D-optimal designs for trigonometric regression models on a partial circle

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Abstract

In the common trigonometric regression model we investigate the D-optimal design problem, where the design space is a partial circle. It is demonstrated that the structure of the optimal design depends only on the length of the design space and that the support points (and weights) are analytic functions of this parameter. By means of a Taylor expansion we provide a recursive algorithm such that the D-optimal designs for Fourier regression models on a partial circle can be determined in all cases. In the linear and quadratic case the D-optimal design can be determined explicitly.

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1 Introduction

Trigonometric regession models of the form

$$y = \beta_0 + \sum_{j=1}^{m} \beta_{2j-1} \sin(jt) + \sum_{j=1}^{m} \beta_{2j} \cos(jt) + \varepsilon, \quad t \in [c, d]; \tag{1.1}$$

$-\infty < c < d < \infty$; are widely used to describe periodic phenomena [see e.g. Mardia (1972), Graybill (1976) or Kitsos, Titterington and Torsney (1988)] and the problem of designing experiments for Fourier regression models has been discussed by several authors [see e.g. Hoel (1965), Karlin and Studden (1966), page 347, Fedorov (1972), page 94, Hill (1978), Lau and Studden (1985), Riccomagno, Schwabe and Wynn (1997)]. Most authors concentrate on the design space $[-\pi, \pi]$, but Hill (1978) and Kitsos, Titterington and Torsney (1988) point out that in many applications it is impossible to take observations on the full circle $[-\pi, \pi]$. We refer to Kitsos, Titterington and Torsney (1988) for a concrete example, who investigated a design problem in rhythmometry involving circadian rhythm exhibited by peak expiratory flow, for which the design region has to be restricted to a partial cycle of the complete 24-hour period.

In the present paper, we address the question of designing experiments in trigonometric models, where the design space is not necessarily the full circle but an arbitrary interval $[c, d] \subset \mathbb{R}$. Recently, Dette and Melas (2001) considered optimal designs for estimating individual coefficients in this model and gave a partial solution to this problem. In the present paper, we consider the D-optimality criterion, which is a reasonable criterion if efficient estimates of all parameters in the model are desired. It is demonstrated in Section 2 that the structure of the D-optimal design depends only on the length $a = (c - d)/2$ of the design space and that there only exist two types of D-optimal designs (this result seems to be even unknown for the complete circle). Our main result of Secion 3 proves that the support points (and weights) of the D-optimal design are analytic functions of the parameter a and that an appropriately scaled version of the D-optimal design converges weakly as $a \to 0$ to a nondegenerate discrete distribution on the interval $[0, 1]$. Following Melas (1978), these results are applied to obtain Taylor expansions for the support points of the D-optimal design (considered as a function of the parameter $a = (d - c)/2$), which allows a complete solution of the D-optimal design problem in the trigonometric regression model (1.1) on the interval $[c, d]$. Finally, some examples are given in Section 4, and in the linear and quadratic trigonometric regression model on the interval $[-a, a]$ D-optimal designs are determined explicitly.

2 Preliminary results for D-optimal designs in trigonometric regression models on a partial circle

Consider the trigonometric regression model (1.1), define $\beta = (\beta_0, \beta_1, \ldots, \beta_{2m})^T$ as the vector of parameters and

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

as the vector of regression functions. An approximate design is a probability measure ξ on the design space $[c, d]$ with finite support [see e.g. Kiefer (1974)]. The support points of the design ξ give the locations, where observations are taken, while the weights give the corresponding proportions of total observations to be taken at these points. Due to the 2π-periodicity of the regression functions we restrict ourselves without loss of generality to design spaces with lenght $d - c \leq 2\pi$. For uncorrelated observations (obtained from an approximate design) the covariance matrix of the least squares estimator for the parameter β is approximately proportional to the matrix

$$M(\xi) = \int f(t) f^T(t) d\xi(t) \in \mathbb{R}^{2m+1 \times 2m+1} , \tag{2.2}$$

which is called 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) or Pukelsheim (1993)].

In this paper, we are interested in D-optimal designs for the trigonometric regression model (1.1) on the interval $[c, d]$, which maximize the determinant

$$\det M(\xi)$$

of the Fisher information matrix in the space of all approximate designs on the interval $[c, d]$. Note that a D-optimal design minimizes the (approximate) volume of the ellipsoid of concentration for the vector β of the unknown parameters in the model (1.1) [see e.g. Fedorov (1972)] and that optimal designs in the trigonometric regression model (1.1) for the full circle $[c, d] = [-\pi, \pi]$ have been determined by numerous authors [see e.g. Karlin and Studden (1966), Fedorov (1972), Lau and Studden (1985), Pukelsheim (1993) or Dette and Haller (1998) among many others].

Our first preliminary result demonstrates that for the solution of the D-optimal design problem on a partial circle it is sufficient to consider only symmetric design spaces. To be precise, let

$$\eta = \begin{pmatrix} t_0 & \ldots & t_n \\ \omega_0 & \ldots & \omega_n \end{pmatrix} \tag{2.3}$$

denote a design on the interval $[c, d]$ with different support points $t_0 < \ldots < t_n$ and positive weights $\omega_0, \ldots, \omega_n$ adding to one and define its affine transformation onto the symmetric interval $[-a, a]$ by

$$\xi_\eta = \begin{pmatrix} \tilde{t}_0 & \ldots & \tilde{t}_n \\ \omega_0 & \ldots & \omega_n \end{pmatrix} \tag{2.4}$$

where $a = (d - c)/2$ and $\tilde{t}_i = t_i - (d + c)/2$, $i = 1, \ldots, n$.

