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REGULAR ARTICLE

D-optimal designs for full and reduced Fourier regression models

Xiaojian Xu[1] · **Xiaoli Shang**[1]

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Abstract The optimal designs for Fourier regression models under the D-optimality criterion are discussed in this article. First, we investigate the D-optimal designs for estimating two coefficients corresponding to either sine or cosine terms in a full Fourier regression model. In many biological applications, estimating such specific pairs of coefficients is of interest. As a result of this article, the D-optimal designs for estimating these "coefficient pairs" can be constructed either explicitly or numerically for Fourier regression models with any order. Our resulting designs are provided for Fourier regression models with order less than 6. Secondly, we discuss the sensitivity of our resulting optimal designs for a full Fourier regression model when the true model is actually a reduced version of the assumed one. Lastly, we provide the algorithm for obtaining the D-optimal designs for a reduced Fourier regression model and the D-optimal designs for a useful reduced Fourier model are constructed. The comparison study shows that the constructed designs incorporating the reduced model are efficient.

Keywords Fourier regression · Least squares estimation · Regression design · Sawtooth wave · Symmetric design

1 Introduction and literature review

A Fourier or trigonometric regression model of a given order m has the form

✉ Xiaojian Xu
xxu@brocku.ca

Xiaoli Shang
xiaol.shang@gmail.com

1 Brock University, St. Catharines, ON, Canada

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$$y = \beta_0 + \sum_{j=1}^{m} \beta_{2j-1} \sin(jt) + \sum_{j=1}^{m} \beta_{2j} \cos(jt) + \varepsilon, \quad t \in I, \tag{1}$$

with regression function $\mathbf{f} = (1, \sin(t), \cos(t), \ldots, \sin(mt), \cos(mt))^T$, and parameter vector $\boldsymbol{\beta} = (\beta_0, \beta_1, \beta_2, \ldots, \beta_{2m})^T$. A literature review on optimal designs for this model has been most recently provided in Xu and Shang (2014). Please also see the references cited therein.

In the present article, we focus on the optimal designs for Fourier regression models under D-optimality criterion. We assume that the random errors ε are uncorrelated with zero mean and positive variance σ^2. Let ξ be a design, which is a probability measure on the design space I. In this paper, when ξ is a discrete design measure, we denote it as a two-row table. The first row of the table represents design support points, and the second represents design allocations which are the proportions of the sample units allocated to the corresponding design support points. For instance, below is a design with l support points:

$$\xi = \begin{pmatrix} t_1 & t_2 & \ldots & t_l \\ w_1 & w_2 & \ldots & w_l \end{pmatrix},$$

with $w_i \geq 0$, and $\sum_{i=1}^{l} w_i = 1$.

In general, we let F_ξ be the distribution function of a design ξ, and define $\mathbf{M}(\xi) = \int_I \mathbf{f}(t)\mathbf{f}(t)^T dF_\xi(t)$. For any linear model with a design matrix $\mathbf{X}$, we have $\mathbf{M}(\xi) = \frac{1}{n}(\mathbf{X}^T\mathbf{X})$; thus, the classical D-optimal design problem is to find an optimal design so that the determinant of $\mathbf{M}^{-1}(\xi)$ can be as small as possible.

In this paper, we first investigate the construction of optimal designs for estimating parameter subsystems in Model (1). In particular, we are interested in the D-optimal design problems for estimating the coefficients pairs $\{\beta_{2i_1}, \beta_{2i_2}\}$ and $\{\beta_{2j_1-1}, \beta_{2j_2-1}\}$, where $i_1, i_2 \in \{0, \ldots, m\}$ and $j_1, j_2 \in \{1, \ldots, m\}$. The precision in estimating such specific pairs of coefficients is important in many biological applications; see Younker and Ehrlich (1977) and Currie et al. (2000), for example. Younker and Ehrlich (1977) have used Fourier expansion for two-dimensional shape analysis. They have revealed that "Fourier analysis in a closed form provides a highly efficient method for measuring overall morphological similarity and identifying specific types of morphological variation". In two-dimensional shape analysis, the shape can be described by a series of terms in a Fourier expansion, where one or two coefficients have a concrete biological interpretation and require particular precision in their estimation. Please also see Dette et al. (2009) (named DMS hereafter) and other references therein for the motivation of optimally designing experiments for estimating such coefficient pairs in a Fourier model.

The problem of constructing optimal designs for the estimation of particular coefficients for Model (1) has been investigated in Dette and Melas (2002, 2003), and Dette et al. (2002, 2007). These authors have also indicated that uniform designs are optimal for estimating a subset of the coefficients $\{\beta_{2j_1-1}, \beta_{2j_1}, \ldots, \beta_{2j_2-1}, \beta_{2j_2}\}$, where $1 < j_1 < \cdots < j_2 < m$.

