d-1}, a^2)$. Then the following conditions must be satisfied

$$\begin{aligned} \frac{\partial \log \phi}{\partial x_i} &= \frac{4x_i}{x_i^2 - a^2} + \frac{\omega'(x_i)}{\omega(x_i)} \\ &\quad + 2\left(\frac{1}{x_i - x_1} + \cdots + \frac{1}{x_i - x_{i-1}} + \frac{1}{x_i - x_{i+1}} + \cdots + \frac{1}{x_i - x_{d-1}}\right) = 0, \end{aligned}$$

for $i = 1, \ldots, d-1$. Let

$$u(x) = \prod_{i=1}^{d-1}(x - x_i) = \sum_{i=0}^{d-1} u_i x^i, \qquad u_{d-1} = 1 \tag{2.3}$$

denote a monic polynomial of degree $d-1$ which has the $d-1$ interior support points of the design in (2.1) as its zeros. It is easy to verify that

$$\frac{u''(x_i)}{u'(x_i)} = 2\left(\frac{1}{x_i - x_1} + \cdots + \frac{1}{x_i - x_{i-1}} + \frac{1}{x_i - x_{i+1}} + \cdots + \frac{1}{x_i - x_{d-1}}\right)$$

(see, Fedorov (1972), Section 2.3). Then the following differential equation holds

$$\frac{4x}{x^2 - a^2} + \frac{\omega'(x)}{\omega(x)} + \frac{u''(x)}{u'(x)} = 0 \tag{2.4}$$

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

To ensure that (2.4) can be solved by techniques as in Theorem 2.3.3 of Fedorov (1972), we have to assume that

$$\frac{\omega'(x)}{\omega(x)} = \frac{p(x)}{q(x)} = \frac{p_m x^m + p_{m-1}x^{m-1} + \cdots + p_0}{q_n x^n + q_{n-1}x^{n-1} + \cdots + q_0} \tag{2.5}$$

is a rational function where $p(x)$ and $q(x)$ are polynomials of degrees m and n, respectively, and the greatest common divisor of $p(x)$ and $q(x)$ is 1. The following lemma characterizes the form of $\omega(x)$ satisfying (2.5). The proof is complicated and deferred to Appendix.

Lemma 2.2. *If $\omega'(x)/\omega(x)$ is a rational function on I, then $\omega(x)$ has the form of*

$$\left(\prod_i |r_i(x)|^{\alpha_i}\right) e^{r(x) + \sum_i \beta_i \tan^{-1}\gamma_i(x+\delta_i)}, \tag{2.6}$$

where $r_i(x)$ is either a monic linear or quadratic polynomial, $r(x)$ is a rational function and α_i, β_i, γ_i, δ_i are real.

Remark. The class (2.6) contains almost all weight functions discussed in the literature on D-optimal designs of weighted polynomial regression. For example, $\omega(x) = 1; (1-x)^{\alpha+1}(1+x)^{\beta+1}$ for $\alpha > -1, \beta > -1; x^{\alpha+1}\exp(-x)$ for $\alpha \geq -1; \exp(-x^2)$ in Theorem 2.3.3 of Fedorov (1970), and $\omega(x) = (1+x^2)^{\alpha+1}$ $\exp(2\beta\tan^{-1}x)$ in Theorem 3.1 of Antille, Dette and Weinberg (2003).

Substituting $\omega'(x)/\omega(x) = p(x)/q(x)$ into (2.4), and multiplying the equation by the common denominator, we obtain $L(x) = 0$ for $x = x_1, \ldots, x_{d-1}$, where

$$L(x) = (x^2 - a^2)q(x)u''(x) + ((x^2 - a^2)p(x) + 4xq(x))u'(x) \tag{2.7}$$

is a second order differential function. Note that $L(x)$ is a polynomial of degree $k+d-1$ where $k = \max(m+1, n)$ and vanishes at $x = x_1, \ldots, x_{d-1}$. Then $u(x)$ is a factor of $L(x)$. Thus there exists an auxiliary polynomial $b(x) = b_k x^k + b_{k-1}x^{k-1} + \cdots + b_0$ such that

$$(x^2 - a^2)q(x)u''(x) + ((x^2 - a^2)p(x) + 4xq(x))u'(x) = b(x)u(x), \tag{2.8}$$

where b_k is the leading coefficient of $L(x)$ and $b_0, \ldots, b_{k-1}$ are k unknown constants.