Lemma 2.1. *Let $M(\eta)$ and $M(\xi_\eta)$ denote the information matrices in the trigonometric regression model (1.1) of the designs η and ξ_η defined by (2.3) and (2.4), respectively, then*

$$\det M(\xi_\eta) = \det M(\eta). \tag{2.5}$$

Proof. If the number of support points satisfies $n+1 < 2m+1$, then both sides of the equation (2.5) vanish and the proof is trivial. Next consider the case $n = 2m$, for which we have [see e.g. Karlin and Studden (1966)]

$$\det M(\xi_\eta) = (\det F(\xi_\eta))^2 \prod_{i=0}^{2m} \omega_i \ , \tag{2.6}$$

where the matrix $F(\xi_\eta) \in \mathbb{R}^{2m+1 \times 2m+1}$ is defined by

$$F(\xi_\eta) = \big(f_i(\tilde{t}_j)\big)_{i=0,\ldots,2m}^{j=0,\ldots,2m} . \tag{2.7}$$

Now it to easy to see that the vector $f(t)$ defined by (2.1) satisfies for any $\alpha \in \mathbb{R}$

$$f(t+\alpha) = Pf(t)$$

where P is a $(2m+1) \times (2m+1)$ diagonal block matrix defined by

$$P = \begin{pmatrix} 1 & & & \\ & Q(\alpha) & & \\ & & \ddots & \\ & & & Q(m\alpha) \end{pmatrix}$$

and $Q(\beta)$ is a 2×2 rotation matrix given by

$$Q(\beta) = \begin{pmatrix} \cos(\beta) & \sin(\beta) \\ -\sin(\beta) & \cos(\beta) \end{pmatrix} .$$

Obviously, we have $\det P = 1$ and obtain from (2.6) and (2.7)

$$\det M(\xi_\eta) = \det M(\eta) \ ,$$

which proves the assertion of the Lemma in the case $n = 2m$. Finally, in the remaining case $n > 2m$, the assertion follows from the Cauchy Binet formula and the arguments given for the case $n = 2m$. $\Box$

From Lemma 2.1 it is clear that it is sufficient to determine the D-optimal designs for symmetric intervals

$$[c,d] = [-a,a], \qquad 0 < a \le \pi$$

and we will restrict ourselves to this case throughout this paper. For fixed $a \in (0,\pi]$ let ξ_a^* denote a D-optimal design for the trigonometric regression model (1.1) on the interval $[-a,a]$. Note that in general the D-optimal design for the trigonometric regression model is not necessarily unique [see e.g. Fedorov (1972), who considered the case $a = \pi$]. However, it is known that the optimal information matrix $M(\xi_a^*)$ is unique and nonsingular [see e.g. Pukelsheim (1993), p. 151]. Moreover, due to the equivalence theorem for D-optimality [see Kiefer (1974)] the design ξ_α^* satisfies

$$d(t,\xi_\alpha^*) \le 0 \quad \text{for all } t \in [-a,a], \tag{2.8}$$

with equality at the support points, where

$$d(t,\xi) = f^T(t)M^{-1}(\xi)f(t) - (2m+1) \tag{2.9}$$

denotes the directional derivative of the function $\xi \to \log\det M(\xi)$ [see Silvey (1980), p.20]. Let $\Xi_a^{(1)}$ denote the set of all designs of the form

$$\xi = \xi(a) = \begin{pmatrix} -t_m & \dots & -t_1 & t_0 & t_1 & \dots & t_m \\ \frac{1}{2m+1} & \dots & \frac{1}{2m+1} & \frac{1}{2m+1} & \frac{1}{2m+1} & \dots & \frac{1}{2m+1} \end{pmatrix} \tag{2.10}$$

where $0 = t_0 < t_1 < \ldots < t_m = a$ and define

$$\Xi^{(2)} = \Big\{ \xi \mid supp(\xi) \subset [-a,a],\ d(t,\xi) = 0 \text{ for all } t \in [-a,a] \Big\} \tag{2.11}$$

as the set of all designs on the interval $[-a,a]$ with vanishing directional derivative for all $t \in [-a,a]$, then we obtain the following auxiliary result.

Lemma 2.2. *Let ξ_a^* denote a D-optimal design on the interval $[-a,a]$, then*

$$\xi_a^* \in \Xi_a^{(1)} \cup \Xi_a^{(2)}.$$

Proof. Due to the equivalence theorem (2.8) any design $\xi \in \Xi_a^{(2)}$ is D-optimal for trigonometric regression model (1.1) on the interval $[-a,a]$. Now assume that

$$\xi \;=\; \begin{pmatrix} u_1 & \dots & u_n \\ \omega_1 & \dots & \omega_n \end{pmatrix}$$

is D-optimal for the trigonometric regression on the interval $[-a,a]$, where the support points satisfy $-a \le u_1 < \ldots < u_n \le a$. If $\xi \notin \Xi_a^{(2)}$, then $d(t,\xi) \not\equiv 0$, but due the equivalence theorem we have