An overview of the design of statistical experiments is presented in Draper and Pukelsheim (1996). The D-optimal designs for estimating the full parameter set in a Fourier regression on a full or partial circle have been examined by Dette et al. (2002) (named DMP hereafter) whereas L-optimal (defined in Sect. 2) designs for estimating a pair of coefficients on a full circle are derived by DMS. Both studies are relevant to the present paper and so their results will be reviewed in detail in the next section. Most recently, Melas et al. (2014) have discussed the optimal choice of the number of empirical Fourier coefficients for comparison of two regression curves whereas Xu and Shang (2014) have studied the classical Q-optimal and minimax robust designs for (1). Among these studies, there are some remaining problems, including the D-optimal design for estimating pairs of coefficients in a Fourier regression model.

We note that both the present article and Xu and Shang (2014) discuss the optimal design problems for (1). However, Xu and Shang (2014) have mainly addressed Q-optimal designs when a prediction problem is targeted and therefore efficiency of estimating a function of all coefficients in the model is of interest whereas this present paper discusses both D-optimal designs for estimating certain coefficient pairs in (1) and D-optimal designs for estimating all coefficients in a reduced Fourier regression model.

We first study the optimal saturated design for estimating all parameters in (1) while the efficiency of estimating a specified pair (both coefficients of cosine terms or both coefficients of sine terms) can be maximized under D-optimality. Namely, we determine a saturated design by minimizing the determinant of the covariance matrix of these two coefficient estimators. In addition, there are many situations that require approximating a function with a certain property via a Fourier model. In such applications, some reduced Fourier regression models have to be utilized. Thus, D-optimal designs for an often-used reduced Fourier regression model will be discussed in the present study as well.

The arrangement for the rest of this paper is as follows: Sect. 2 provides the detailed reviews on previous results for D-optimal designs for estimating the full parameter set and L-optimal designs for estimating coefficient pairs in a full Fourier regression model; Sect. 3 derives our resulting D-optimal designs for estimating the pair of coefficients in a full Fourier regression model and also gives a comparison study between our resulting designs and the L-optimal designs obtained by DMS; and Sect. 4 discusses the optimal designs for Fourier regression models with a reduced form, provides the algorithm of deriving the D-optimal designs for such reduced model, and presents a comparison study on the efficiencies of our resulting designs.

2 Reviews on previous results

DMP has investigated the D-optimal design problem for estimating the full parameter set in Model (1), where the design space is a partial or full circle, $[-a, a]$, with $0 < a \leq \pi$.

For uncorrelated observations, the covariance matrix of the least squares estimator for the parameter $\boldsymbol{\beta}$ is proportional to the inverse of the information matrix, where the information matrix is given by

$$\mathbf{M}(\xi) = \int \mathbf{f}(t)\mathbf{f}(t)^T dF_\xi(t) \in \mathbb{R}^{(2m+1)\times(2m+1)}. \tag{2}$$

DMP has provided a solution of the D-optimal design problem which maximizes the determinant of (2) for Model (1) on the design space $[-a,\ a]$. DMP has obtained

$$\det \mathbf{M}(\xi) = \frac{2^{2m^2}}{(2m+1)^{2m+1}} \prod_{i=1}^{m} \left(1 - x_i^2\right)(1 - x_i)^2 \prod_{1\le i<j\le m} \left(x_j - x_i\right)^4,$$

with $x_i = \cos(t_i)$ $(i = 1, \ldots, m)$, and constructed the following:

(i) If $a \ge \pi(1 - 1/(2m+1))$, the D-optimal design with equal allocations is having $2m+1$ support points at

$$0 \text{ and } t_i = \pm 2\pi \frac{i}{2m+1}, \quad i = 1, \ldots, m.$$

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

$$\xi^* = \begin{pmatrix} -a & -a\tau^*_{m-1}(a) & \cdots & -a\tau^*_1(a) & 0 & a\tau^*_1(a) & \cdots & a\tau^*_{m-1}(a) & a \\ \frac{1}{2m+1} & \frac{1}{2m+1} & \cdots & \frac{1}{2m+1} & \frac{1}{2m+1} & \frac{1}{2m+1} & \cdots & \frac{1}{2m+1} & \frac{1}{2m+1} \end{pmatrix},$$

where τ^*_i is a real analytic function defined as $\tau^*_i(a) = \dfrac{\arccos x^*_i}{a}$, $i = 1, \ldots, m-1$, where x^*_i is the ith element of the unique solution $\mathbf{x}^*$—a $(m-1)$ dimensional vector—which maximizes function

$$\phi(\mathbf{x},\ a) = \prod_{i=1}^{m} \left(1 - x_i^2\right)(1 - x_i)^2 \prod_{1\le i\le j\le m} \left(x_j - x_i\right)^4,$$

over $\mathbf{x} \in \chi = \{(x_1, \ldots, x_{m-1})^T | x_i = \cos(a\tau_i),\ i = 1, \ldots, m-1\}$ and $x_m = \cos(a)$.

