

# OPTIMAL DESIGNS FOR ESTIMATING INDIVIDUAL COEFFICIENTS IN FOURIER REGRESSION MODELS

BY HOLGER DETTE AND VIATCHESLAV B. MELAS

*Ruhr-Universität Bochum and St. Petersburg State University*

In the common trigonometric regression model, we investigate the optimal design problem for the estimation of the individual coefficients, where the explanatory variable varies in the interval  $[-a, a]$ ,  $0 < a \leq \pi$ . It is demonstrated that the structure of the optimal design depends sensitively on the size of the design space. For many important cases, optimal designs can be found explicitly, where the complexity of the solution depends on the value of the parameter  $a$  and the order of the term, for which the corresponding coefficient has to be estimated. The main tool of our approach is the reduction of the problem for the trigonometric regression model to a design problem for a polynomial regression. In particular, we determine the optimal designs for estimating the parameters corresponding to the cosine terms explicitly, if the design space is sufficiently small, and prove that under this condition all optimal designs for estimating the parameters corresponding to the sine terms are supported at the same points.

## 1. Introduction. Trigonometric regression models of the form

$$(1.1) \quad y = \beta_0 + \sum_{j=1}^m \beta_{2j-1} \sin(jt) + \sum_{j=1}^m \beta_{2j} \cos(jt) + \varepsilon, \quad t \in [-a, a], \quad 0 < a \leq \pi,$$

are widely used to describe periodic phenomena [see, e.g., Mardia (1972), Graybill (1976) and Kitsos, Titterton and Torsney (1988) or the recent collection of research papers in biology edited by Lestrel (1997)]. The problem of designing experiments for Fourier regression models has been discussed by several authors [see, e.g., Karlin and Studden (1966), page 347, Fedorov (1972), page 94, Hill (1978), Lau and Studden (1985) and Riccomagno, Schwabe and Wynn (1997)]. While most authors concentrate on the design space  $[-\pi, \pi]$  much less attention has been paid to the case of a smaller design space [see, e.g., Hill (1978) and Wu (2002)]. This situation is of practical importance because in many applications it is impossible to take observations on the full circle  $[-\pi, \pi]$ . We refer to Kitsos, Titterton and Torsney (1988), who investigated a design problem in rhythmometry involving the circadian rhythm exhibited by peak expiratory flow,

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for which the design region has to be restricted to a partial circle of the complete 24-hour period. Further applications can be found in McCool (1979) in the context of precision engineering. A rather different field of application of trigonometric regression models on an incomplete circle is in agronomy, where these models are used for the prediction of the length of growth processes [see, e.g., Weber and Liebig (1981)].

It is the purpose of the present paper to study the optimal design problem for the estimation of the individual coefficients  $\beta_k$  in the trigonometric regression model (1.1) on the interval  $[-a, a]$ . The estimation of the individual coefficients and the corresponding optimal designs is of importance for several reasons. First, the precise estimation of the top coefficients is useful for model diagnostics, more precisely, for the investigation of the degree of regression [see, e.g., Dette and Haller (1998)]. In particular, if Fourier series are used as curve estimators, the degree corresponds to some kind of smoothing parameter and it is important to estimate these coefficients with sufficient efficiency. Moreover, there are several applications of trigonometric regression models in two-dimensional shape analysis in biology, where the coefficients of lower order are of particular importance, because they have a specific meaning in the biological context. We refer for concrete examples to Younker and Ehrlich (1977) and Currie, Ganeshanandam, Noiton, Garrick, Shelbourne and Oraguzie (2000). Second, the optimal designs for the individual coefficients are the basis of all standardized optimality criteria introduced by Dette (1997), and  $E$ -optimal designs can often be found as convex combinations of the optimal designs for the estimation of the individual coefficients [see Pukelsheim and Studden (1993), Melas (2000), Imhof and Studden (2001) and Dette and Melas (2002)]. Third, optimal designs are useful as benchmarks in evaluating the performance of other designs and therefore provide a means of identifying efficient designs. Here it is of practical importance to know the efficiency of the designs for the estimation of the top individual coefficients, because, in practice, these coefficients are tested for significance in order to reduce the number of parameters in the model. Consider, for example, the quadratic trigonometric regression model on the full circle  $[-\pi, \pi]$ . Table 1 shows the efficiencies of the (equally spaced)  $D$ -optimal design for estimating the top coefficients  $\beta_2, \beta_3, \beta_4$  in the trigonometric model on various design spaces. The  $D$ -optimal design on the interval  $[-\pi, \pi]$  is taken from Pukelsheim (1993), Chapter 9, the  $D$ -optimal designs on the intervals  $[-\frac{\pi}{2}, \frac{\pi}{2}]$  and  $[-\frac{\pi}{4}, \frac{\pi}{4}]$  can be found in Dette, Melas and Pepelyshev (2002), while the optimal designs for estimating the coefficients  $\beta_2, \beta_3, \beta_4$  are obtained from the results given in this paper (see Sections 2–4). We observe that the  $D$ -optimal design (in other words, the uniform and commonly believed optimal allocation of observations) is not a good choice for model diagnostics in a quadratic trigonometric regression model on the interval  $[-\pi, \pi]$ , because it does not allow efficient testing of the top coefficients in this model. On the other hand, on a small design space, say  $[-\frac{\pi}{2}, \frac{\pi}{2}]$

TABLE 1  
*Efficiencies of the  $D$ -optimal design for a quadratic trigonometric regression on the intervals  $[-\pi, \pi]$ ,  $[-\frac{\pi}{2}, \frac{\pi}{2}]$  and  $[-\frac{\pi}{4}, \frac{\pi}{4}]$  model with respect to various optimality criteria*

Interval	Efficiency		
	$\beta_2$	$\beta_3$	$\beta_4$
$[-\pi, \pi]$	50%	50%	50%
$[-\frac{\pi}{2}, \frac{\pi}{2}]$	89.41%	77.32%	79.77%
$[-\frac{\pi}{4}, \frac{\pi}{4}]$	85.27%	74.31%	82.68%

or  $[-\frac{\pi}{4}, \frac{\pi}{4}]$ , the situation changes completely. Here the  $D$ -optimal design (not necessarily a uniform distribution) produces reasonable efficiencies for testing the top coefficients in the quadratic regression model. A similar statement can be made for higher order degree models and a simple rule of thumb would be to recommend  $D$ -optimal designs only for inference in trigonometric regression models with a “small” range for the explanatory variable, because only in this case do they have reasonable efficiency for model diagnostics.

In Section 2, we introduce the general notation and state several preliminary results. The main tool of our approach is the reduction of the design problem for the trigonometric regression model to a design problem for a polynomial regression model. On incomplete intervals, we study the support points and weights of the optimal designs as functions of the length of the design space. In Section 3, we consider the optimal design problem for the estimation of the coefficients of the cosine terms. The optimal design problem for the estimation of the parameter  $\beta_k$  can be solved analytically for any  $k \in \{0, 2, \dots, 2m\}$ , provided that the design space  $[-a, a]$  is sufficiently small (see Theorem 3.1), where the critical value of  $a$  depends on the index of the coefficient and is always larger than  $\pi/2$ . In this case, the supports of the optimal designs for estimating the coefficients  $\beta_0, \beta_2, \dots, \beta_{2m}$  are the same and can be expressed through the extremal points of a Chebyshev polynomial of the first kind. Section 4 considers the problem of estimating individual coefficients of the sine terms, for which the situation is more difficult. For sufficiently small design spaces  $[-a, a]$ , we prove that the supports of the optimal designs for estimating the coefficients  $\beta_1, \beta_3, \dots, \beta_{2m-1}$  are the same and can be characterized as the extremal points of a function (see Theorem 4.5). However, neither this function nor these points can be found in an explicit form. Only the limit of the support points and the weights (after renormalization) can be found analytically, if the length of the design space tends to 0. Moreover, the points and weights considered as functions of the length of the design interval are real analytic and for this reason the optimal designs can be obtained numerically by a Taylor expansion. Finally, some conclusions are given in Section 5 and the proofs and technical details are deferred to the Appendix.

**2. Optimal designs for estimating individual coefficients.** Consider the trigonometric regression model (1.1), define  $\beta = (\beta_0, \beta_1, \dots, \beta_{2m})^T$  and let

$$(2.1) \quad f(t) = (1, \sin t, \cos t, \dots, \sin(mt), \cos(mt))^T = (f_0(t), \dots, f_{2m}(t))^T$$

denote the vector of regression functions. An approximate design is a probability measure  $\xi$  on the design space  $[-a, a]$  with finite support [see, e.g., Kiefer (1974)]. The support points of the design  $\xi$  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 by some rounding procedure), the covariance matrix of the least squares estimator for the parameter  $\beta$  is approximately given by

$$\frac{\sigma^2}{n} M^{-1}(\xi),$$

where  $n$  denotes the sample size and the matrix

$$(2.2) \quad M(\xi) = \int_{-a}^a f(t) f^T(t) d\xi(t) \in \mathbb{R}^{2m+1 \times 2m+1}$$

is called the information matrix in the design literature. An optimal design minimizes (or maximizes) an appropriate convex (or concave) function of the information matrix and there are numerous criteria proposed in the literature, which can be used for the discrimination between competing designs [see, e.g., Fedorov (1972), Silvey (1980) and Pukelsheim (1993)].