$$d(u,\xi) \le 0 \quad \forall\, u \in [-a,a]$$

$$d(u_i,\xi) = 0 \quad \forall\, i = 1,\ldots,n \tag{2.12}$$

$$\frac{d}{du} d(u,\xi)|_{u=u_i} = 0 \quad \forall\, i = 2,\ldots,n-1.$$

If $\tilde{\xi}$ denotes the reflection of ξ at the origin, then it is easy to see that $\det M(\xi) = \det M(\tilde{\xi})$ and consequently $\tilde{\xi}$ is also D-optimal. Moreover, the concavity of the D-criterion implies that the symmetric design $\xi^* = (\xi + \tilde{\xi})/2$ is also D-optimal in the trigonometric regression (1.1) on the interval $[-a,a]$. Note that there exists a permutation matrix $P \in \mathbb{R}^{2m+1 \times 2m+1}$ such that

$$PM(\xi)P^T = \begin{pmatrix} M_1(\xi) & M_2(\xi) \\ M_2^T(\xi) & M_3(\xi) \end{pmatrix}, \tag{2.13}$$

where

$$M_1(\xi) = \int_{-a}^{a} f_c(t) f_c^T(t) d\xi(t) \in \mathbb{R}^{m+1\times m+1}$$

$$M_2(\xi) = \int_{-a}^{a} f_c(t) f_s^T(t) d\xi(t) \in \mathbb{R}^{m+1\times m} \tag{2.14}$$

$$M_3(\xi) = \int_{-a}^{a} f_s(t) f_s^T(t) d\xi(t) \in \mathbb{R}^{m\times m}$$

and $f_c(t) = (1, \cos(t), \dots, \cos(mt))^T$, $f_s(t) = (\sin(t), \dots, \sin(mt))^T$. Because the information matrix of the D-optimal design is unique [see Pukelsheim (1993)], we obtain (note that ξ^* is symmetric)

$$M_2(\xi) = M_2(\tilde{\xi}) = M_2(\xi^*) = 0 \in \mathbb{R}^{m+1\times m},$$

which implies for the directional derivative in (2.9)

$$\begin{aligned} g(t) = d(t,\xi) &= {f_c}^T(t) M_1^{-1}(\xi) f_c(t) + {f_s}^T(t) M_3^{-1}(\xi) f_s(t) - (2m+1) \\ &= \sum_{i=0}^{2m} \gamma_i \cos(it) \end{aligned} \tag{2.15}$$

for appropriate constants $\gamma_0, \dots, \gamma_{2m}$ (note that the last representation follows by well known trigonometric formulas). From $\xi \notin \Xi_a^{(2)}$ we obtain that the polynomial $g(t)$ is not identically zero and the equivalence theorem shows that every suppport point is a zero of the function g. Moreover, the functions $\{1, \cos t, \dots, \cos(2mt)\}$ form a Chebyshev system on the interval $[0, a]$ and a Chebyshev system on the interval $[-a, 0]$. Consequently, g has at most $2m + 1$ roots in the interval $[0, a]$ and at most $2m + 1$ zeros in the interval $[-a, 0]$ (including counting of multiplicities) [see Karlin and Studden (1966)]. Consider the case $[0, a]$ and substitute $t = \arccos x$, then it follows, observing the definition of the Chebyshev polynomials of the first kind

$$T_i(x) = \cos(i \arccos x), \tag{2.16}$$

[see Rivlin (1974)] that $g(\arccos x)$ is a nonpositive polynomial of degree $2m$ on the interval $[\cos a, 1]$. Consequently, if $g(\arccos x)$ has exactly $2m$ roots (including counting of multiplicities), the boundary points $\cos a$ and 1 have to be roots of $g(\arccos x)$. Note that a similar argument applies to the interval $[-a, 0]$ and therefore the nonpositive function g defined in (2.15) has at most $4m$ roots (including counting of multiplicities) in the interval $[-a, a]$. Because the number of regression functions is $2m + 1$, it therefore follows from (2.12) that any D-optimal design $\eta \notin \Xi_a^{(2)}$ has exactly $2m+1$ support points in the interval $[-a, a]$ including the boundary points $-a, a$. A standard argument shows that all weights of the D-optimal design have to be equal, i.e. $\omega_j = 1/(2m+1)$, $j = 1, \dots, 2m+1$. If $\xi \notin \Xi_a^{(1)}$, then $\xi \neq \tilde{\xi}$ and consequently $\xi^* = (\xi + \tilde{\xi})/2$ is a D-optimal design for the trigonometric regression model (1.1) on interval $[-a, a]$ with more than $2m + 1$ support points, which is impossible, by the above discussion. This shows $\xi \in \Xi_a^{(1)}$ and proves Lemma 2.2.

□

3 Analytic properties of D-optimal designs in trigonometric regression models on a partial circle

Lemma 2.2 motivates the consideration of designs of the form (2.10) and our next Lemma gives an explicit representation for the determinant of the information matrix of this type of design.