3. Taylor Expansions for Unknown Constants

Substituting $u(x) = \sum_{i=0}^{d-1} u_i x^i$ into (2.8) and comparing the coefficients on both sides, we obtain an equation, in matrix-vector form,

$$(1, x, \ldots, x^{k+d-2})Au \,=\, 0, \tag{3.1}$$

where $A = (a_{i,j}) = D - B$, $i = 0, \ldots, k+d-2$, $j = 0, \ldots, d-1$, $u = (u_0, \ldots, u_{d-1})^T$, and

$$D = \begin{pmatrix}
0 & d_{0,1} & d_{0,2} & 0 & \cdots & \cdots & \cdots & 0 \\
0 & d_{1,1} & d_{1,2} & d_{1,3} & \ddots & & & \vdots \\
0 & d_{2,1} & d_{2,2} & d_{2,3} & \ddots & \ddots & & \vdots \\
\vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \ddots & \vdots \\
 & & & & & d_{d-4,d-3} & d_{d-4,d-2} & 0 \\
 & & & & & & d_{d-3,d-2} & d_{d-3,d-1} \\
 & & & & & & & d_{d-2,d-1} \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & d_{k,1} & & & & & & \\
0 & d_{k+1,1} & d_{k+1,2} & & & & & \\
0 & 0 & d_{k+2,2} & d_{k+2,3} & & & & \\
\vdots & \vdots & \ddots & \ddots & \ddots & \vdots & \vdots & \vdots \\
\vdots & \vdots & & \ddots & \ddots & d_{k+d-4,d-3} & d_{k+d-4,d-2} & d_{k+d-4,d-1} \\
\vdots & \vdots & & & \ddots & d_{k+d-3,d-3} & d_{k+d-3,d-2} & d_{k+d-3,d-1} \\
0 & 0 & \cdots & \cdots & \cdots & 0 & d_{k+d-2,d-2} & d_{k+d-2,d-1}
\end{pmatrix}_{(k+d-1)\times d} \tag{3.2}$$

is a banded matrix with bandwidth $k+3$, $d_{i,j} = j(-a^2[(j-1)q_{i-j+2} + p_{i-j+1}] + [j+3]q_{i-j} + p_{i-j-1})$ is the coefficient of $x^i u_j$ in $L(x)$, $p_i = 0$ if $i < 0$ or $i > m$, $q_i = 0$ if $i < 0$ or $i > n$, and B is a lower banded matrix which has bandwidth

$k+1$ and constant values along negative-sloping diagonals,

$$B = \begin{pmatrix} b_0 & 0 & \cdots & \cdots & 0 \\ b_1 & b_0 & \ddots & & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ b_{k-1} & & \ddots & \ddots & 0 \\ b_k & b_{k-1} & & \ddots & b_0 \\ 0 & b_k & \ddots & & b_1 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & b_k & b_{k-1} \end{pmatrix}_{(k+d-1)\times d} . \tag{3.3}$$

Now the D-optimal design problem is reduced to finding the $k+d-1$ unknown constants $b = (b_0, \ldots, b_{k-1})^T$ and $\{u_0, \ldots, u_{d-2}\}$ such that

$$Au = 0, \tag{3.4}$$

or that u is orthogonal to the row space of A. Note that if $k = 0$, then the $d-1$ unknown constants u can be solved directly from (3.4) since A is a real matrix. If the k unknown constants $b, k \geq 1$, are available, then u can be solved by a backward-substitution process from the following matrix equation

$$A_{k-1}u = 0, \tag{3.5}$$

where A_{k-1} consists of the last $k-1$ rows of A. Noting that the last row in (3.5) implies $u_{d-2} = -a_{k+d-2,d-1}/a_{k+d-2,d-2}$. The last second row can be solved for $u_{d-3} = -(a_{k+d-3,d-1} + a_{k+d-3,d-2}u_{d-2})/a_{k+d-3,d-3}$. Continuing in this fashion yields $u_0 = -\sum_{i=1}^{d-1} a_{k,i}u_i/a_{k,0}$. If $k = 1$, then $A_{k-1} = A$, b_0 is an eigenvalue of A, and u is the unique eigenvector of A corresponding to b_0. A special form of this case is considered in Dette, Melas and Biedermann (2002). Apparently, there is no literature on how to solve for D-optimal designs with $k > 1$.