In this paper, we are interested in optimal designs for the estimation of the individual coefficients  $\beta_k$  in the trigonometric regression model (1.1). To be precise, let  $e_k \in \mathbb{R}^{2m+1}$  denote the  $(k+1)$ st unit vector ( $k = 0, \dots, 2m$ ) and  $A^-$  be a generalized inverse of the matrix  $A \in \mathbb{R}^{2m+1 \times 2m+1}$ ; then a design  $\xi$  is called  $e_k$ -optimal or optimal for estimating the coefficient  $\beta_k$ , if  $\beta_k$  is estimable by the design  $\xi$  [i.e.,  $e_k \in \text{Range}(M(\xi))$ ] and  $\xi$  minimizes the function

$$(2.3) \quad \Phi_k(\eta) = e_k^T M^-(\eta) e_k$$

in the set of all designs  $\eta$  such that  $\beta_k$  is estimable by the design  $\eta$ . The  $e_k$ -optimal designs have been discussed by several authors, mainly for the case of polynomial regression on the interval  $[-1, 1]$  [see, e.g., Studden (1968) and Sahn (2000)], but nothing is known for the trigonometric case.

It follows by standard arguments [see Pukelsheim (1993), Chapters 4 and 5] that  $\Phi$  is a convex function on the set of designs on the interval  $[-a, a]$ , which is invariant with respect to a reflection of the design at the origin. Consequently, there exists a symmetric  $e_k$ -optimal design (which is not necessarily unique), and we will restrict ourselves to the determination of optimal designs in the set  $\Xi_s$  of all symmetric designs on the interval  $[-a, a]$ . As pointed out by Dette and Haller (1998), this set can be mapped in a one-to-one manner onto the set of designs on

the interval  $[\alpha, 1]$ , where  $\alpha = \cos a$ . More precisely, define for a symmetric design  $\xi$  on the interval  $[-a, a]$  its projection  $\eta_\xi$  as the design on the interval  $[\alpha, 1]$  given by

$$(2.4) \quad \eta_\xi(\cos x) = \begin{cases} \xi(x) + \xi(-x), & \text{if } 0 < x \leq a, \\ \xi(0), & \text{if } x = 0. \end{cases}$$

It is now easy to see that after an appropriate permutation  $P \in \mathbb{R}^{2m+1 \times 2m+1}$  on the order of the regression functions the information matrix  $\tilde{M}(\xi) = PM(\xi)P$  of a symmetric design is block diagonal with diagonal blocks given by

$$(2.5) \quad \begin{aligned} M_c(\xi) &= \left( \int_{-a}^a \cos(it) \cos(jt) d\xi(t) \right)_{i,j=0}^m \\ &= \left( \int_\alpha^1 T_i(x)T_j(x) d\eta_\xi(x) \right)_{i,j=0}^m, \end{aligned}$$

$$(2.6) \quad \begin{aligned} M_s(\xi) &= \left( \int_{-a}^a \sin(it) \sin(jt) d\xi(t) \right)_{i,j=1}^m \\ &= \left( \int_\alpha^1 (1-x^2)U_i(x)U_j(x) d\eta_\xi(x) \right)_{i,j=0}^{m-1}, \end{aligned}$$

where  $T_i(x) = \cos(i \arccos x)$  and  $U_i(x) = \sin((i + 1) \arccos x)/\sin(\arccos x)$  denote the Chebyshev polynomials of the first and second kind, respectively [see, e.g., Rivlin (1974)]. Note that this transformation transfers the optimal design problem for the estimation of the individual coefficients in a trigonometric regression model to a design problem for the estimation of the coefficients in the weighted polynomial regression models

$$(2.7) \quad y = \sum_{j=0}^m \delta_j T_j(x) + \varepsilon, \quad x \in [\alpha, 1],$$

$$(2.8) \quad y = \sqrt{1-x^2} \sum_{j=0}^{m-1} \delta_j U_j(x) + \varepsilon, \quad x \in [\alpha, 1].$$

The following result will be used frequently in the proofs of a number of subsequent results. Its proof is straightforward and therefore omitted.

LEMMA 2.1. (i) A symmetric design  $\xi^*$  on the interval  $[-a, a]$  is optimal for estimating the coefficient  $\beta_{2l}$  ( $0 \leq l \leq m$ ) in the trigonometric regression (1.1) if and only if the design  $\eta_{\xi^*}$  obtained by the transformation (2.4) is optimal for estimating the parameter  $\delta_l$  in the Chebyshev regression model (2.7).

(ii) Similarly, a symmetric design  $\xi^*$  on the interval  $[-a, a]$  is optimal for estimating the coefficient  $\beta_{2l-1}$  ( $1 \leq l \leq m$ ) in the trigonometric regression

model (1.1) if and only if the design  $\eta_{\xi^*}$  obtained by the transformation (2.4) is optimal for estimating the coefficient  $\delta_{l-1}$  in the weighted Chebyshev regression model (2.8).

Lemma 2.1 relates our problem to a corresponding design problem in a polynomial model. Our main application of this result is the derivation of bounds on the number of support points of the optimal designs [for a proof, see Dette and Melas (2001)].

**THEOREM 2.2.** *If  $\xi_k^*$  denotes a symmetric optimal design for estimating the parameter  $\beta_k$  in the trigonometric regression model (1.1), then*

$$\begin{aligned} \max\{2l + 1, m - l + 1\} &\leq \#\text{supp}(\xi_{2l}^*) \leq 2m + 1, \\ \max\{2l, m - l + 1\} &\leq \#\text{supp}(\xi_{2l-1}^*) \leq 2m, \end{aligned}$$

whenever  $0 \leq l \leq m$ .

It turns out that the optimal designs for estimating the top individual coefficients in the trigonometric regression model (1.1) with design space  $[-\pi, \pi]$  can be found explicitly. As indicated in Section 1, these designs are of particular importance from a practical viewpoint. The following lemma is proved in the Appendix and will be frequently used in subsequent sections.

**LEMMA 2.3.** *Consider the trigonometric regression model (1.1) on the design space  $[-\pi, \pi]$ .*

(a) *For any  $l$  such that  $m/3 < l \leq m$  and any  $\delta \in [0, \frac{1}{2l}]$ , the design*

$$(2.9) \quad \xi_{2l}^* = \begin{pmatrix} -\pi & -\pi + \frac{\pi}{l} & \cdots & -\pi + \frac{2l-1}{l}\pi & \pi \\ \frac{1}{2l} - \delta & \frac{1}{2l} & \cdots & \frac{1}{2l} & \delta \end{pmatrix}$$

*is optimal for estimating the parameter  $\beta_{2l}$ . Moreover, in this case,  $\Phi_{2l}(\xi_{2l}^*) = 1$ .*

(b) *For any  $l$  such that  $m/3 < l \leq m$ , the design  $\xi_{2l}^*$  defined by (2.9) is optimal for the estimation of the intercept  $\beta_0$ .*

(c) *For any  $l$  such that  $m/3 < l \leq m$ , the design*

$$\xi_{2l-1}^* = \begin{pmatrix} -\pi + \frac{\pi}{2l} & -\pi + \frac{3\pi}{2l} & \cdots & -\pi + \frac{2l-3}{2l}\pi & \frac{-\pi}{2l} + \pi \\ \frac{1}{2l} & \frac{1}{2l} & \cdots & \frac{1}{2l} & \frac{1}{2l} \end{pmatrix}$$

*is optimal for estimating the coefficient  $\beta_{2l-1}$ . Moreover, in this case,  $\Phi_{2l-1}(\xi_{2l-1}^*) = 1$ .*

**3. Optimal designs for estimating individual coefficients of cosine terms on a partial circle.** In this section we investigate the  $e_{2l}$ -optimal design ( $0 \leq l \leq m$ ) for the trigonometric regression model (1.1) with design space  $[-a, a]$  in more detail. It will be demonstrated that there exists a point, say  $a_l^* \in (0, \pi]$ , such that for all  $a \leq a_l^*$  the optimal design for estimating the parameter  $\beta_{2l}$  can be found explicitly. Our second result gives the lower bound  $a_l^* \geq \pi/2$  ( $l = 0, \dots, m$ ) for  $a_l^*$ , and for lower order trigonometric regression we observe numerically  $a_l^* \geq 0.7\pi$ . Finally, it is indicated at the end of this section that an explicit solution of the  $e_{2l}$ -optimal design problem for any value of  $a$  satisfying  $a_l^* < a \leq \pi$  can only be found in particular cases.