On the other hand, using Theorem 7.20 in Pukelsheim (1993), Dette et al. (2007) have shown that for any $n \ge 2m+1$, a design that assigns equal allocation $1/n$ to each of n equispaced support points $(\alpha + 2j\pi/n) \bmod 2\pi$, $j = 1, \ldots, n$, with $\alpha \in [0,\ 2\pi)$ is Φ_p-optimal for the estimation of a subset of the coefficients $\{\beta_{2i_1-1},\ \beta_{2i_1}, \ldots, \beta_{2i_r-1},\ \beta_{2i_r}\}$, where $1 \le i_1 < \cdots < i_r \le m$, $r \in \{1, \ldots, m\}$, in Model (1) when $I = [0,\ 2\pi]$. This result has provided a general solution to the optimal design problem for the estimation of $\{\beta_{2i-1},\ \beta_{2i}\}$, where $i = 1, \ldots, m$.

DMS has also constructed the L-optimal design (with $\mathbf{e}_k$ being the kth unit vector and L matrix being $\mathbf{e}_{2i_1}\mathbf{e}^T_{2i_1} + \mathbf{e}_{2i_2}\mathbf{e}^T_{2i_2}$ and $\mathbf{e}_{2j_1-1}\mathbf{e}^T_{2j_1-1} + \mathbf{e}_{2j_2-1}\mathbf{e}^T_{2j_2-1}$, respectively) for estimating pairs of coefficients $\{\beta_{2i_1},\ \beta_{2i_2}\}$ and $\{\beta_{2j_1-1},\ \beta_{2j_2-1}\}$, where $i_1,\ i_2 \in \{0, \ldots, m\}$ and $j_1,\ j_2 \in \{1, \ldots, m\}$. We define the notation of $\lfloor\cdot\rfloor$ as the floor function mapping a real number to the largest previous integer. For several special coefficient pairs (but not all) they obtained explicit L-optimal designs, which can be expressed as follows:

(iii) When $m > 3$, the design

$$\xi^*_{(2\lfloor \frac{m}{2} \rfloor-1,\,4\lfloor \frac{m}{2} \rfloor-1)} = \begin{pmatrix} -t_n & -t_{n-1} & \cdots & -t_1 & t_1 & \cdots & t_{n-1} & t_n \\ \frac{1}{2n} & \frac{1}{2n} & \cdots & \frac{1}{2n} & \frac{1}{2n} & \cdots & \frac{1}{2n} & \frac{1}{2n} \end{pmatrix},$$

with

$$n = 2\left\lfloor \frac{m}{2} \right\rfloor, \quad x = \frac{2\arctan(\sqrt[4]{5})}{n}, \quad \text{and} \quad t_i = 2\left\lfloor \frac{i}{2} \right\rfloor \frac{\pi}{n} + (-1)^{(i-1)}x,$$

is L-optimal for estimating $\left\{\beta_{2\lfloor \frac{m}{2} \rfloor-1},\ \beta_{4\lfloor \frac{m}{2} \rfloor-1}\right\}$.

(iv) For any $\alpha \in [0,\ w_n]$, the design

$$\xi^*_{(2\lfloor \frac{m}{2} \rfloor,\,4\lfloor \frac{m}{2} \rfloor)} = \begin{pmatrix} -\pi & -t_{n-1} & \cdots & -t_1 & 0 & t_1 & \cdots & t_{n-1} & \pi \\ w_n-\alpha & w_{n-1} & \cdots & w_1 & w_0 & w_1 & \cdots & w_{n-1} & \alpha \end{pmatrix},$$

with

$$n = 2\left\lfloor \frac{m}{2} \right\rfloor, \quad t_i = \frac{(i-1)\pi}{n}, \quad i = 2, \ldots, n,$$
$$w_0 = \sqrt{5}w_1, \quad w_1 = \frac{\sqrt{5}-1}{4n}, \quad \text{and} \quad w_i = w_{i-2}, \quad i = 2, \ldots, n,$$

is L-optimal for estimating $\left\{\beta_{2\lfloor \frac{m}{2} \rfloor},\ \beta_{4\lfloor \frac{m}{2} \rfloor}\right\}$.

(v) The L-optimal design for estimating $\left\{\beta_0,\ \beta_{2\lfloor \frac{m}{2} \rfloor}\right\}$ coincides with $\xi^*_{(2\lfloor \frac{m}{2} \rfloor,\,4\lfloor \frac{m}{2} \rfloor)}$ in (iv).

We note that the explicit solutions above have partially solved the L-optimal design problem for estimating coefficient pairs. However, the full solution for such a problem remains. In addition, L-optimality does not account for the correlations between the estimators for the coefficient pairs. The following section will tackle this open problem under the D-optimality criterion that will take these correlations into consideration in the design construction.