A recursive procedure to approximate the k ($k \geq 1$) unknown constants b is described in the following. Our approach, based on (3.4), is algebraic. The method is an extension of Dette, Melas and Biedermann (2002), which combines algebraic and functional approaches to study D-optimal designs for trigonometric regression models on a partial circle.

First we relate (3.4) to an optimization problem that reduces to solving a system of k polynomial equations in b and a fixed parameter a^2. Note that $u^T A^T A u = 0$ by (3.4). Consider $G(b, a^2) = \det(A^T A)$, non-negative since $A^T A$ is a positive semidefinite matrix. The unknown constants b_i's in (2.8) are functions of a^2 ($b_0^*, \ldots, b_{k-1}^*$, say), which is a global minimum point of G for any fixed a, i.e., $\min_b G(b, a^2) = G(b^*, a^2) = 0$, where $b^* = (b_0^*, \ldots, b_{k-1}^*)^T$. Therefore

$$g(b^*, a^2) = 0 \in \Re^k, \tag{3.6}$$

where $g = (g_0, \ldots, g_{k-1})^T$ and $g_i = \partial G(b, a^2)/\partial b_i$. If the the Jacobian matrix $J_g(a) = (\partial g_i/\partial b_j)_{i,j=0}^{k-1}$ is nonsingular at $a = 0$, that is $\det[J_g(0)] \neq 0$, then from the implicit function theorem (see, Khuri (2002), Theorem 7.6.2), the b_i^*'s are analytical functions of a^2 on the interval $(-\bar{a}, \bar{a})$ where $\bar{a}$ is a function of $\omega(x)$ and d. This implies that the Taylor series of b_i^* at the origin exists for $i = 0, \ldots, k-1$.

The constant term of the Taylor series of b_i^* can be calculated as follows. As a tends to 0, all optimal support points converge to 0, and the limiting supporting polynomial is $\widehat{u}(x) = x^{d-1}$. Let $\widehat{b}_i = \lim_{a \to 0} b_i^*$. Then by (2.8) the $\widehat{b}_i$'s satisfy

$$\widehat{b}(x) = (d-1)[(d-2)q(x) + xp(x) + 4q(x)], \tag{3.7}$$

where $\widehat{b}(x) = \widehat{b}_0 + \cdots + \widehat{b}_{k-1}x^{k-1} + b_k x^k$.

Consider the Taylor expansions of b_i^*'s, $b^*(a^2) = \sum_{j=0}^{\infty} b_{(j)}(a^2)^j, b_{(0)} = \widehat{b}$, where $\widehat{b} = (\widehat{b}_0, \ldots, \widehat{b}_{k-1})^T$ and $b_{(j)} = (b_{(0,j)}, \ldots, b_{(k-1,j)})^T$. Denote the Taylor polynomials of degree n by $b_{<n>}(a^2) = \sum_{j=0}^{n} b_{(j)}(a^2)^j, b_{(0)} = \widehat{b}$, where $b_{<n>}(a^2) = (b_{<0,n>}, \ldots, b_{<k-1,n>})^T$. The coefficients $b_{(j)}$ can be computed recursively as

$$b_{(n+1)} = -\frac{1}{(n+1)!} J_g^{-1}(0) \left. \frac{d^{n+1}}{d(a^2)^{n+1}} g(b_{<n>}(a^2), a^2) \right|_{a=0}, \qquad n = 0, 1, \ldots$$

which has been explicitly found in Dette, Melas and Pepelyshev (2004).

4. Examples

An illustration of the method presented in Section 3 is given in the following two examples.