In many cases,  $c$ -optimal designs for regression models are supported at the extremal points of an equi-oscillating function [see Kiefer and Wolfowitz (1959) and Studden (1968)]. For this reason, we consider the set of extremal points

$$(3.1) \quad t_i = t_i(a) = \arccos \left\{ \frac{1 - \alpha}{2} \cos \frac{i\pi}{m} + \frac{1 + \alpha}{2} \right\}, \quad i = 0, \dots, m,$$

$x_i = \cos t_i$  ( $i = 0, \dots, m$ ), of the  $m$ th Chebyshev polynomial  $T_m((2x - 1 - \alpha)/(1 - \alpha))$  of the first kind on the interval  $[\alpha, 1] = [\cos a, 1]$  (with  $\alpha = \cos a$ ) as a candidate for the support of the optimal design for estimating the individual coefficient in the Chebyshev regression model (2.4). The optimal weights corresponding to these points can be obtained by standard methods [see, e.g., Pukelsheim and Torsney (1991) and Dette and Melas (2001)],

$$(3.2) \quad w_0 = \frac{A_0}{\sum_{j=1}^m A_j}, \quad w_i = \frac{A_i}{2 \sum_{j=1}^m A_j}, \quad i = 1, \dots, m,$$

where

$$(3.3) \quad A_i = A_i(a) = (-1)^{m-l+i} \int_{-1}^1 l_i(x) T_l(x) \frac{dx}{\sqrt{1-x^2}}, \quad i = 0, \dots, m,$$

and

$$(3.4) \quad l_i(x) = \prod_{\substack{j=1 \\ i \neq j}}^n \frac{x - x_j}{x_i - x_j}$$

denotes the  $i$ th Lagrange interpolation polynomial with nodes  $x_i = \cos t_i$  ( $i = 0, \dots, m$ ). The following result shows that this design is indeed optimal for a sufficiently small design space.

**THEOREM 3.1.** *Consider the trigonometric regression model (1.1) on the interval  $[-a, a]$ . For any  $l \in \{0, \dots, m\}$ , the quantity*

$$(3.5) \quad a_l^* = a_{l,m}^* = \sup \{ z \in (0, \pi] \mid A_i(a) > 0 \text{ for all } i = 0, \dots, m \text{ and for all } a \in (0, z) \}$$

is always positive and the design

$$(3.6) \quad \xi_{2l,a}^* = \begin{pmatrix} -t_m & \cdots & -t_1 & t_0 & t_1 & \cdots & t_m \\ w_m & \cdots & w_1 & w_0 & w_1 & \cdots & w_m \end{pmatrix},$$

with support points (3.1) and weights (3.2), is optimal for estimating the parameter  $\beta_{2l}$ , whenever  $a \leq a_l^*$ .

The critical bound  $a_l^*$  can be determined numerically from (3.5) and (3.3) by standard numerical integration. Table 2 gives some values of the critical point  $a_l^*$  for various degrees of the trigonometric regression model. Note that Theorem 3.1 covers a relatively large range of the interval  $[0, \pi]$ . The following theorem shows that the critical bound in (3.5) is at least  $\pi/2$  independent of the degree of the trigonometric model and of the parameter that has to be estimated.

**THEOREM 3.2.** *Let  $x_l^*$  denote the smallest root of the polynomial*

$$(3.7) \quad \left(\frac{d}{dx}\right)^l \{(x+1)U_{m-1}(x)\}, \quad l = 1, \dots, m-1,$$

and  $x_m^* = 0$ . Then for any  $l \in \{1, \dots, m\}$  the critical value  $a_l^*$  defined in (3.5) satisfies

$$a_l^* \geq a_l^{**} = \arccos \frac{x_l^* + 1}{x_l^* - 1}.$$

In particular, we have  $a_l^* \geq a_l^{**} > \pi/2$  for all  $l \in \{1, \dots, m\}$  and for any fixed  $l$  we have

$$\lim_{m \rightarrow \infty} a_l^{**} = \frac{\pi}{2}.$$

**EXAMPLE 3.3.** Consider the case of estimating the coefficient of the highest cosine term, that is,  $l = m$  in Theorem 3.2. In this case, the polynomial defined in (3.7) is constant, which implies  $a_m^{**} = a_m^* = \pi$ , and the  $e_{2m}$ -optimal design is

TABLE 2  
Critical values  $a_l^*$  defined in (3.5) for various values of  $l$  and  $m$

	$m = 2$	$m = 3$	$m = 4$	$m = 5$
1	$2\pi/3$	$0.6881\pi$	$0.7411\pi$	$0.7666\pi$
$\cos(x)$	$0.6082\pi$	$0.7323\pi$	$0.7311\pi$	$0.7765\pi$
$\cos(2x)$	$\pi$	$2\pi/3$	$0.7576\pi$	$0.7598\pi$
$\cos(3x)$		$\pi$	$0.7048\pi$	$0.7709\pi$
$\cos(4x)$			$\pi$	$0.7323\pi$
$\cos(5x)$				$\pi$



given by (3.6) for any  $a \in (0, \pi]$ . Moreover, the weights of the  $e_{2m}$ -optimal design can be found explicitly by a careful inspection of the proof of Theorem 3.2, which shows that the corresponding design problem in the model (2.7) is the  $D_1$ -optimal design in an ordinary polynomial regression on the interval  $[\alpha, 1]$ . The  $D_1$ -optimal design for polynomial regression has been determined by many authors on the interval  $[-1, 1]$  [see, e.g., Studden (1980) and Spruill (1990)] and puts masses  $\frac{1}{2m}, \frac{1}{m}, \dots, \frac{1}{m}, \frac{1}{2m}$  at the points  $x_0, x_1, \dots, x_m$ , where  $x_i = \cos t_i$  ( $i = 0, \dots, m$ ) and the nodes  $t_i$  are defined by (3.1). Observing the transformation (2.4), it follows that for any  $a \in (0, \pi]$  an optimal design for estimating the coefficient  $\beta_{2m}$  is given by

$$\xi_{2m}^* = \begin{pmatrix} -t_m & -t_{m-1} & \dots & -t_1 & t_0 & t_1 & \dots & t_{m-1} & t_m \\ \frac{1}{4m} & \frac{1}{2m} & \dots & \frac{1}{2m} & \frac{1}{2m} & \frac{1}{2m} & \dots & \frac{1}{2m} & \frac{1}{4m} \end{pmatrix},$$

where the support points  $t_i$  are defined in (3.1).

EXAMPLE 3.4. In the second example of this section, we will present a complete solution of the design problem for the estimation of the cosine terms in a quadratic trigonometric regression. It is easy to see that for  $a \geq \frac{2}{3}\pi$  the uniform distribution at the points  $-\frac{2\pi}{3}, 0, \frac{2\pi}{3}$  is optimal for estimating the intercept in the trigonometric regression of degree 2 on the interval  $[-a, a]$ . If  $a \leq \frac{2}{3}\pi$ , the situation changes and the design

$$(3.8) \quad \xi_{0,a}^* = \begin{pmatrix} -a & t^* & 0 & t^* & a \\ w_2^* & w_1^* & w_0^* & w_1^* & w_2^* \end{pmatrix},$$

with

$$(3.9) \quad t^* = t^*(a) = \arccos(\cos(a)/2 + 1/2)$$

and

$$(3.10) \quad w_1^* = w_1^*(a) = \frac{1 + 2 \cos a}{5 + 6 \cos a + \cos^2 a}, \quad w_2^* = \frac{1 + (\cos a)/2}{5 + 6 \cos a + \cos^2 a},$$

is  $e_0$ -optimal on the interval  $[-a, a]$  (see Theorem 3.1). The optimal design for the estimation of the coefficient of  $\cos t$  on the interval  $[-a, a]$  is obtained as

$$(3.11) \quad \xi_{2,a}^* = \begin{pmatrix} -a & -\pi + a & \pi - a & a \\ \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} \end{pmatrix}$$

if  $\arccos(-1/3) \leq a \leq \pi$  (see Lemma 2.3 and note that  $\alpha^* = 0$  for  $m = 2$ ) and as

$$(3.12) \quad \xi_{2,a}^* = \begin{pmatrix} -a & -t^* & 0 & t^* & a \\ w_2^* & \frac{1}{4} & w_0^* & \frac{1}{4} & w_2^* \end{pmatrix}$$

in the case  $0 \leq a \leq \arccos(-1/3)$ , where  $t^*$  is defined by (3.9) and the weights  $w_0^*$  and  $w_2^*$  are given by

$$(3.13) \quad w_2^* = \frac{1 \cos a + 3}{16 \cos a + 1}, \quad w_0^* = \frac{1}{2} - 2w_2^*$$

(see Theorem 3.1). Finally, the design for estimating the coefficient of  $\cos(2t)$  on the interval  $[-a, a]$  is given by

$$(3.14) \quad \xi_{4,a}^* = \begin{pmatrix} -a & -t^* & 0 & t^* & a \\ \frac{1}{8} & \frac{1}{4} & \frac{1}{4} & \frac{1}{4} & \frac{1}{8} \end{pmatrix},$$

where the point  $t^*$  is defined by (3.9) (see Example 3.3).