Lemma 3.1. *Let ξ denote a design of the form (2.10) and $x_i = \cos t_i$, $i = 0, \ldots, m$, then*

$$\det M(\xi) = \frac{2^{2m^2}}{(2m+1)^{2m+1}} \prod_{i=1}^{m} (1-x_i^2)(1-x_i)^2 \prod_{1 \le i < j \le m} (x_j - x_i)^4. \tag{3.1}$$

Proof. For any design ξ of the form (2.10) we have

$$\det M(\xi) = \det M_1(\xi) \det M_3(\xi),$$

where the matrices $M_1(\xi), M_2(\xi), M_3(\xi)$ are defined by (2.14). Define the design η_ξ by

$$\eta_\xi = \begin{pmatrix} x_0 & x_1 & \ldots & x_m \\ \frac{1}{2m+1} & \frac{2}{2m+1} & \ldots & \frac{2}{2m+1} \end{pmatrix},$$

then it is straightforward to see, that

$$M_1(\xi) = \left(\int_{-1}^{1} T_i(x) T_j(x) d\eta_\xi(x) \right)_{i,j=0}^{m}, \tag{3.2}$$

$$M_3(\xi) = \left(\int_{-1}^{1} (1-x^2) U_i(x) U_j(x) d\eta_\xi(x) \right)_{i,j=0}^{m-1} \tag{3.3}$$

where $T_i(x)$ is the Chebyshev polynomial of the first kind defined in (2.16) and

$$U_i(x) = \frac{\sin((i+1)\arccos x)}{\sin(\arccos x)} \tag{3.4}$$

is the Chebyshev polynomial of the second kind [see Rivlin (1974)]. Because $T_i(x)$ is a polynomial of degree i with leading coefficient 2^{i-1}, it follows that $M_1(\xi)$ is essentially a Vandermonde determinant, i.e.

$$\det M_1(\xi) = 2^{m(m-1)} \frac{2^m}{(2m+1)^{m+1}} \Big(\det \big((x_j^i)_{i=0,\ldots,m}^{j=0,\ldots,m} \big) \Big)^2 =$$

$$= \frac{2^{m^2}}{(2m+1)^{m+1}} \prod_{i=1}^{m} (1-x_i)^2 \prod_{1 \le i < j \le m} (x_j - x_i)^2$$

(note that $x_0 = 1$). Note that the support point x_0 of η_ξ has a vanishing contribution to the matrix $M_3(\xi)$ and that the leading coefficient of $U_i(x)$ is 2^i. Therefore we have by similar arguments

$$\det M_3(\xi) = \frac{2^{m^2}}{(2m+1)^m} \prod_{i=1}^{m} (1 - x_i^2) \prod_{1 \le i < j \le m} (x_j - x_i)^2$$

and a combination of these formulas yields (3.1), which proves the assertion of Lemma 3.1. $\square$

We are now studying the function

$$\phi(x, a) = \prod_{i=1}^{m} (1 - x_i^2)(1 - x_i)^2 \prod_{1 \le i < j \le m} (x_j - x_i)^4 \tag{3.5}$$

as a function of the length a of the design space. To this end we note that $x_m = \cos(a)$ and introduce the set

$$T = \{(\tau_1, \ldots, \tau_{m-1})^T \ \mid \ 0 < \tau < \ldots < \tau_{m-1} < 1\} \tag{3.6}$$

$$\mathcal{X} = \{(x_1, \ldots, x_{m-1})^T \mid \ x_i = \cos(a\tau_i), \ i = 1, \ldots, m-1, \ (\tau_1, \ldots, \tau_{m-1})^T \in T\} \tag{3.7}$$

Note that any design $\xi \in \Xi_a^{(1)}$ of the form (2.10) is uniquely determined by a point $\tau = (\tau_1, \ldots, \tau_{m-1})^T \in T$ or its corresponding function $x = (x_1, \ldots, x_{m-1})^T \in \mathcal{X}$ by the transformation $t_i = a\tau_i = \arccos x_i$, $i = 1, \ldots, m-1$ (note that $t_0 = 0, t_m = a$) and by Lemma 3.1 the determinant of $M(\xi)$ is proportional to the function ϕ given in (3.5). By standard arguments it can now be verified that for fixed $a \in (0, \pi]$ the function ϕ in (3.5) is a strictly concave function of $x = (x_1, \ldots, x_{m-1})^T \in \mathcal{X}$. Therefore (for fixed a) the function $\phi(x, a)$ has a unique maximum in $\mathcal{X}$, which will be denoted by $x^*(a)$ (because of its dependence on the length of the design space). The function ϕ is obviously differentiable and $x^*(a)$ can be obtained as the unique solution of the equations

$$\frac{\partial}{\partial x} \phi(x, a) = 0 \in \mathbb{R}^{m-1}. \tag{3.8}$$

Moreover, for any $x \in \mathcal{X}$ the matrix of the second partial derivatives

$$G(x, a) = \left(\frac{\partial^2}{\partial x_i \partial x_j} \phi(x, a) \right)_{i,j=1}^{m-1} \tag{3.9}$$

is positive definite and in particular the matrix

$$J(a) = G(x^*(a), a) \tag{3.10}$$

is positive definite for all $a \in (0, \pi]$. It therefore follows from the implicit function theorem [see Gunning and Rossi (1965)] that the function

$$x^* : \begin{cases} (0, \pi] & \to & \mathcal{X} \\ a & \to & x^*(a) \end{cases} \tag{3.11}$$

defined as the solution of the equation (3.8) is real analytic. In other words: for any point $a_0 \in (0, \pi]$ there exists a neighbourhood U_0 of a_0, such that the function $x^*|_{U_0}$ can be expanded in a convergent Taylor series. Observing the symmetry $\phi(x, a) = \phi(x, -a)$, it therefore follows that the function

$$
\tau^* : \begin{cases} [-\pi, \pi]\backslash\{0\} \to T \\ a \to \tau^*(a) = \left(\frac{\arccos x_1^*(|a|)}{a}, \dots, \frac{\arccos x_{m-1}^*(|a|)}{a}\right)^T \end{cases} \tag{3.12}
$$

is also real analytic. The following result shows that the function τ^* can be extended to a real analytic function on the full circle $[-\pi, \pi]$.