3 D-optimal designs for full Fourier regression models

3.1 D-optimal designs for estimation of coefficient pairs

With a full circle design space, DMP has shown that if the set of designs cannot make the directional derivative of the function $\xi \longrightarrow \log\det \mathbf{M}(\xi)$ equal to zero for all $t \in [-\pi,\ \pi]$, then all allocations of the D-optimal design have to be equal. We note that the directional derivative referred here is the Fréchet derivative of $\log\det \mathbf{M}$ at ξ in the direction of η, and it is defined as

$$\lim_{\alpha\to 0} \frac{1}{\alpha}\{\log\det \mathbf{M}[(1-\alpha)\xi + \alpha\eta] - \log\det \mathbf{M}(\xi)\};$$

see Sect. 3.5 of Silvey (1980) for details. Moreover, if ξ is D-optimal, it is easy to see that ξ', the reflection of ξ at the origin, is also D-optimal. The concavity of the D-criterion implies that the symmetric design $\xi^* = (\xi + \xi')/2$ is also D-optimal for the Fourier regression, where the notation of $(\xi + \xi')/2$ is the average over two designs ξ and ξ'. This "average" operation can be taken by two steps: first add the reflected values of the design support points of each of ξ and ξ' if they are not symmetric around the origin so that each design is modified to be symmetrical around the origin for its first row, and these added support points have allocation of zero; then carry the same operation as a matrix average, namely, after the first step modification each element of $(\xi + \xi')/2$ is the average of the corresponding elements in ξ and ξ'.

Therefore in this section, we seek optimal designs in the set of symmetric designs on $[-\pi, \pi]$ that have support points 0 and $\pm t_i$ $(i = 1, \ldots, m)$ with equal allocations.

Consider Model (1) with $I = [-\pi, \pi]$, for a symmetric design ξ after an appropriate permutation $\mathbf{P} \in \mathbb{R}^{(2m+1)\times(2m+1)}$ of the order of the regression functions, the information matrix (2) will be transformed to a block diagonal matrix. According to DMP, this transformation can be expressed as

$$\widetilde{\mathbf{M}}(\xi) = \mathbf{P}\mathbf{M}(\xi)\mathbf{P}^T = \begin{pmatrix} \mathbf{M}_c(\xi) & \mathbf{0} \\ \mathbf{0} & \mathbf{M}_s(\xi) \end{pmatrix}$$

with the blocks given by

$$\mathbf{M}_c(\xi) = \left(\int_{-\pi}^{\pi} \cos(it)\cos(jt)dF_\xi(t)\right)_{i,j=0}^{m} \in \mathbb{R}^{(m+1)\times(m+1)},$$

and

$$\mathbf{M}_s(\xi) = \left(\int_{-\pi}^{\pi} \sin(it)\sin(jt)dF_\xi(t)\right)_{i,j=1}^{m} \in \mathbb{R}^{m\times m}.$$

It is easy to show that $\det(\mathbf{M}(\xi)) = \det(\widetilde{\mathbf{M}}(\xi)) = \det(\mathbf{M}_c(\xi)) \cdot \det(\mathbf{M}_s(\xi))$, and hence $\det(\mathbf{M}^{-1}(\xi)) = \det(\widetilde{\mathbf{M}}^{-1}(\xi)) = \det(\mathbf{M}_c^{-1}(\xi)) \cdot \det(\mathbf{M}_s^{-1}(\xi))$.

Taking n $(\geq 2m+1)$ uncorrelated observations, the design matrix $\mathbf{X}$ can be expressed as

$$\mathbf{X} = \begin{pmatrix} 1 & \sin t_1 & \cos t_1 & \cdots & \sin(mt_1) & \cos(mt_1) \\ 1 & \sin t_2 & \cos t_2 & \cdots & \sin(mt_2) & \cos(mt_2) \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & \sin t_n & \cos t_n & \cdots & \sin(mt_n) & \cos(mt_n) \end{pmatrix}_{n\times(2m+1)}.$$

Since $\mathbf{M} = \frac{1}{n}(\mathbf{X}^T\mathbf{X})$, after the permutation transformation with $\mathbf{P}$, matrix $\mathbf{X}^T\mathbf{X}$ becomes block diagonal with the form

$$\widetilde{\mathbf{X}^T\mathbf{X}} = \mathbf{P}\left(\mathbf{X}^T\mathbf{X}\right)\mathbf{P}^T = \begin{pmatrix} n\mathbf{M}_c(\xi) & \mathbf{0} \\ \mathbf{0} & n\mathbf{M}_s(\xi) \end{pmatrix}.$$

More importantly, its determinant does not change. Therefore, the inverse of $\widetilde{\mathbf{X}^T\mathbf{X}}$ can be written as

$$\widetilde{\mathbf{X}^T\mathbf{X}}^{-1} = \begin{pmatrix} \frac{1}{n}\mathbf{M}_c^{-1}(\xi) & \mathbf{0} \\ \mathbf{0} & \frac{1}{n}\mathbf{M}_s^{-1}(\xi) \end{pmatrix}.$$

In order to solve the D-optimal design problems for estimating the pairs $\{\beta_{2k},\ \beta_{2l}\}$ and $\{\beta_{2k-1},\ \beta_{2l-1}\}$, $0 \le k < l \le m$, we direct our attention to obtaining the determinant of $\mathrm{Cov}(\hat{\beta}_{2k},\ \hat{\beta}_{2l})$ and $\mathrm{Cov}(\hat{\beta}_{2k-1},\ \hat{\beta}_{2l-1})$.