**4. Optimal designs for estimating individual coefficients of the sine terms on a partial circle.** In this section, we concentrate on the optimal design problem for the estimation of the individual coefficients corresponding to the sine terms in the trigonometric regression model (1.1). In this case, the situation is substantially more difficult, because in most cases the design points cannot be found explicitly. The difficulties will be illustrated in the following example.

EXAMPLE 4.1. Consider the quadratic trigonometric regression model on the interval  $[-a, a]$ . We are interested in the optimal designs for estimating the coefficient of the terms  $\sin t$  and  $\sin(2t)$ . Define  $z^*$  as the unique positive solution of the equation

$$z^4 + 2z^3 \cos a + z^2 \sin a - 2z \cos a - 1 = 0$$

and

$$(4.1) \quad t^* = t^*(a) = \arccos z^*.$$

Note that the uniqueness of  $z^*$  follows easily from Descartes' rule of signs [see Karlin and Studden (1966), page 27, and Pólya and Szegő (1971), page 43]. If  $\frac{\pi}{2} \leq a \leq \pi$ , the optimal design  $\xi_{1,a}^*$  for estimating the coefficient of  $\sin t$  on the interval  $[-a, a]$  has equal masses at the points  $-\frac{\pi}{2}$  and  $\frac{\pi}{2}$  (see Corollary 4.2), while for  $0 < a \leq \frac{\pi}{2}$  the design

$$(4.2) \quad \xi_{1,a}^* = \begin{pmatrix} -a & -t^* & t^* & a \\ \frac{1}{2} - w_1^* & w_1^* & w_1^* & \frac{1}{2} - w_1^* \end{pmatrix},$$

with  $t^*$  defined by (4.1) and

$$(4.3) \quad w_1^* = w_1^*(a) = \frac{1 \cos(a)}{2 (\cos(a) - e)} \times \frac{(\cos(a) - 1)(\cos(a) + 1)(\cos(a)e - 2e^2 + 1)}{(\cos(a)e^3 + (3 - 2 \cos(a))^2 e^2 - 2 \cos(a)e + \cos(a)^3 e + \cos(a)^2 - 2)}$$

is  $e_1$ -optimal on the interval  $[-a, a]$  (see Example 4.3). Similarly, if  $\frac{3}{4}\pi \leq a \leq \pi$ , the design  $\xi_{3,a}^*$  with equal masses at the points  $-\frac{3\pi}{4}, \frac{\pi}{4}, \frac{\pi}{4}$  and  $\frac{3\pi}{4}$  is optimal for estimating the coefficient of  $\sin(2t)$  (see Corollary 4.2), while for  $0 < a \leq \frac{3}{4}\pi$  the  $e_3$ -optimal design is of the form (4.2) with  $t^*$  given by (4.1) and weight  $w_1^*$  defined by

$$(4.4) \quad \begin{aligned} w_1^* &= w_1^*(a) \\ &= \frac{1}{2} \frac{(\cos(a) - 1)(\cos(a) + 1)(e \cos(a) + 1 - 2e^2)}{(\cos(a) - e)(\cos(a) + e \cos(a)^2 - e^2 \cos(a) - e^3)} \end{aligned}$$

(see Theorem 4.4).

Example 4.1 indicates that the  $e_1$ - and  $e_3$ -optimal designs for the quadratic trigonometric model have the same support points whenever  $a \leq \frac{\pi}{2}$ . One of the main results of this section shows that this property is also true for general degree  $m \geq 2$ . In other words, if  $a$  is sufficiently small (which will be made precise later), the support points of the  $e_{2m-1}$ -optimal design in the trigonometric regression model (1.1) on the interval  $[-a, a]$  coincide with the support points of the  $e_{2l-1}$ -optimal design for any  $l \in \{1, \dots, m\}$ . Note that this property simplifies the optimal design problem for estimating the coefficients of the sine terms substantially. As soon as the  $e_{2m-1}$ -optimal design has been identified and the design space is sufficiently small, only the weights of the  $e_{2l-1}$ -optimal designs have to be determined, which can be done by standard techniques [see Pukelsheim and Torsney (1991)].

For this reason, we will start our investigations of the sine case with a careful discussion of the optimal design problem for the estimation of the parameter  $\beta_{2m-1}$  in the trigonometric regression model (1.1). In this case, we determine the optimal design numerically using a technique, which was introduced by Melas (1978) in the context of optimal design. Our next result considers the case  $a > \pi(1 - 1/2m)$  and is an immediate consequence of Lemma 2.3.

**COROLLARY 4.2.** *Let  $m/3 < l \leq m$  and  $\pi(1 - 1/2l) \leq a \leq \pi$ . Then the optimal design for estimating the coefficient  $\beta_{2l-1}$  in the trigonometric regression model (1.1) on the interval  $[-a, a]$  is given by the design  $\xi_{2l-1}^*$  defined in part (c) of Lemma 2.3.*

Let us now consider the case  $0 < a \leq \pi(1 - 1/2m)$ . It can be shown [see Dette and Melas (2001)] that the optimal design for estimating the coefficient  $\beta_{2m-1}$  in the trigonometric regression model is of the form

$$(4.5) \quad \xi_{2m-1,a}^* = \begin{pmatrix} -a & at_2^*(a) & \cdots & at_m^*(a) & -at_m^*(a) & \cdots & -at_2^*(a) & a \\ \frac{1}{2}w_1^*(a) & \frac{1}{2}w_2^*(a) & \cdots & \frac{1}{2}w_m^*(a) & \frac{1}{2}w_m^*(a) & \cdots & \frac{1}{2}w_2^*(a) & \frac{1}{2}w_1^*(a) \end{pmatrix},$$

where the weights are given by

$$(4.6) \quad w_i^* = w_i^*(a) = \frac{(-1)^{m-i} \{\sqrt{1-x_i^2} \prod_{j \neq i} (x_i - x_j)\}^{-1}}{\sum_{k=1}^m (-1)^{m-k} \{\sqrt{1-x_k^2} \prod_{j \neq k} (x_k - x_j)\}^{-1}},$$

with  $x_1 = \cos a$ ,  $x_i = \cos(at_i^*(a))$ . Moreover, the support points and weights of the optimal design for the coefficient  $\xi_{2m-1,a}^*$  are real analytic functions of the parameter  $a$ . This result can be used for the determination of these quantities by elementary Taylor expansions. The calculation of the coefficients in this expansion is complicated and can be found in the technical report of Dette and Melas (2001). The algorithm in this reference allows the determination of the support points and weights of the  $e_{2m-1}$ -optimal design with arbitrary precision. We will illustrate the application of this method in the following example.

EXAMPLE 4.3. In the case  $m = 3$ , the support points of the optimal design for the coefficient of  $\sin(3x)$  in the cubic trigonometric regression model (1.1) on the interval  $[-a, a]$  for  $0 < a < 5\pi/6$  are given by  $-a$ ,  $at_2^*(a)$ ,  $at_3^*(a)$ ,  $-at_3^*(a)$ ,  $-at_2^*(a)$ ,  $a$  and the weights are obtained from (4.6). It is easy to see that  $t_i^*(a)$  defines an even function and Table 3 shows the first six nonvanishing coefficients of the expansion

$$(4.7) \quad t_i^*(a) = \sum_{j=0}^{\infty} \frac{t_{i,2j}^*}{(2j)!} \left(\frac{a}{\pi}\right)^{2j}.$$

The optimal designs are depicted in Figure 1 for  $a \in (0, 5\pi/6)$ .