Example 4.1. Consider quadratic polynomial regression with $\omega(x) = 2x^2 + x + 1$ on the interval $[-a, a]$. Then $p(x) = 4x + 1$ and $q(x) = 2x^2 + x + 1$. The second-order differential equation in (2.8) is given by $(x^2 - a^2)(4x+1) + 4x(2x^2 + x + 1) = (12x^2 + b_1 x + b_0)(x + u_0)$. We can rewrite the equation above in the matrix-vector form $(1, x, x^2)A(u_0, 1)^T = 0$, where

$$A = \begin{pmatrix} -b_0 & -a^2 \\ -b_1 & 4 - 4a^2 - b_0 \\ -12 & 5 - b_1 \end{pmatrix}.$$

From (3.7) the limit of $b^*(a^2)$ when a tends to 0 is given by $\widehat{b} = (\widehat{b}_0, \widehat{b}_1)^T = (4, 5)^T$. The Taylor expansion of $b_{<5>}(a^2) = (b_{<0,5>}, b_{<1,5>})^T$ is $(4 - \frac{11}{4}a^2 + \frac{103}{64}a^4, 5 + 3a^2 + \frac{33}{16}a^4)^T$. Then by (3.4)

$$\begin{pmatrix} -4 + \frac{11}{4}a^2 - \frac{103}{64}a^4 & -a^2 \\ -5 - 3a^2 - \frac{33}{16}a^4 & -\frac{5}{4}a^2 - \frac{103}{64}a^4 \\ -12 & -3a^2 - \frac{33}{16}a^4 \end{pmatrix} \begin{pmatrix} u_0 \\ 1 \end{pmatrix} \approx \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}.$$

Solving (3.5) gives $u_0 = -a^2/4 - 11a^4/64$. For example, if $a = 0.3$, then the zero of the supporting polynomial $u(x) = x - a^2/4 - 11a^4/64$ is 0.024. Then the design computed from above is

$$\xi = \begin{pmatrix} -0.3 & 0.024 & 0.3 \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix}.$$

The numerical result shows that ξ is a D-optimal design on the interval $[-0.3, 0.3]$ in the sense of the D-Equivalence criterion (see Kiefer and Wolfowitz (1960)) satisfying $\max_{x\in[-a,a]} |d(x,\xi) - 3| \le 10^{-3}$, where $d(x,\xi) = \omega(x)f^T(x)M^{-1}(\xi)f(x)$.

The coefficients of the u_i's and the Taylor expansions for the b_i's for $d = 2, 3, 4, 5$ are given in Table 1.

Table 1. The coefficients of u_i's and Taylor expansions for b_i's.

	j	0	1	2	3	4	5
$d=2$	b_0	4	−2.75000	1.60938	1.11914	−0.17511	−1.34727
	b_1	5	3.00000	2.06250	0.21094	−1.52417	−1.57846
	u_0	0	−0.25000	−0.17188	−0.01758	0.12701	0.13154
$d=3$	b_0	10	−4.53333	1.20415	−1.61573	2.30525	−0.71317
	b_1	12	4.26667	−3.94430	−0.77807	1.25073	−2.25860
	u_0	0	−0.20000	−0.06400	−0.02958	−0.04288	0.02770
	u_1	0	−0.26667	0.24652	0.04863	−0.07817	0.14116
$d=4$	b_0	18	−6.16071	1.24477	1.37457	−0.03039	−2.15460
	b_1	21	5.35714	−6.02029	5.23264	−2.06192	3.18621
	u_0	0	0.00000	0.05357	−0.01122	0.02499	−0.01195
	u_1	0	−0.42857	−0.06997	−0.06236	0.10328	−0.01851
	u_2	0	−0.26786	0.30102	−0.26163	0.10310	−0.15931
$d=5$	b_0	28	−7.73333	1.33666	2.41879	−4.76908	3.78370
	b_1	32	6.40000	−7.57977	7.63099	−4.97560	1.45153
	u_0	0	0.00000	0.04762	0.01411	0.00933	−0.01927
	u_1	0	0.00000	0.11429	−0.08093	0.07060	−0.06925
	u_2	0	−0.66667	−0.07055	−0.06736	0.20346	−0.24073
	u_3	0	−0.26667	0.31582	−0.31796	0.20732	−0.06048

Example 4.2. Consider the problem of the radius $\bar{a}$ of convergence for the Taylor expansion of $b^*(a^2)$. In general, a closed form for $\bar{a}$ seems intractable. Even the task of computing the numerical values of $\bar{a}$ is formidable, since the length of expressions involved in computing of Taylor expansion growths quickly as n increases. Therefore we consider the radius $\bar{a}_n$ of convergence for $b_{<n>}(a^2)$. The convergence criterion for $b_{<n>}(a^2)$ used here is