Lemma 3.2. *The function τ^* defined by (3.12) can be extended to a real analytic function on the interval $[-\pi, \pi]$, where*

$$
\tau^*(0) = \lim_{a \to 0} \tau(a) = (\tau_1^*, \dots, \tau_{m-1}^*)^T ,
$$

$\tau_1^* < \ldots < \tau_{m-1}^*$ are the positive roots of the polynomial

$$
P_{m-1}^{(1,1/2)}(2x^2 - 1) \;=\; \frac{1}{2x} P_{2m-1}^{(1,1)}(x) \;=\; \frac{1}{(2m+1)x} P'_{2m}(x)
$$

and $P_i^{(\alpha,\beta)}(x)$ denotes the ith Jacobi polynomial orthogonal with respect to the measure $(1-x)^\alpha (1+x)^\beta dx$ and $P_{2m}(x)$ is the $2m$th Legendre polynomial orthogonal with respect to the Lebesgue measure on the interval $[-1, 1]$.

Proof. The assertion of Lemma 3.2 follows if we prove the existence of $\lim_{a\to 0} \tau^*(a)$ and the claimed form of its components. Let $x_\tau = (\cos(a\tau_1), \dots, \cos(a\tau_{m-1}))^T$, then the expansions $\sin t = t + o(t)$, $\cos t = 1 - t^2/2 + o(t^2)$ show that for $a \to 0$

$$
\phi(x_\tau, a) = \frac{a^{2m(2m+1)}}{2^{2m^2}} \prod_{i=1}^{m} \tau_i^6 \prod_{1 \le i < j \le m} (\tau_i^2 - \tau_j^2)^4 (1 + o(a))
$$

($\tau_m = 1$) and consequently, the limit $\lim_{a\to 0} \tau^*(a)$ exists and can be obtained by maximizing the function

$$
\bar{\phi}(\tau) = \prod_{i=1}^{m} \tau_i^3 (1 - \tau_i^2)^2 \prod_{1 \le i < j \le m-1} (\tau_i^2 - \tau_j^2)^2 \tag{3.13}
$$

over the set T defined in (3.6). Note that standard arguments show the strict concavity of the function $\bar{\phi}$ and consequently, the point $\tau^* = (\tau_1^*, \dots, \tau_{m-1}^*)^T$ where the maximum is obtained is unique. Taking partial derivatives of the logarithm of $\bar{\phi}$ yields the system

$$
\frac{3}{\tau_i} + \frac{4\tau_i}{\tau_i^2 - 1} + \sum_{j=1, j\neq i}^{m-1} \frac{4\tau_i}{\tau_i^2 - \tau_j^2} \;=\; 0 \;, \qquad i = 1 \dots m-1 \tag{3.14}
$$

and substituting $\tau_i^2 = y_i \in (0,1)$ gives

$$\frac{3}{y_i} + \frac{4}{y_i - 1} + \sum_{j=1, j\neq i}^{m-1} \frac{4}{y_i - y_j} \;=\; 0\;, \qquad i = 1 \ldots m-1\;. \tag{3.15}$$

Similar arguments as given in Karlin and Studden (1966) or Fedorov (1972) show that the polynomial $\psi(y) = \prod_{i=1}^{m-1}(y - y_i)$ satisfies the differential equation

$$y(1-y)\psi''(y) + (3/2 - 7/2y)\psi'(y) + (m-1)(m+3/2)\psi(y) = 0. \tag{3.16}$$

It is well known [see e.g. Szegö (1975), Sect. 4.21] that the unique polynomial solution of this differential equation is given by the polynomial

$$P_{m-1}^{(1/2,1)}(1-2y)$$

and the assertion of the Lemma now follows from transformation $y = \tau^2$ and the equation $P_n^{(\alpha,\beta)}(-x) = (-1)^n P_{m-1}^{(\beta,\alpha)}(x)$ [see Szegö (1975), formula (4.1.3)]. The alternative representations of the polynomial $P_{m-1}^{(1,1/2)}(2x^2-1)$ are a consequence of $P_n^{(0,0)}(x) = P_n(x)$ and Theorem 4.1 in Szegö (1975). $\Box$

Table 1: *Values of the components $\tau_1^*(0), \ldots, \tau_{m-1}^*(0)$ of the vector $\tau^*(0)$ defined in Lemma 3.2 and the polynomial solution of the differential equation (3.16) for various values of m.*

m	$\psi(y)$ and $\tau_j(0)$
2	$\psi(y) = y - 3/7$
	$\tau_1^*(0) = \sqrt{3/7} \approx 0.6546$
3	$\psi(y) = y^2 - 10/11y + 5/33$
	$\tau_1^*(0) \approx 0.4688, \tau_2^*(0) \approx 0.8302$
4	$\psi(y) = y^3 - 7/5y^2 + 7/13y - 7/143$
	$\tau_1^*(0) \approx 0.3631, \tau_2^*(0) \approx 0.6772, \tau_3^*(0) \approx 0.8998$
5	$\psi(y) = y^4 - 36/19y^3 + 378/323y^2 - 84/323y + 63/4199$
	$\tau_1^*(0) \approx 0.2958, \tau_2^*(0) \approx 0.5652, \tau_3^*(0) \approx 0.7845, \tau_4^*(0) \approx 0.9340$