Observing the results of Section 3, it is natural to investigate if the  $e_{2l-1}$ -optimal design has the same support points as the  $e_{2m-1}$ -optimal design. By Lemma 2.1, this is equivalent to investigating if the  $e_{m-1}$ - and  $e_{l-1}$ -optimal designs for the weighted Chebyshev regression model (2.8) have the same support

TABLE 3  
Coefficients in the Taylor expansion (4.7) for the interior negative support points  $t_2^*(a)$ ,  $t_3^*(a)$  of the  $e_5$ -optimal designs in the cubic trigonometric regression model (1.1) on the interval  $[-a, a]$ . The  $e_1$ - and  $e_3$ -optimal designs have the same support points if  $a \leq b_l^*$ ,  $l = 1, 2$ , where  $b_l^*$  is defined in (4.10)

$j$	0	2	4	6	8	10
$t_{3,2j}^*$	-0.8090	0.1839	0.1490	0.0683	-0.0254	-0.0825
$t_{2,2j}^*$	-0.3090	0.1839	-0.0412	-0.0099	0.0148	-0.0049

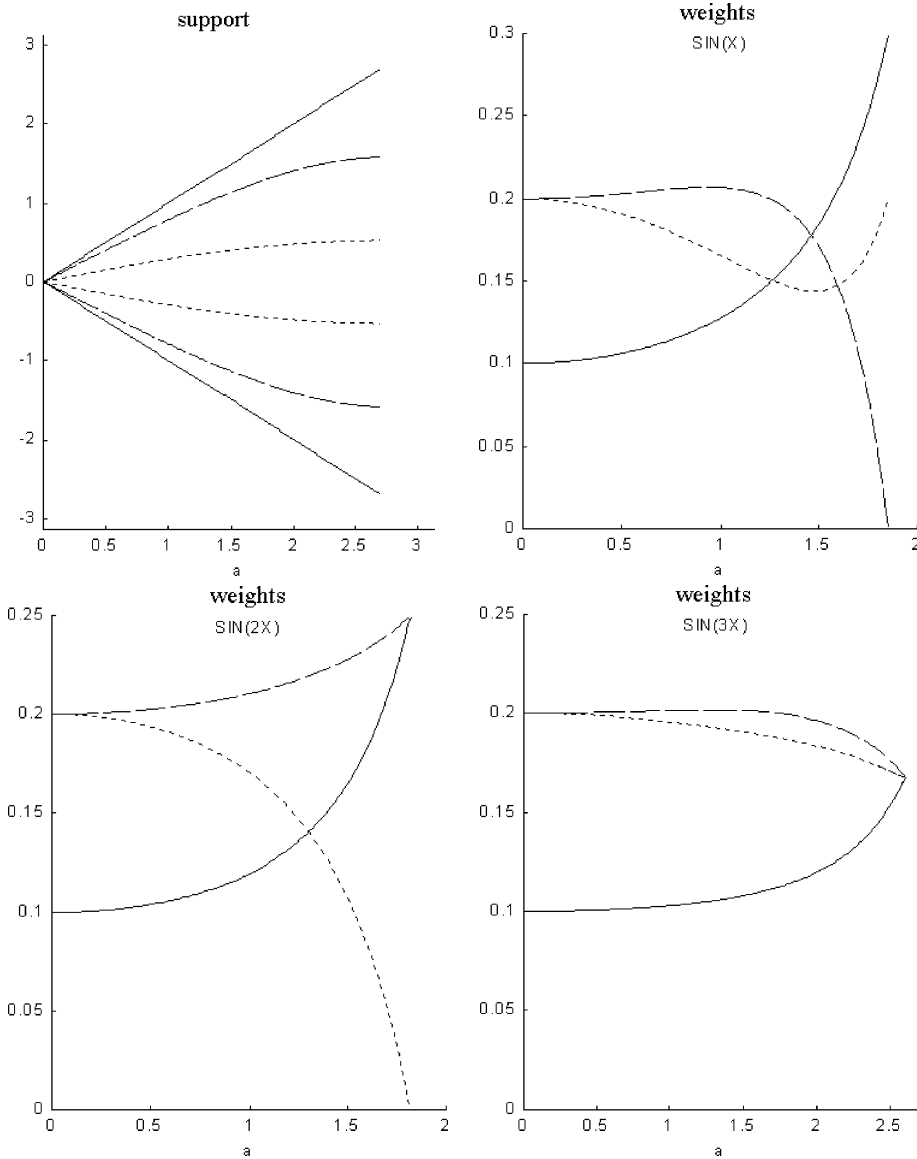


FIG. 1. Support points and weights of the  $e_1$ -,  $e_3$ - and  $e_5$ -optimal design in the cubic trigonometric regression model ( $m = 3$ ). The support points are calculated by the Taylor expansion (4.7) (upper left figure), while the weights are obtained from the support points using formula (4.6).

points. Let  $-a = at_1^*(a) < at_2^*(a) < \dots < at_m^*(a) < 0$  denote the negative support points of the  $e_{2m-1}$ -optimal design and define  $x_i = \cos(at_i^*(a))$  ( $i = 1, \dots, m$ ). The optimal weights [for the  $e_{l-1}$ -optimality criterion in the model (2.8)] at these

points are then given by

$$(4.8) \quad w_i^* = w_i^*(a) = \frac{|B_i|}{\sum_{j=1}^m |B_j|}, \quad i = 1, \dots, m,$$

where

$$(4.9) \quad B_i = B_i(a) = \int_{-1}^1 \prod_{j \neq i} \frac{x - x_j}{x_i - x_j} \sqrt{\frac{1 - x^2}{1 - x_i^2}} U_{l-1}(x) dx, \quad i = 1, \dots, m,$$

[see Pukelsheim and Torsney (1991) and Dette and Melas (2001)]. The proof of the following theorem can be found in Dette and Melas (2001).

**THEOREM 4.4.** *If  $1 \leq l \leq m - 1$ , then the quantity*

$$(4.10) \quad \begin{aligned} b_l^* &:= b_{l,m}^* \\ &:= \sup \left\{ z \in \left( 0, \pi \left( 1 - \frac{1}{2l} \right) \right) \mid w_i^*(a) > 0 \right. \\ &\quad \left. \text{for all } i = 1, \dots, m \text{ and all } a \in (0, z) \right\} \end{aligned}$$

*is always positive. If  $a < b_l^*$ , then the  $e_{2l-1}$ - and  $e_{2m-1}$ -optimal designs have the same supports while the weights of the  $e_{2l-1}$ -optimal design at the support points  $\pm at_i^*(a)$  are given by  $w_i^*(a)/2$ ,  $i = 1, \dots, m$ , where  $t_1^*(a) = -1$  and the weights  $w_i^*(a)$  are defined in (4.8).*

For trigonometric regression of lower order, the critical bounds are listed in Table 4. If  $a$  is smaller than the corresponding bound, the  $e_{2l-1}$ -optimal design in the trigonometric regression model (1.1) has the same support points as the optimal design for estimating the coefficient of  $\sin(mx)$ , which can be obtained numerically. Moreover, for any  $l \in \{1, \dots, m - 1\}$ , it can be shown that  $b_l^* \geq \pi/2$

TABLE 4  
 Critical values  $b_l^*$  defined in (4.10) for various values of  $l$  and  $m$ .  
 The optimal design for estimating the coefficient  $\beta_{2l-1}$   
 in the trigonometric regression model (1.1) on the interval  $[-a, a]$   
 has the same support points as the  $e_{2m-1}$ -optimal design, whenever  $a \leq b_l^*$

	$m = 2$	$m = 3$	$m = 4$	$m = 5$
$\sin(x)$	$\pi/2$	$0.59\pi$	$0.66\pi$	$0.66\pi$
$\sin(2x)$	.	$0.53\pi$	$0.65\pi$	$0.69\pi$
$\sin(3x)$	.	.	$0.63\pi$	$0.71\pi$
$\sin(4x)$	.	.	.	$0.67\pi$

[see Dette and Melas (2001)]. The corresponding weights are found by numerical integration using formula (4.8).

We have illustrated these calculations in the cubic trigonometric regression model in Figure 1, which shows the support points and corresponding weights of the optimal designs for estimating the coefficient of  $\sin x$ ,  $\sin(2x)$  and  $\sin(3x)$ , respectively. For example, in the cubic trigonometric regression model on the interval  $[-1, 1]$ , all optimal designs for estimating the coefficients of the sine terms have the same support points, namely,  $-1, -0.655, -0.251, 0.251, 0.655, 1$ . The masses of the  $e_1$ -optimal designs are given by  $0.125, 0.209, 0.166, 0.166, 0.209, 0.125$ , while the  $e_3$ - and  $e_5$ -optimal designs have masses  $0.119, 0.210, 0.171, 0.171, 0.210, 0.119$  and  $0.103, 0.201, 0.196, 0.196, 0.201, 0.103$  at these points, respectively.

Note the clear sensitivity of the weights of the optimal designs for estimating the coefficients of  $\sin x$  and  $\sin(3x)$  with respect to the length of the design space. If  $a$  approaches the critical value  $b_l^*$  ( $l = 1, 2$ ), the weight at one support point tends to 0 and the  $e_{2l-1}$ -optimal design in the trigonometric regression on the interval  $[-b_l^*, b_l^*]$  is a four-point design. Moreover, there exists an interval  $I_l = [b_l^*, b_l^* + \varepsilon)$  such that for any  $a \in I_l$  the  $e_{2l-1}$ -optimal design for the cubic trigonometric regression model is only supported at four points ( $l = 1, 2$ ).