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

where $\hat{\xi}$ is a design computed from $b_{<n>}(a^2)$. The constant $\bar{a}_n$ is the maximum a such that (4.1) holds. Table 2 lists $\bar{a}_n$ for various weight functions, $d = 2, 3, 4, 5$ and $n = 5, 10$. For example, if $\omega(x) = 2x^2 + x + 1$ and $d = 2$, then $\bar{a}_n$ for $n = 5$ and 10 is 0.644 and 0.752, respectively. For any $\omega(x)$, $\bar{a}_5$ is always less than $\bar{a}_{10}$. Numbers in bold face satisfy $d = 2$ and $\omega'(0) = 0$. The numerical values of $b_{<n>}$ are quadratic functions in a. Thus the radius of convergence $\bar{a}_n$ is a constant.

Table 2. Radius $\bar{a}_n$ of convergence for $b_{<n>}(a^2)$.

$\omega(x)$	k	n	$d=2$	$d=3$	$d=4$	$d=5$
$x+2$	1	5	1.470	1.610	1.773	1.303
		10	1.471	1.681	1.787	1.796
$2x^2+x+1$	2	5	0.644	0.601	0.564	0.591
		10	0.752	0.740	0.692	0.677
$\frac{1}{x^2+1}$	2	5	∞	0.781	0.757	0.520
		10	∞	0.975	0.940	0.800
e^x	1	5	1.559	2.430	2.249	2.220
		10	1.844	2.692	3.341	4.070
$e^{\frac{1}{x-1}}$	2	5	0.569	0.641	0.666	0.455
		10	0.566	0.660	0.719	0.674
$(x+1)e^x$	2	5	0.548	0.636	0.704	0.503
		10	0.631	0.798	0.870	0.767
$\frac{e^x}{(x+1)^2}$	2	5	0.723	0.660	0.649	0.392
		10	0.858	0.829	0.840	0.695
$e^{\tan^{-1} x}$	2	5	0.980	0.880	0.784	0.625
		10	1.152	1.058	0.934	0.863
$e^{\tan^{-1} \frac{x}{x-1}}$	2	5	0.643	0.620	0.535	0.442
		10	0.753	0.745	0.711	0.633
$(x^2+1)e^{\tan^{-1} x}$	2	5	0.842	0.756	0.670	0.590
		10	0.904	0.908	0.905	0.827
$\frac{e^{\tan^{-1} x}}{x^2+1}$	2	5	0.881	0.790	0.602	0.527
		10	0.941	0.891	0.823	0.810
x^2+1	2	5	**1.352**	0.930	0.838	0.727
		10	**1.352**	1.331	1.156	1.011
x^4+1	4	5	**1.773**	0.945	0.832	0.609
		10	**1.773**	1.150	0.995	0.951
e^{x^2}	2	5	**1.389**	1.047	1.223	1.145
		10	**1.389**	1.435	1.602	1.728
$e^{\tan^{-1} x^2}$	4	5	**1.353**	0.874	0.793	0.635
		10	**1.353**	1.097	0.993	0.930
$\frac{x^2+1}{x^4+1}$	6	5	**1.179**	0.718	0.734	0.473
		10	**1.179**	1.038	0.902	0.887

Appendix. Proof of Lemma 2.2

Any rational function $p(x)/q(x)$ in (2.5) can be written as $s(x)+t(x)/q(x)$, where $s(x), t(x)$ and $q(x)$ are polynomials and the degree of $t(x) <$ the degree of $q(x)$. From the Partial-Fraction Decomposition Theorem (see, Grossman (1993), Section 7.7) we have

$$\frac{t(x)}{q(x)}=\sum_{i=1}^{k_1}\sum_{j=1}^{m_i}\frac{A_{ij}}{(x-A_i)^j}+\sum_{i=1}^{k_2}\sum_{j=1}^{n_i}\frac{B_{ij}x+C_{ij}}{(x^2+B_ix+C_i)^j},$$

where $A_{ij}, B_{ij}, C_{ij}, A_i, B_i, C_i$, are constants and each $x^2+B_ix+C_i$ is an irreducible quadratic polynomial. It is well-known that