Table 1 shows the polynomial $P_{m-1}^{(1,1/2)}(2y-1)$ (normalized such that the leading coefficient is 1) and the corresponding values $\tau_i^* = \sqrt{y_i}$ for lower degrees $m = 2, 3, 4, 5$. The following result shows that for small designs space, i.e.

$$a \leq \pi(1 - 1/(2m+1)),$$

the solution of the optimal design problem can be obtained by a Taylor expansion of the function τ^* in (3.12) at the point $a = 0$, where the ith component $\tau_i^*(0)$ of the vector $\tau^*(0)$ is the ith positive root of the polynomial $P_{m-1}^{(1,1/2)}(2x^2-1)$.

Theorem 3.3. *Consider the trigonometric regression model (1.1) with design space $[-a, a]$, where $0 < a \leq \pi$.*

(i) *If $a > \pi(1 - 1/(2m+1))$, then the design ξ_a^* with equal masses at the $2m+1$ points*

$$t_i^* = 2\pi \frac{i-1-m}{2m+1}, \quad i = 1, \dots, 2m+1 \tag{3.17}$$

is a D-optimal design.

(ii) *If $a < \pi(1 - 1/(2m+1))$, the D-optimal design is unique and of the form*

$$\xi_a^* = \begin{pmatrix} -a & -a\tau_{m-1}^*(a) & \dots & -a\tau_1^*(a) & 0 & a\tau_1^*(a) & \dots & a\tau_{m-1}^*(a) & a \\ \frac{1}{2m+1} & \frac{1}{2m+1} & \dots & \frac{1}{2m+1} & \frac{1}{2m+1} & \frac{1}{2m+1} & \dots & \frac{1}{2m+1} & \frac{1}{2m+1} \end{pmatrix} \tag{3.18}$$

where τ^* is a real analytic function on the interval $[-\pi, \pi]$ defined by (3.12) and Lemma 3.2.

Proof. Recall the definition of the set $\Xi_a^{(2)}$ in (2.11) and assume that the design $\xi^* \in \Xi_a^{(2)}$ is D-optimal for the trigonometric regression model (1.1) on interval $[-a, a]$. Because $d(t, \xi^*) = 0$ for all $t \in [-a, a]$ it follows from the Chebyshev property of the functions $\{1, \sin t, \cos t, \dots, \sin mt, \cos mt\}$ that the directional derivative $d(t, \xi^*)$ also vanishes on the full circle $[-\pi, \pi]$ [see Karlin and Studden (1966), p. 20]. Consequently, ξ^* is also D-optimal for the trigonometric regression on the interval $[-\pi, \pi]$, which implies [by the uniqueness of the D-optimal information matrix]

$$M(\xi^*) = \text{diag}(1, 1/2, \dots, 1/2),$$

$$\det M(\xi^*) = 2^{-2m}.$$

On the other hand we have

$$\lim_{a \to 0} \max_{\xi} \det M(\xi) = 0 \ ,$$

and consequently for sufficiently small a the D-optimal design cannot be an element of the set $\Xi_a^{(2)}$. From Lemma 2.2 it follows that the D-optimal design must belong to the set $\Xi_a^{(1)}$ and the discussion in the first part of this section shows that for sufficiently small a the D-optimal design is unique and of the form (3.18). Now let ξ_a^* denote the design defined by (3.18) and

$$\begin{aligned} a^* &= \sup\{a \in (0, \pi] \mid \xi_a^* \text{ is D-optimal}\} \\ &= \sup\{a \in (0, \pi] \mid \det M(\xi^*) < 2^{-2m}\} \end{aligned} \tag{3.19}$$

(note that the second equality follows by continuity and Lemma 2.2). It is well known [see Fedorov (1972) or Pukelsheim (1993)] that the uniform distribution ξ_u at the $2m+1$ points defined by (3.17) is D-optimal for the trigonometric regression model on the interval

$[-\pi, \pi]$. If $\hat{a} = \pi(1 - 1/(2m+1))$ denotes the largest support point of this design, then it follows that $\xi^*_{\hat{a}} = \xi_u$. Consequently, the design $\xi^*_{\hat{a}}$ specified in part (i) of Theorem 3.3 is also D-optimal for the trigonometric regression on the interval $[-\hat{a}, \hat{a}]$ and the D-optimality of $\xi^*_{\hat{a}}$ on $[-\pi, \pi]$ shows

$$\xi^*_{\hat{a}} \in \Xi^{(1)}_{\hat{a}} \cap \Xi^{(2)}_{\hat{a}} ,$$

which implies for the critical bound in (3.18) the inequality $a^* \leq \hat{a}$. Now for any design of the form

$$\xi = \xi(a) = \begin{pmatrix} -t_m & \ldots & -t_1 & t_0 & t_1 & \ldots & t_m \\ \frac{1}{2m+1} & \ldots & \frac{1}{2m+1} & \frac{1}{2m+1} & \frac{1}{2m+1} & \ldots & \frac{1}{2m+1} \end{pmatrix} \tag{3.20}$$