**5. Summary.** In this paper, the problem of designing experiments for estimating individual coefficients in Fourier regression models on the interval  $[-a, a]$  is studied. On a complete design space  $[-a, a] = [-\pi, \pi]$ , the optimal designs for estimating the top coefficients can be determined explicitly (see Lemma 2.3) and these designs have a similar structure as the classical  $D$ -optimal design for the trigonometric regression model (but they are not identical). On an incomplete interval ( $0 < a < \pi$ ), the optimal design problem is substantially more difficult. If the design space is sufficiently small, then the optimal designs for estimating the coefficients corresponding to the cosine terms can be found explicitly. In particular, all designs are supported at the same points, which are the extremal points of a scaled Chebyshev polynomial (see Theorem 3.1). A sufficient condition for this property is  $a \leq \frac{\pi}{2}$  (see Theorem 3.2), but for lower order trigonometric regression the range is substantially larger. Similarly, the optimal designs for estimating the coefficients corresponding to the sine terms are all supported at the same set of points provided that the design space  $[-a, a]$  is sufficiently small (see Theorem 4.4), and the condition  $a \leq \frac{\pi}{2}$  is sufficient for this property. The common support points vary analytically with the parameter  $a$  but cannot be determined explicitly. For this reason, a numerical construction based on a Taylor expansion is applied, which allows us to determine the support points of the optimal designs for estimating the individual coefficients corresponding to the sine terms with arbitrary precision. The results of this paper are based on certain relations between the trigonometric and the polynomial regression models. In many important cases,

the optimal designs for estimating individual coefficients in the Fourier regression model can be determined, either explicitly or numerically. However, there are still some remaining open cases, for which the optimal design problem cannot be solved by the methods proposed in this paper and which require further research in the future.

## APPENDIX: PROOFS AND TECHNICAL DETAILS

**A.1. Preliminaries.** We begin with a couple of technical lemmas, which are required for the proofs of the main results in the previous sections. Our first result is an important tool for the determination of optimal designs and gives a slightly different formulation of the equivalence theorem for  $e_k$ -optimal designs than is usually stated in the literature [see, e.g., Pukelsheim (1993), Section 2, and Studden (1968)]. The result is stated here for general regression models and a proof can be found in Dette, Melas and Pepelyshev (2000).

**LEMMA A.1.** For  $k = 0, 1, \dots, d$ , let  $\bar{f}_k(t) = (f_0(t), \dots, f_{k-1}(t), f_{k+1}(t), \dots, f_d(t))^T$  denote the vector obtained by omitting the component  $f_k(t)$  in the vector  $f(t) = (f_0(t), \dots, f_d(t))^T$ . A design  $\xi^*$  is optimal for estimating the parameter  $\beta_k$  in the model

$$y = \sum_{j=0}^d \beta_j f_j(t) + \varepsilon, \quad t \in \tau \subset \mathbb{R},$$

if and only if there exist a positive number  $h$  and a vector  $q \in \mathbb{R}^d$  such that the function  $\varphi(t) = f_k(t) - q^T \bar{f}_k(t)$  satisfies:

- (i)  $h\varphi^2(t) \leq 1$  for all  $t \in \tau$ ;
- (ii)  $\text{supp}(\xi^*) \subset \{t \in \tau \mid h\varphi^2(t) = 1\}$ ;
- (iii)  $\int_{\tau} \varphi(t) \bar{f}_k(t) d\xi^*(t) = 0 \in \mathbb{R}^d$ .

Moreover, in this case  $h = \Phi_k(\xi^*)$ ; the function  $\varphi$  is called an extremal polynomial.

Note that there is an alternative formulation of Lemma 2.1 (see Section 2) in terms of  $c$ -optimality in the ordinary polynomial regression model. A  $c$ -optimal design minimizes the variance of the least squares estimator for the linear combination  $\sum_{j=0}^d \delta_j c_j$ , where  $c = (c_0, \dots, c_d)^T \in \mathbb{R}^{d+1}$  is a given vector and  $d \in \{m-1, m\}$  corresponding to the cases (2.8) and (2.7), respectively [see Pukelsheim (1993)]. To be precise, let  $T \in \mathbb{R}^{m+1 \times m+1}$  and  $U \in \mathbb{R}^{m \times m}$  denote the matrix of the coefficients of the Chebyshev polynomials of the first and second



kind, that is,

$$(A.1) \quad \begin{aligned} (T_0(x), \dots, T_m(x))^T &= T \cdot (1, x, \dots, x^m)^T, \\ (U_0(x), \dots, U_{m-1}(x))^T &= U \cdot (1, x, \dots, x^{m-1})^T. \end{aligned}$$

Defining  $t(l) = T^{-1}e_l$  ( $l = 0, \dots, m$ ) and  $u(l) = U^{-1}e_l$  ( $l = 0, \dots, m - 1$ ), we obtain by straightforward algebra the following auxiliary result.

LEMMA A.2. *A symmetric design  $\xi^*$  on the interval  $[-a, a]$  is optimal for estimating the individual coefficient  $\beta_{2l}$  ( $0 \leq l \leq m$ ) in the trigonometric regression (1.1) if and only if the design  $\eta_{\xi^*}$  obtained by the transformation (2.4) is  $t(l)$ -optimal in the ordinary polynomial regression model of degree  $m$  on the interval  $[\alpha, 1]$ .*

*Similarly, a symmetric design  $\xi^*$  on the interval  $[-a, a]$  is optimal for estimating the coefficient  $\beta_{2l-1}$  ( $1 \leq l \leq m$ ) in the trigonometric regression model (1.1) if and only if the design  $\eta_{\xi^*}$  obtained by the transformation (2.4) is  $u(l - 1)$ -optimal in the ordinary weighted polynomial regression model of degree  $m - 1$  with efficiency function  $\lambda(x) = 1 - x^2$  on the interval  $[\alpha, 1]$ .*

**A.2. Proof of Lemma 2.3.** We will only consider the first case (a), the remaining parts being treated similarly. The proof follows essentially by an application of Lemma A.1 and the discrete orthogonality properties of the Chebyshev polynomials of the first kind. To be precise, let  $t_i = -\pi + \frac{i}{2l}\pi$  ( $i = 0, \dots, 2l$ ) and consider the trigonometric polynomial  $\varphi(t) = \cos(lt)$ , which obviously satisfies conditions (i) and (ii) of Lemma A.1 with  $h = 1$ . To prove the remaining condition (iii), we have to establish the identities

$$(A.2) \quad s_{2j} = \int_{-\pi}^{\pi} \varphi(t) f_{2j}(t) d\xi_{2l}^*(t) = \frac{1}{2l} \sum_{i=0}^{2l-1} \cos(jt_i) \cos(lt_i) = 0$$

for all  $j = 0, 1, \dots, l - 1, l + 1, \dots, m$ , and

$$(A.3) \quad s_{2j-1} = \int_{-\pi}^{\pi} \varphi(t) f_{2j-1}(t) d\xi_{2l}^*(t) = \frac{1}{2l} \sum_{i=0}^{2l-1} \sin(jt_i) \cos(lt_i) = 0$$

for all  $j = 1, \dots, m$ . Note that the relation (A.3) is obvious by the symmetry of the design  $\xi_{2l}^*$ . For the quantities  $s_{2j}$ , we obtain, with the notation  $x_i = \cos(t_i) = \cos(-t_i) = \cos(t_{2l-i})$ ,  $i = 0, \dots, l$ ,

$$s_{2j} = \frac{1}{2l} \{T_j(x_0)T_l(x_0) + T_j(x_l)T_l(x_l)\} + \frac{1}{l} \sum_{i=1}^{l-1} T_j(x_i)T_l(x_i).$$

Note that  $x_0, \dots, x_l$  are the extremal points of the Chebyshev polynomial of the first kind and that the orthogonality properties of these polynomials with respect

to discrete measures [see Rivlin (1974), Exercise 1.5.28] show that  $s_{2j} = 0$  if and only if for all  $j \in \{0, \dots, l-1\} \cup \{l+1, \dots, m\}$  the quantities  $l+j$  and  $|l-j|$  are not multiples of  $2l$ . A simple calculation shows that this is obviously satisfied if  $l > m/3$ , which completes the proof of the first assertion of Lemma 2.3.