$$\int\frac{A_{ij}}{(x-A_i)^j}\,dx=\begin{cases}A_{ij}\log|x-A_i|+C & \text{if } j=1,\\ \dfrac{A_{ij}}{1-j}(x-A_i)^{-j+1}+C & \text{if } j=2,3,\ldots,\end{cases}\tag{A.1}$$

$$\int\frac{B_{ij}x+C_{ij}}{(x^2+B_ix+C_i)^j}\,dx=\begin{cases}\alpha_1\log|x^2+B_ix+C_i|+\alpha_2\tan^{-1}(\alpha_3(x+B_i/2))+C & \text{if } j=1,\\ r(x)+\beta_1\tan^{-1}(\beta_2(x+B_i/2))+C & \text{if } j=2,3,\ldots\end{cases}\tag{A.2}$$

where $\alpha_1,\alpha_2,\alpha_3,\beta_1,\beta_2$ are constants, C is the constant of integration, and $r(x)$ is a rational function. Note that the inverse tangent satisfies the addition formula

$$\tan^{-1}a+\tan^{-1}b=\begin{cases}\tan^{-1}\frac{a+b}{1-ab}-\pi & \text{if } a<0 \text{ and } b<0,\\ \tan^{-1}\frac{a+b}{1-ab}+\pi & \text{if } a>0 \text{ and } b>0,\\ \tan^{-1}\frac{a+b}{1-ab} & \text{if } ab\le 0.\end{cases}$$

Combining this with (A.1) and (A.2), we have

$$\begin{aligned}\int\frac{\omega'(x)}{\omega(x)}\,dx&=\log|\omega(x)|+C\\ &=\int s(x)+\sum_{i=1}^{k_1}\sum_{j=1}^{m_i}\frac{A_{ij}}{(x-A_i)^j}+\sum_{i=1}^{k_2}\sum_{j=1}^{n_i}\frac{B_{ij}x+C_{ij}}{(x^2+B_ix+C_i)^j}\,dx\\ &=\log|r_1(x)|+r_2(x)+\tan^{-1}r_3(x)+C,\end{aligned}$$

the desired result.

Acknowledgements

This research was supported by the National Science Council of the Republic of China (Grant No. 91-2118-M-110-004-). The author is indebted to two referees for their constructive comments and suggestions on an earlier version of this paper.

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.

Chang, F.-C. (1998). On asymptotic distribution of optimal design for polynomial-type regression. *Statist. Probab. Lett.* **36**, 421-425.

Chang, F.-C. and Lin, G.-C. (1997). D-optimal designs for weighted polynomial regression. *J. Statist. Plann. Inference* **55**, 371-387.

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

Dette, H., Melas, V. B. and Biedermann, S. (2002). A functional-algebraic determination of D-optimal designs for trigonometric regression models on a partial circle. *Statist. Probab. Lett.* **58**, 389-397.

Dette, H., Melas, V. B. and Pepelyshev, A. (2002). D-optimal designs for trigonometric regression models on a partial circle. *Ann. Inst. Statist. Math.* **54**, 945-959.

Dette, H., Melas, V.B. and Pepelyshev, A. (2004). Optimal designs for estimating individual coefficients–a functional approach. *J. Statist. Plann. Inference* **118**, 201-219.

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

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

Grossman, S. I. (1993). *Calculus*. 5th edition. Hartcourt Bruce, Orlando, Florida.

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.

Khuri, A. I. (2002). *Advanced Calculus with Applications in Statistics*. 2nd edition. Wiley, New York.

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

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

Melas, V. B. (2000). Analytic theory of E-optimal designs for polynomial regression. In *Advances in Stochastic Simulation Methods*, 85-116. Birkhäuser, Boston.

Melas, V. B. (2001). Analytical properties of locally D-optimal designs for rational models. In *MODA 6 – Advances in Model-Oriented Data Analysis and Experimental Design* (Edited by A. C. Atkinson, P. Hackl and W. G. Müller), 201-209. Physica, Heidelberg.

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

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

Wolfram, S. (2003). *The Mathematica Book*. 5th edition. Wolfram Media/Cambridge University Press.

Department of Applied Mathematics, National Sun Yat-sen University, Kaohsiung, Taiwan 804, R.O.C.

E-mail: changfc@math.nsysu.edu.tw

(Received September 2003; accepted March 2004)