with $0 < t_1 < \ldots < t_m \leq \pi$ it follows from Lemma 3.1 that

$$\det M(\xi) = C \prod_{i=1}^{m} (1 - x_i^2)(1 - x_i)^2 \prod_{1 \leq i < j \leq m} (x_j - x_i)^4 =: h(x_\xi)$$

with $C = 2^{2m^2}/(2m+1)^{2m+1}$, $x_\xi = (x_1, \ldots, x_m)^T$, $x_i = \cos t_i$ $(i = 1, \ldots, m)$. The discussion at the beginning of this section shows that h is strictly concave. Additionally, we have for the design $\xi^*_{\hat{a}}$

$$h(x_{\xi^*_{\hat{a}}}) = 2^{-2m}$$

and for any other design ξ of the form (3.20)

$$h(x_\xi) < 2^{-2m}$$

(because otherwise a convex combination of $\xi^*_{\hat{a}}$ and ξ_a would have an information matrix with a determinant larger than 2^{-2m}, which is impossible). Consequently, because ξ^*_u is of the form (3.20) it follows for the quantity a^* defined by (3.19) that $a^* = \hat{a}$.
If $a \geq \hat{a}$, the discussion of this proof shows that the design specified by part (i) of Theorem 3.3 is D-optimal. If $a < \hat{a}$, the definition (3.19) shows that the D-optimal design is in the set $\Xi^{(1)}_a$ and Lemma 3.1 and 3.2 (with their corresponding proofs) imply that the D-optimal design for the trigonometric regression on the interval $[-a, a]$ is of the form (3.18), which completes the proof of the theorem. □

Note that Theorem 3.3 provides a complete solution of the D-optimal design problem. In the case (i) with $a \geq \pi(1 - 1/(2m+1))$ a D-optimal design for the trigonometric regression model (1.1) on the interval $[-a, a]$ is explicitly given by the uniform distribution at the support points specified by (3.17), but is not necessarily unique. If $a < \pi(1 - 1/(2m+1))$ the D-optimal design is unique and specified by (3.18), where the vector $\tau^*(a) = (\tau^*_1(a), \ldots, \tau^*_{m-1}(a))^T$ can be obtained by means of a Taylor expansion at the point $a = 0$

$$\tau^*(a) = \sum_{i=0}^{\infty} \tau^*_{(i)} a^i \tag{3.21}$$

and the vector $\tau^*_{(0)} = \tau^*(0)$ is given in Lemma 3.2. It is shown in Dette, Melas and Pepelyshev (2000) that the coefficients in the above expansion can be calculated by the recursive relations

$$\tau^*_{(s+1)} = -\frac{1}{(s+1)!} J^{-1}(0) \left(\frac{d}{da}\right)^{s+1} g(\tau^*_{<s>}(a), a)\Big|_{a=0}$$

$s = 0, 1, 2, \ldots$, where

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

denotes the Taylor polynomial of degree $s \in \{0, 1, 2, \ldots\}$,

$$J(0) = \left(\frac{\partial^2}{\partial\tau_i \partial\tau_j} \phi(x_\tau, a)\right)_{i,j=1}^{m-1}\Big|_{\tau=\tau^*(0)}$$

and

$$g(\tau, a) = \frac{\partial}{\partial\tau} \phi(x_\tau, a) \in \mathbb{R}^{m-1}.$$

Note that in general an exact determination of the radius of convergence for the Taylor expansion (3.21) seems to be intractable. In general several re-expansions could be needed to obtain the D-optimal design for any $a \in (0, \pi(1 - 1/(2m+1))$. However, our numerical calculations in the following section indicate that the expansion at the point $a = 0$ always gives the D-optimal design for the trigonometric regression model (1.1) on the interval $[-a, a]$ for any $a \in (0, \pi(1 - 1/(2m+1))$.

4 Examples

Example 4.1. Our first example considers the linear trigonometric regression model ($m = 1$) on the interval $[-a, a]$, for which the solution is rather obvious. If $a \geq 2\pi/3$, the design

$$\xi^*_a = \begin{pmatrix} -\frac{2\pi}{3} & 0 & \frac{2\pi}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix}$$

is D-optimal, while for $a < 2\pi/3$ the D-optimal design for the linear trigonometric regression model on the interval $[-a, a]$ is given by

$$\xi^*_a = \begin{pmatrix} -a & 0 & a \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix}.$$

This follows directly from Theorem 3.3.

Example 4.2. In the quadratic regression model the situation is more complicated. If $a \geq 4\pi/5$, then part (i) of Theorem 3.3 shows that the design

$$\xi^*_a = \begin{pmatrix} -\frac{4\pi}{5} & -\frac{2\pi}{5} & 0 & \frac{2\pi}{5} & \frac{4\pi}{5} \\ \frac{1}{5} & \frac{1}{5} & \frac{1}{5} & \frac{1}{5} & \frac{1}{5} \end{pmatrix}$$

is D-optimal. If $a < 4\pi/5$, the D-optimal design can be obtained by means of a Taylor expansion as indicated in the second part of Theorem 3.3. However, in this particular case an explicit solution is possible by a careful inspection of the arguments given in Section 3. Part (ii) of Theorem 3.3 shows that the D-optimal design in the quadratic trigonometric regression model is in the set $\Xi_a^{(1)}$, whenever $a < 4\pi/5$ and consequently only one support point $t_1^* = t_1^*(a)$ has to be determined. This can be done by a direct differentation of the function $\phi(x, a)$ in (3.5). Note that $m = 2$, $x_2 = \cos a$ and therefore $\phi(x, a)$ is a function of only one variable, say $x_1 \in (-1, 1)$. Elementary calculus yields that the derivative of ϕ has zeros at the points $x_1 = \cos a$, $x_2 = 1$ and

$$x_{3,4} = \frac{1}{8}\Big[2\cos(a) - 1 \mp \sqrt{33 + 12\cos(a) + 4\cos(a)^2}\Big].$$