**A.3. Proof of Theorem 3.1.** First, we will prove that if the parameter  $a$  approaches 0 the quantities  $A_i$  defined in (3.3) are all positive. To this end, let  $s_i = \cos(i\pi/m)$  denote the extremal points of the Chebyshev polynomial of the first kind  $T_m(x)$ . Then we have

$$\begin{aligned}
 2^{m-1} \prod_{j=0, j \neq i}^m (s_i - s_j) &= \frac{d}{dx}(x^2 - 1)U_{m-1}(x) \Big|_{x=s_i} \\
 &= \frac{d}{dx}(T_{m+1}(x) - xT_m(x)) \Big|_{x=s_i} \\
 &= (m+1)U_m(s_i) - ms_i U_{m-1}(s_i) - T_m(s_i) \\
 &= \frac{(-1)^i}{\gamma_i},
 \end{aligned}
 \tag{A.4}$$

where  $\gamma_0 = \gamma_m = 1/(2m)$  and  $\gamma_i = 1/m$  if  $1 \leq i \leq m-1$ . For the derivation of this identity, we use the well-known facts [see Szegő (1959)]  $T'_k(x) = kU_{k-1}(x)$ ,  $U_m(s_i) = (-1)^i$  if  $1 \leq i \leq m-1$  and  $U_k(1) = (-1)^k U_k(-1) = k+1$ . This implies, for the weights in (3.3),

$$\begin{aligned}
 A_i &= (-1)^{m-l+i} \int_{-1}^1 \prod_{j=0, j \neq i}^m \frac{x - x_j}{x_i - x_j} T_l(x) \frac{dx}{\sqrt{1-x^2}} \\
 &= \frac{2^{m-1}(-1)^{m-l}}{(1-\alpha)^m} \gamma_i \int_{-1}^1 \prod_{j=0, j \neq i}^m (2x - 1 - \alpha - \{1-\alpha\}s_j) T_l(x) \frac{dx}{\sqrt{1-x^2}}.
 \end{aligned}
 \tag{A.5}$$

This means, for  $a \rightarrow 0$  (which implies  $\alpha = \cos a \rightarrow 1$ ),

$$\begin{aligned}
 \lim_{a \rightarrow 0} (1-\alpha)^m A_i &= 2^{2m-1} (-1)^{m-l} \gamma_i \int_{-1}^1 (x-1)^m T_l(x) \frac{dx}{\sqrt{1-x^2}} \\
 &= \gamma_i 2^{2m-1} \int_{-1}^1 (1+x)^m T_l(x) \frac{dx}{\sqrt{1-x^2}} \\
 &= \gamma_i 2^{3m-1} \frac{\Gamma(\frac{1}{2})\Gamma(m+\frac{1}{2})}{\Gamma(m+1)} \frac{P_l^{(m, -m-1)}(-1)}{P_l^{(m, -m-1)}(1)} \\
 &= \gamma_i 2^{3m-1} \frac{\Gamma(\frac{1}{2})\Gamma(m+\frac{1}{2})}{\Gamma(m+1-l)} \frac{\Gamma(m+1)}{\Gamma(m+1+l)},
 \end{aligned}
 \tag{A.6}$$

where  $P_n^{(\alpha,\beta)}(x)$  denotes the  $n$ th Jacobi polynomial [see, e.g., Szegö (1959)]. The second equality follows by the substitution  $x \rightarrow -x$  and  $T_l(-x) = (-1)^l T_l(x)$ ; the third equality is obtained from the identity (4.10.11) in Szegö (1959), which reduces in the present context to the equation  $(\alpha = \beta = -\frac{1}{2}, \mu = m + \frac{1}{2}, x = -1)$

$$2^m \frac{P_l^{(m,-m-1)}(-1)}{P_l^{(m,-m-1)}(1)} = \frac{\Gamma(m+1)}{\Gamma(\frac{1}{2})\Gamma(m+\frac{1}{2})} \int_{-1}^1 \frac{(1+y)^{m+1/2}}{(1-y)^{1/2}} \frac{P_l^{(-1/2,-1/2)}(y)}{P_l^{(-1/2,-1/2)}(y)} dy$$

[note that  $T_l(y) = 2^l(l!)^2/(2l)!P_l^{(-1/2,-1/2)}(y)$ ]. The final equality is a consequence of the relations  $P_l^{(\alpha,\beta)}(1) = \Gamma(l+\alpha+1)/\{\Gamma(\alpha+1)\Gamma(l+1)\}$  and  $P_l^{(\alpha,\beta)}(-x) = P_l^{(\beta,\alpha)}(x)(-1)^l$  [see formulas (4.1.1) and (4.1.3) in the same reference]. Consequently, if  $a \rightarrow 0$  all quantities  $A_i$  defined in (3.3) are positive and by continuity the supremum  $a_l^*$  defined by (3.5) is also positive.

For the proof of the second assertion of Theorem 3.1, recall that by Lemma 2.1 the  $e_{2l}$ -optimality of the design  $\xi_{2l,a}^*$  defined by (3.6) in the trigonometric regression model (1.1) is equivalent to the  $e_l$ -optimality of the design

$$\eta_{\xi_{2l,a}^*} = \begin{pmatrix} x_0 & x_1 & \cdots & x_m \\ w_0 & 2w_1 & \cdots & 2w_m \end{pmatrix}$$

in the Chebyshev regression model (2.7) on the interval  $[\cos a, 1]$ . We will now use Lemma A.1 to establish this optimality. To this end, assume that  $a_l^* > a$  and define

$$(A.7) \quad \varphi(x) = T_m\left(\frac{2x-1-\alpha}{1-\alpha}\right)\varphi_l = \sum_{j=0}^m b_j T_j(x),$$

where the coefficient  $\varphi_l$  is defined by the condition that the coefficient  $b_l$  of  $T_l(x)$  in the above expansion of  $\varphi$  equals 1 and  $\alpha = \cos a$ . This polynomial obviously satisfies conditions (i) and (ii) of Lemma A.1 with  $h = 1/\varphi_l$ . It can be shown by a straightforward calculation [see Dette and Melas (2001)] that condition (iii) of this lemma is equivalent to the existence of a solution of the equation

$$(A.8) \quad FDw = 0,$$

with positive coefficients, where  $D = \text{diag}(1, -1, \dots, (-1)^m)$  and the matrix  $F$  is defined by

$$(A.9) \quad F = \begin{bmatrix} T_0(x_0) & \cdots & T_0(x_m) \\ \vdots & \vdots & \vdots \\ T_{l-1}(x_0) & \cdots & T_{l-1}(x_m) \\ T_{l+1}(x_0) & \cdots & T_{l+1}(x_m) \\ \vdots & \vdots & \vdots \\ T_m(x_0) & \cdots & T_m(x_m) \end{bmatrix} \in \mathbb{R}^{m \times m+1}.$$

However, it is easy to see that the vector  $(A_0, -A_1, \dots, (-1)^m A_m)$  is always a solution of  $F\mu = 0$ . Because  $A_i > 0$  ( $i = 0, \dots, m$ ) whenever  $a < a_l^*$ , it follows that the vector  $\tilde{w} = (\tilde{w}_0, \dots, \tilde{w}_m)^T$ , with

$$\tilde{w}_i = \frac{A_i}{\sum_{j=0}^m A_j}, \quad i = 0, \dots, m,$$

is a solution of (A.8) with positive coefficients. Consequently, by Lemma A.1 the design with masses  $\tilde{w}_0, \tilde{w}_1, \dots, \tilde{w}_m$  at the points  $x_0, x_1, \dots, x_m$  is optimal for estimating the parameter  $\delta_l$  in the Chebyshev regression model (2.7). The assertion now follows from the above discussion, which shows that the design  $\xi_{2l,a}^*$  defined in (3.6) is optimal for estimating the coefficient  $\beta_{2l}$  in the trigonometric regression (1.1) on the interval  $[-a, a]$  whenever  $a < a_l^*$ . The remaining assertion for  $a = a_l^*$  follows by continuity.