Assuming that the blocked matrix

$$\mathbf{A} = \begin{pmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{pmatrix}, \tag{3}$$

is symmetric and invertible, by the well-known Frobenius formula (see for example, Theorem 2.2, P42 in Zhang 1999), we have

$$\begin{aligned} \det(\mathbf{A}) &= \det(\mathbf{A}_{11}) \cdot \det\left(\mathbf{A}_{22} - \mathbf{A}_{21}\mathbf{A}_{11}^{-1}\mathbf{A}_{12}\right) \\ &= \det(\mathbf{A}_{22}) \cdot \det\left(\mathbf{A}_{11} - \mathbf{A}_{12}\mathbf{A}_{22}^{-1}\mathbf{A}_{21}\right), \end{aligned}$$

and

$$\mathbf{A}^{-1} = \begin{pmatrix} \mathbf{A}_{11}^{-1} + \mathbf{A}_{11}^{-1}\mathbf{A}_{12}\mathbf{B}^{-1}\mathbf{A}_{21}\mathbf{A}_{11}^{-1} & -\mathbf{A}_{11}^{-1}\mathbf{A}_{12}\mathbf{B}^{-1} \\ -\mathbf{B}^{-1}\mathbf{A}_{21}\mathbf{A}_{11}^{-1} & \mathbf{B}^{-1} \end{pmatrix},$$

with $\mathbf{B} = \mathbf{A}_{22} - \mathbf{A}_{21}\mathbf{A}_{11}^{-1}\mathbf{A}_{12}$. Hence, matrix $n\mathbf{M}_c$ can be partitioned into four blocks as in (3), where

$$\mathbf{A}_{11} = \begin{pmatrix} n & \sum_{i=1}^n \cos t_i & \cdots & \sum_{i=1}^n \cos(mt_i) \\ \sum_{i=1}^n \cos t_i & \sum_{i=1}^n \cos^2 t_i & \cdots & \sum_{i=1}^n \cos t_i \cos(mt_i) \\ \vdots & \vdots & \ddots & \vdots \\ \sum_{i=1}^n \cos((k-1)t_i) & \sum_{i=1}^n \cos t_i \cos((k-1)t_i) & \cdots & \sum_{i=1}^n \cos((k-1)t_i)\cos(mt_i) \\ \sum_{i=1}^n \cos((k+1)t_i) & \sum_{i=1}^n \cos t_i \cos((k+1)t_i) & \cdots & \sum_{i=1}^n \cos((k+1)t_i)\cos(mt_i) \\ \vdots & \vdots & \ddots & \vdots \\ \sum_{i=1}^n \cos((l-1)t_i) & \sum_{i=1}^n \cos t_i \cos((l-1)t_i) & \cdots & \sum_{i=1}^n \cos((l-1)t_i)\cos(mt_i) \\ \sum_{i=1}^n \cos((l+1)t_i) & \sum_{i=1}^n \cos t_i \cos((l+1)t_i) & \cdots & \sum_{i=1}^n \cos((l+1)t_i)\cos(mt_i) \\ \vdots & \vdots & \ddots & \vdots \\ \sum_{i=1}^n \cos(mt_i) & \sum_{i=1}^n \cos t_i \cos(mt_i) & \cdots & \sum_{i=1}^n \cos^2(mt_i) \end{pmatrix}, \quad \text{and}$$

$$\mathbf{A}_{22} = \begin{pmatrix} \sum_{i=1}^n \cos^2(kt_i) & \sum_{i=1}^n \cos(kt_i)\cos(lt_i) \\ \sum_{i=1}^n \cos(kt_i)\cos(lt_i) & \sum_{i=1}^n \cos^2(lt_i) \end{pmatrix}.$$

This implies

$$\det\left(\mathrm{Cov}\left(\hat{\beta}_{2k},\ \hat{\beta}_{2l}\right)\right) = \det\left(\mathbf{A}_{22} - \mathbf{A}_{21}\mathbf{A}_{11}^{-1}\mathbf{A}_{12}\right)^{-1} = \frac{\det(\mathbf{A}_{11})}{\det(n\mathbf{M}_c)}$$
$$= \frac{1}{2^{m^2}} \frac{\det(\mathbf{A}_{11})}{\prod_{i=1}^{m}(1-\cos t_i)^2 \prod_{1\le i<j\le m}(\cos t_j - \cos t_i)^2}.$$