It is easy to see that only one of these two points yields to a solution in the interval $[\cos a, 1]$ and consequently the D-optimal design for the quadratic trigonometric regression model on the interval $[-a, a]$ with $0 < a \le 4\pi/5$ is given by

$$\xi_a^* = \begin{pmatrix} -a & -t_1^*(a) & 0 & t_1^*(a) & a \\ \frac{1}{5} & \frac{1}{5} & \frac{1}{5} & \frac{1}{5} & \frac{1}{5} \end{pmatrix}$$

where

$$t_1^*(a) = \arccos\left(\frac{1}{8}\Big[2\cos(a) - 1 + \sqrt{33 + 12\cos(a) + 4\cos(a)^2}\Big]\right).$$

Example 4.3. In the general the case $m \ge 3$ the second part of Theorem 3.3 has to be applied if $a \le \pi(1 - 1/(2m+1))$ (note that in the remaining case a D-optimal design is explicitly given in part (i) of Theorem 3.3). From Table 1 we obtain the values of $\tau_i^*(0)$, $i = 1, \ldots, m-1$ (provided $m \le 5$) and the nontrivial support points $\tau_i^*(a)$ for $0 < a < \pi(1 - 1/(2m+1))$ can now be calculated by means of a Taylor expansion as indicated at the end of Section 3. Table 2 shows the values of the first coefficients in the expansion

$$\tau_i^*(a) = \sum_{l=0}^{\infty} \tau_{i(l)}^* \left(\frac{a}{\pi}\right)^l, \; i = 1, \ldots, m-1 \tag{4.1}$$

for $m = 2, 3, 4, 5$. It can easily be shown that $\tau_i^*(a)$ is an even function of the parameter a and consequently the odd coefficients vanish and only the even coefficients are displayed.

Consider as a concrete example the case $m = 3$. If $a \ge 6\pi/7$ a D-optimal design for the cubic trigonometric regression model on the interval $[-a, a]$ is given by part (i) of Theorem 3.3, i.e.

$$\xi_a^* = \begin{pmatrix} -\frac{6\pi}{7} & -\frac{4\pi}{7} & -\frac{2\pi}{7} & 0 & \frac{2\pi}{7} & \frac{4\pi}{7} & \frac{6\pi}{7} \\ \frac{1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{1}{7} \end{pmatrix}$$

Table 2: *Coefficients in the expansion (4.1). The D-optimal design in the trigonometric regression model (1.1) on the interval* $[-a, a]$ *with* $0 < a < \pi(1-1/(2m+1))$ *has equal masses at the points* $-a,\ -t_{m-1}, \ldots, -t_1,\ 0,\ t_1, \ldots, t_{m-1},\ a,$ *where* $t_i = a\tau_i^*(a)$, $i = 1, \ldots, m-1$.

	i	0	2	4	6	8	10
$m = 2$	$\tau^*_{1\,(i)}$	.65465	-.21977	-.07747	.04852	.06118	-.02116
$m = 3$	$\tau^*_{1\,(i)}$	.46885	-.19145	-.00875	.02584	-.00184	-.00283
	$\tau^*_{2\,(i)}$	.83022	-.13502	-.10286	-.05465	-.00161	.03946
$m = 4$	$\tau^*_{1\,(i)}$	.36312	-.15556	.00820	.01117	-.00368	-.00011
	$\tau^*_{2\,(i)}$	.67719	-.18093	-.07349	.00094	.02393	.01100
	$\tau^*_{3\,(i)}$	.89976	-.08456	-.07603	-.06025	-.03806	-.01256
$m = 5$	$\tau^*_{1\,(i)}$	.29576	-.12851	.01204	.00501	-.00238	.00036
	$\tau^*_{2\,(i)}$	.56524	-.18316	-.03971	.01585	.01178	-.00245
	$\tau^*_{3\,(i)}$	.78448	-.14366	-.08805	-.03360	.00483	.01980
	$\tau^*_{4\,(i)}$	.93400	-.05677	-.05431	-.04874	-.03965	-.02762

If $0 < a < 6\pi/7$ the D-optimal design can be calculated from the expansion (4.1) and Table 2. For example if $a = 1$ we obtain that the D-optimal design for the cubic trigonometric regression model on the interval $[-1, 1]$ is given by

$$\xi_a^* = \begin{pmatrix} -1 & -0.8154 & -0.4494 & 0 & 0.4494 & 0.8154 & 1 \\ \frac{1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{1}{7} \end{pmatrix}.$$

Figure 1 shows the support points of D-optimal designs as a function of the length a of the design space for $m = 2, 3, 4, 5$. The support points have been determined by a Taylor expansion as indicated in Section 3 and the D-optimal design puts equal masses at these points.

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