**A.4. Proof of Theorem 3.2.** Note that by Lemma A.2 a design  $\xi_{2l}^*$  is  $e_{2l}$ -optimal in the trigonometric regression if and only if the measure  $\eta_{\xi_{2l}^*}$  induced by the transformation (2.4) is  $t(l)$ -optimal in the ordinary polynomial regression on the interval  $[\alpha, 1]$ , where  $t(l) = T^{-1}e_l$  and  $T$  denotes the matrix of coefficients of the Chebyshev polynomial of the first kind defined by (A.2). Let  $t_{i,j}$  denote the entries of the matrix  $T^{-1}$ . Then it follows by Cramer’s rule that  $t_{i,j} = 0$  whenever  $i + j$  is odd and  $t_{i,j} = 0$  whenever  $i < j$ . Moreover, the nonvanishing coefficients in the Chebyshev expansions of the monomials  $x^k = \sum_{j=0}^k \eta_{k,j} T_j(x)$  ( $k = 0, \dots, m$ ) are all positive [see, e.g., Rivlin (1974), Exercise 1.5.32], and, as a consequence, the vector  $t(l) = T^{-1}e_l$  can be written as

$$(A.10) \quad t(l) = \sum_{j=0}^{\lfloor (m-l)/2 \rfloor} \alpha_{l,j} e_{l+2j},$$

with positive coefficient  $\alpha_{l,j}$  ( $j = 0, \dots, \lfloor (m-l)/2 \rfloor; l = 0, \dots, m$ ). We will now investigate the  $e_{l+2j}$ -optimal designs in ordinary polynomial regression using recent results of Sahn (2000). Note that the design space, which has to be considered, is the interval  $[\alpha, 1]$ , where  $\alpha \rightarrow 1$  as  $a \rightarrow 0$ . Sahn (2000) showed that the structure of the optimal design for estimating the  $i$ th coefficient in an ordinary polynomial regression on the interval  $[\alpha, 1]$  is determined by the symmetry parameter  $s(\alpha) = (\alpha + 1)/(\alpha - 1)$ . In particular, he proved that the  $e_i$ -optimal design for the ordinary polynomial regression is supported at the transformed Chebyshev points

$$(A.11) \quad x_j = \cos(t_j) = \frac{1 - \alpha}{2} \cos\left(\frac{j\pi}{m}\right) + \frac{1 + \alpha}{2}, \quad j = 0, \dots, m,$$

whenever  $s(\alpha) = (\alpha + 1)/(\alpha - 1) < x_i^*$ , where  $x_i^*$  is the smallest 0 of the polynomial

$$k_i(x) = \left(\frac{d}{dx}\right)^i \{(x + 1)U_{m-1}(x)\},$$

if  $0 \leq i \leq m - 1$  and  $x_m^* = 0$ . Now it is easy to see that the roots of the polynomials  $k_i(x)$  and  $k_{i+1}(x)$  are interlacing, and, consequently, we have for the smallest roots of these polynomials  $x_i^* < x_j^*$  whenever  $i < j$ . This implies that, whenever

$$a < a_l^{**} = \arccos \frac{x_l^* + 1}{x_l^* - 1},$$

we have

$$a < \arccos \frac{x_i^* + 1}{x_i^* - 1}, \quad i = l, l + 1, \dots, m.$$

Consequently, it follows from Sahm (2000) that in this case for all  $i = l, l + 1, \dots, m$  the  $e_i$ -optimal designs in the ordinary polynomial regression on the interval  $[\alpha, 1]$  are supported at the points in (A.11). We will now prove that the  $t(l)$ -optimal design in the ordinary polynomial regression [which is the  $e_l$ -optimal design for the Chebyshev regression (2.7)] is also supported at the full set of Chebyshev points defined in (A.11) whenever  $a < a_l^{**}$ . If this assertion has been proved, we obtain by a standard calculation [see Dette and Melas (2001)] that the weights of the design  $\eta_{\xi_{2l}^*}$  are given by

$$(A.12) \quad w_i = \frac{|u_i|}{\sum_{j=1}^n |u_j|}, \quad i = 1, \dots, n,$$

where the quantities  $u_i$  are given by

$$(A.13) \quad u_i = \int_{-1}^1 l_i(x) T_l(x) \frac{dx}{\sqrt{1-x^2}}, \quad i = 1, \dots, n,$$

and  $l_i(x)$  denotes the  $i$ th Lagrange interpolation polynomial with nodes  $x_1, \dots, x_n$  defined in (3.4). This implies that the quantities  $A_i = (-1)^{m-l+i} u_i$  defined in (3.3) are positive for all  $a \in (0, a_l^{**})$ . This follows because by the first part of this proof the quantities  $A_i$  are positive if  $a \rightarrow 0$  and they have to be of the same sign, and because we will prove below that for all  $a \in (0, a_l^{**})$  the design  $\eta_{\xi_{2l}^*}$  is supported at the full set of Chebyshev points.

To this end, recall that for  $0 < a < a_l^{**}$  the  $e_{l+2j}$ -optimal design ( $j = 0, \dots, \lfloor (m-l)/2 \rfloor$ ) is supported at the Chebyshev points defined in (A.11) with extremal polynomial given by (A.7). Lemma A.1 for the vector  $f(x) = (1, x, \dots, x^m)^T$  shows that the corresponding vector of optimal weights  $w^j = (w_0^j, \dots, w_m^j)^T$  satisfies

$$G_j D w^j = 0, \quad j = 0, \dots, \left\lfloor \frac{m-l}{2} \right\rfloor,$$

where the matrix  $D$  is given by  $D = (-1)^{m-l} \cdot \text{diag}(1, -1, \dots, (-1)^m)$  and the matrices  $G_j$  are obtained from the matrix  $\tilde{G} = (x_j^i)_{i,j=0,\dots,m}$  by deleting

the  $(l + 2j + 1)$ st row. Condition (ii) of the same lemma implies, for some  $h_j > 0$ ,

$$\bar{G}Dw^j = \frac{1}{h_j}e_{l+2j}, \quad j = 0, \dots, \left\lfloor \frac{m-l}{2} \right\rfloor,$$

which yields that for all  $j \in \{0, \dots, \lfloor (m - j)/2 \rfloor\}$  the  $(k + 1)$ st component of the vector  $\bar{G}^{-1}e_{l+2j}$  is nonzero and has sign  $(-1)^{k+l+m}$  (by the pattern of the diagonal elements of the matrix  $D$ ). Introducing the notation [see Studden (1968)]

$$D_v(c) = \begin{pmatrix} 1 & \cdots & 1 & 1 & \cdots & 1 & c_0 \\ x_0 & \cdots & x_{v-1} & x_{v+1} & \cdots & x_m & c_1 \\ \vdots & & \vdots & \vdots & & \vdots & \vdots \\ x_0^m & \cdots & x_{v-1}^m & x_{v+1}^m & \cdots & x_m^m & c_m \end{pmatrix}, \quad v = 0, \dots, m,$$

for a vector  $c = (c_0, \dots, c_m) \in \mathbb{R}^{m+1}$ , we obtain for this component the representation

$$(A.14) \quad 0 \neq e_k^T \bar{G}^{-1}e_{l+2j} = (-1)^{m-k} \frac{D_k(e_{l+2j})}{\det \bar{G}},$$

$$j = 0, \dots, \left\lfloor \frac{m-l}{2} \right\rfloor, k = 0, \dots, m,$$

and, consequently,  $D_k(e_{l+2j})$  has sign  $(-1)^l$  for all  $j = 0, \dots, \lfloor (m - l)/2 \rfloor$ . Therefore, it follows from the representation (A.10) that

$$(A.15) \quad D_k(t(l)) = \sum_{j=0}^{\lfloor (m-l)/2 \rfloor} \alpha_{l,j} D_k(e_{l+2j}) \neq 0$$

for all  $k = 0, \dots, m$ , and the results of Studden (1968) show that the  $t(l)$ -optimal design in the ordinary polynomial regression is supported on the full set of Chebyshev points defined by (A.11) whenever  $0 < a < a_l^{**}$ .

By the argument in the paragraph following formula (A.13), the quantities  $A_i$  defined in (3.3) are all positive for  $a \in (0, a_l^{**})$ , which implies  $a_l^{**} \leq a_l^*$  and completes the proof of the first part of the theorem.

For the second part, we note that all roots of the polynomial  $(x + 1)U_{m-1}(x)$  are real and located in the interval  $[-1, 1]$  [see, e.g., Szegő (1959)], and, consequently, the roots of the  $l$ th derivative have the same property, which implies  $x_l^* > -1$  or, equivalently,  $a_l^{**} > \arccos 0 = \pi/2$ . Similarly, the roots of  $(x + 1)U_{m-1}(x)$  become dense in the interval  $[-1, 1]$  as  $m \rightarrow \infty$  [see Szegő (1959)], and by the interlacing property the roots the  $l$ th derivative have the same property, which implies, for any fixed  $l$ ,

$$\lim_{m \rightarrow \infty} a_l^{**} = \lim_{m \rightarrow \infty} \arccos \frac{x_l^* + 1}{x_l^* - 1} = \arccos 0 = \frac{\pi}{2}$$

and completes the proof of the theorem.

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FAKULTÄT FÜR MATHEMATIK  
 RUHR-UNIVERSITÄT BOCHUM  
 44780 BOCHUM  
 GERMANY  
 E-MAIL: holger.dette@ruhr-uni-bochum.de

DEPARTMENT OF MATHEMATICS  
 ST. PETERSBURG STATE UNIVERSITY  
 ST. PETERSBURG  
 RUSSIA  
 E-MAIL: v.melas@pobox.spbu.ru