For the pairs corresponding to sine terms, we let $\tilde{\mathbf{A}}_{11}$ represent the $(m-2)\times(m-2)$ submatrix of $n\mathbf{M}_s$ with its kth, lth rows and kth, lth columns being removed, and

$$\tilde{\mathbf{A}}_{22} = \begin{pmatrix} \sum_{i=1}^{n}\sin^2(kt_i) & \sum_{i=1}^{n}\sin(kt_i)\sin(lt_i) \\ \sum_{i=1}^{n}\sin(kt_i)\sin(lt_i) & \sum_{i=1}^{n}\sin^2(lt_i) \end{pmatrix}_{2\times 2}$$

be the 2×2 submatrix of $n\mathbf{M}_s$ only containing the elements at its kth, lth rows and kth, lth columns. Similarly, we have

$$\det\left(\mathrm{Cov}\left(\hat{\beta}_{2k-1},\ \hat{\beta}_{2l-1}\right)\right) = \frac{1}{2^{m^2}} \frac{\det(\tilde{\mathbf{A}}_{11})}{\prod_{i=1}^{m}(1-\cos^2 t_i) \prod_{1\le i<j\le m}(\cos t_j - \cos t_i)^2}.$$

For instance, when $m = 2$,

$$\det\left(\mathrm{Cov}\left(\hat{\beta}_{2k},\ \hat{\beta}_{2l}\right)\right) = \frac{\sum_{i=1}^{n}\cos^2(ht_i)}{16(1-\cos t_1)^2(1-\cos t_2)^2(\cos t_1 - \cos t_2)^2}, \tag{4}$$

and

$$\det\left(\mathrm{Cov}\left(\hat{\beta}_{2k-1},\ \hat{\beta}_{2l-1}\right)\right) = \frac{1}{16(1-\cos^2 t_1)(1-\cos^2 t_2)(\cos t_1 - \cos t_2)^2},$$

with an integer h, satisfying $0 \le h \le 2$ and $h \ne k,\ l$. When $m = 3$,

$$\det\left(\mathrm{Cov}\left(\hat{\beta}_{2k},\ \hat{\beta}_{2l}\right)\right)$$
$$= \frac{\left(\sum_{i=1}^{n}\cos^2(gt_i)\right)\left(\sum_{i=1}^{n}\cos^2(ht_i)\right) - \left(\sum_{i=1}^{n}\cos(gt_i)\cos(ht_i)\right)^2}{64\prod_{i=1}^{3}(1-\cos t_i)^2\prod_{1\le i<j\le 3}(\cos t_j - \cos t_i)^2}, \tag{5}$$

and

$$\det\left(\mathrm{Cov}\left(\hat{\beta}_{2k-1},\ \hat{\beta}_{2l-1}\right)\right) = \frac{\sum_{i=1}^{n}\sin^2(ht_i)}{64\prod_{i=1}^{3}(1-\cos^2 t_i)\prod_{1\le i<j\le 3}(\cos t_j - \cos t_i)^2}, \tag{6}$$

with integers g and h, satisfying $0 \le g,\ h \le 2$ and $g,\ h \ne k,\ l$.

It is difficult to determine the general analytic results for a large m. Nevertheless, in the case of m being large, we can find D-optimal design for estimating coefficient pairs numerically in order to minimize $\det(\mathrm{Cov}(\hat{\beta}_{2k},\ \hat{\beta}_{2l}))$ or $\det(\mathrm{Cov}(\hat{\beta}_{2k-1},\ \hat{\beta}_{2l-1}))$. We will present analytic results for $m \leq 3$ in Sect. 3.2 and some numerical results for $m > 3$ in Sect. 3.3.

3.2 D-optimal designs obtained for $m \leq 3$

In this subsection, we search for D-optimal symmetric design with equal mass and $2m + 1$ support points for Model (1) on $[-\pi, \pi]$ when $m \leq 3$. We let $-t_m, -t_{m-1}, \ldots, -t_1, 0, t_1, \ldots, t_{m-1}, t_m$ be the support points, with $0 < t_1 < t_2 < \cdots < t_m \leq \pi$, and let $\xi^*_{(i,k)}$ be a D-optimal design for estimating the pair $\{\beta_i, \beta_k\}$.

When $m = 1$, the design support points are: $-t$, 0, and t. Immediately, we derive $\det(\mathbf{X}^T\mathbf{X}) = 4\sin^2 t(\cos t - 1)^2$. Then, we construct D-optimal design on $[-\pi, \pi]$ for estimating $\{\beta_0, \beta_2\}$ in order to minimize $\det(Cov(\widehat{\beta}_0, \widehat{\beta}_2))$, where $\det(Cov(\widehat{\beta}_0, \widehat{\beta}_2)) \propto \frac{1}{2(\cos t - 1)^2}$. Consequently, the design

$$\xi^*_{(0,2)} = \begin{pmatrix} -\pi & 0 & \pi \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix},$$

is D-optimal for estimating $\{\beta_0, \beta_2\}$. We note that this result can be extended to the case when the design space is a partial circle $[-a, a]$, $0 < a \leq \pi$. In this situation, $t = a$ minimizes $\det(Cov(\widehat{\beta}_0, \widehat{\beta}_2))$. Therefore, a general D-optimal design is given by

$$\xi^*_{(0,2)} = \begin{pmatrix} -a & 0 & a \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix},$$

for any $0 < a \leq \pi$.

When $m = 2$, the design support points are: $-t_2, -t_1, 0, t_1, t_2$. Then, we have

$$\det(5\mathbf{M}_s) = 16\sin^2 t_1 \sin^2 t_2 (\cos t_1 - \cos t_2)^2,$$

and

$$\det(5\mathbf{M}_c) = 16(\cos t_1 - 1)^2 (\cos t_2 - 1)^2 (\cos t_1 - \cos t_2)^2.$$

The problem of finding a D-optimal design for estimating the coefficient pair $\{\beta_1, \beta_3\}$ is equivalent to maximizing the determinant of $\mathbf{M}_s$, namely,

$$\min \det\left(\mathrm{Cov}\left(\widehat{\beta}_1, \widehat{\beta}_3\right)\right) \Leftrightarrow \max \det(\mathbf{M}_s).$$

We maximize $\det(\mathbf{M}_s)$ over t_1 and t_2 with the restriction $0 < t_1 < t_2 \leq \pi$. Then, the resulting D-optimal design $\xi^*_{(1,3)}$ is given by

$$\xi^*_{(1,3)} = \begin{pmatrix} -\pi + t^* & -t^* & 0 & t^* & \pi - t^* \\ \frac{1}{5} & \frac{1}{5} & \frac{1}{5} & \frac{1}{5} & \frac{1}{5} \end{pmatrix},$$

where $t^* = \arctan\sqrt{2}$.

By the definitions of $\tilde{\mathbf{A}}_{11}$ and $\mathbf{A}_{11}$, for $m = 2$ we have $\tilde{\mathbf{A}}_{11} = 1$ and

$$\mathbf{A}_{11} = \sum_{i=1}^{n} \cos^2(ht_i),$$

with $0 \leq h \leq 2$ and $h \neq k,\ l$.

From (4), we then obtain

$$\det\left(\mathrm{Cov}\left(\widehat{\beta}_2,\ \widehat{\beta}_4\right)\right) = \frac{5}{16(\cos t_1 - 1)^2(\cos t_2 - 1)^2(\cos t_1 - \cos t_2)^2},$$

$$\det\left(\mathrm{Cov}\left(\widehat{\beta}_0,\ \widehat{\beta}_4\right)\right) = \frac{2\cos^2(t_1) + 2\cos^2(t_2) + 1}{16(\cos t_1 - 1)^2(\cos t_2 - 1)^2(\cos t_1 - \cos t_2)^2},$$

and

$$\det\left(\mathrm{Cov}\left(\widehat{\beta}_0,\ \widehat{\beta}_2\right)\right) = \frac{2\cos^2(2t_1) + 2\cos^2(2t_2) + 1}{16(\cos t_1 - 1)^2(\cos t_2 - 1)^2(\cos t_1 - \cos t_2)^2}.$$

Now, we maximize $\det(\mathrm{Cov}^{-1}(\widehat{\beta}_{2k},\ \widehat{\beta}_{2l}))$ over t_1 and t_2 with the restriction $0 < t_1 < t_2 \leq \pi$. In result, we obtain the following D-optimal designs:

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

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

and

$$\xi^*_{(0,2)} = \begin{pmatrix} -0.8137\pi & -0.3479\pi & 0 & 0.3479\pi & 0.8137\pi \\ \frac{1}{5} & \frac{1}{5} & \frac{1}{5} & \frac{1}{5} & \frac{1}{5} \end{pmatrix}.$$

When $m = 3$, the design support points are: $-t_3,\ -t_2,\ -t_1,\ 0,\ t_1,\ t_2,\ t_3$, where $0 < t_1 < t_2 < t_3 \leq \pi$. From (5), we can have

$$\det\left(\mathrm{Cov}\left(\hat{\beta}_4,\ \hat{\beta}_6\right)\right) = \frac{\begin{pmatrix} 2(\cos t_1 - \cos t_2)^2 + 2(\cos t_1 - \cos t_3)^2 + 2(\cos t_2 - \cos t_3)^2 \\ +(\cos t_1 - 1)^2 + (\cos t_2 - 1)^2 + (\cos t_3 - 1)^2 \end{pmatrix}}{64(\cos t_1 - 1)^2(\cos t_2 - 1)^2(\cos t_3 - 1)^2(\cos t_1 - \cos t_2)^2(\cos t_1 - \cos t_3)^2(\cos t_2 - \cos t_3)^2}.$$

By minimizing $\det(\mathrm{Cov}(\hat{\beta}_4,\ \hat{\beta}_6))$, a D-optimal design is found to be:

$$\xi^*_{(4,6)} = \begin{pmatrix} -\pi & -0.6422\pi & -0.3735\pi & 0 & 0.3735\pi & 0.6422\pi & \pi \\ \frac{1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{1}{7} & \frac{1}{7} \end{pmatrix}.$$

The D-optimal designs for other coefficient pairs can be constructed in a similar manner by minimizing either (5) or (6). Table 1 provides the support points of the

Table 1 The design support points for estimating $\{\beta_{2k},\ \beta_{2l}\}$ and $\{\beta_{2k-1},\ \beta_{2l-1}\}$ when $m = 2$ and 3

$m=2$	$\{\beta_0,\beta_2\}$	$\{\beta_0,\beta_4\}$	$\{\beta_2,\beta_4\}$				$\{\beta_1,\beta_3\}$		
t_1	0.3479π	$\pi/2$	$\pi/2$				$\arctan\sqrt{2}$		
t_2	0.8137π	π	π				$\pi-\arctan\sqrt{2}$		
$m=3$	$\{\beta_0,\beta_2\}$	$\{\beta_0,\beta_4\}$	$\{\beta_0,\beta_6\}$	$\{\beta_2,\beta_4\}$	$\{\beta_2,\beta_6\}$	$\{\beta_4,\beta_6\}$	$\{\beta_1,\beta_3\}$	$\{\beta_1,\beta_5\}$	$\{\beta_3,\beta_5\}$
t_1	0.2710π	0.2407π	0.3404π	0.3443π	0.3041π	0.3735π	0.3108π	0.1959π	0.2003π
t_2	0.6436π	0.5319π	0.6672π	0.5968π	0.6959π	0.6422π	0.3559π	0.5000π	0.5000π
t_3	π	0.8917π	π	π	π	π	0.6702π	0.8040π	0.8000π

Table 2 The design support points for estimating $\{\beta_{2k},\ \beta_{2l}\}$ and $\{\beta_{2k-1},\ \beta_{2l-1}\}$ when $m = 4$

Pairs	t_1	t_2	t_3	t_4	Pairs	t_1	t_2	t_3	t_4
$\{\beta_0,\beta_2\}$	0.20π	0.45π	0.70π	0.90π	$\{\beta_1,\beta_3\}$	0.20π	0.40π	0.60π	0.80π
$\{\beta_0,\beta_4\}$	0.20π	0.45π	0.65π	0.90π	$\{\beta_1,\beta_5\}$	0.20π	0.4667π	0.5333π	0.80π
$\{\beta_0,\beta_6\}$	0.25π	0.40π	0.65π	π	$\{\beta_1,\beta_7\}$	0.1333π	0.40π	0.60π	0.8667π
$\{\beta_0,\beta_8\}$	0.25π	0.50π	0.75π	π	$\{\beta_3,\beta_5\}$	0.20π	0.40π	0.60π	0.80π
$\{\beta_2,\beta_4\}$	0.15π	0.45π	0.65π	0.95π	$\{\beta_3,\beta_7\}$	0.1333π	0.3333π	0.6667π	0.8667π
$\{\beta_2,\beta_6\}$	0.05π	0.30π	0.70π	0.95π	$\{\beta_5,\beta_7\}$	0.1333π	0.40π	0.60π	0.8667π
$\{\beta_4,\beta_6\}$	0.35π	0.50π	0.65π	π					
$\{\beta_6,\beta_8\}$	0.30π	0.50π	0.75π	π					

D-optimal designs for all pairs of the coefficients corresponding to cosine terms and sine terms, respectively, when $m = 2$ and 3.

As a result, we have the following observation: (a) when $m = 2$, D-optimal designs for the estimation of pair $\{\beta_0,\ \beta_4\}$ and $\{\beta_2,\ \beta_4\}$ are precisely uniform, (b) when $m = 3$, some support points in $\xi^*_{(0,2)}$, $\xi^*_{(1,5)}$ and $\xi^*_{(3,5)}$ are closer to 0 while the support points in $\xi^*_{(1,3)}$ have two clusters around ± 1, each containing two design points, and they are relatively close to each other. It suggests that the experimenter can place relatively more experiment units at ± 1, (c) for $m = 3$, the D-optimal designs for the estimation of pairs $\{\beta_0,\ \beta_4\}$ and $\{\beta_0,\ \beta_6\}$ are more uniform than those for other pairs.

3.3 Resulting D-optimal designs for $m > 3$

When $m > 3$, the design support points of a D-optimal design for estimating any coefficient pair $\{\beta_{2k},\ \beta_{2l}\}$ or $\{\beta_{2k-1},\ \beta_{2l-1}\}$ cannot always be expressed explicitly; however, they can be obtained numerically in order to minimize $\det(\mathrm{Cov}(\hat{\beta}_{2k},\ \hat{\beta}_{2l}))$ or $\det(\mathrm{Cov}(\hat{\beta}_{2k-1},\ \hat{\beta}_{2l-1}))$. The support points of our resulting designs for $m = 4$ and 5 are provided in Tables 2 and 3, respectively. When $m = 4$, the D-optimal design support points for estimating pairs of $\{\beta_0,\ \beta_8\}$, $\{\beta_2,\ \beta_8\}$, and $\{\beta_4,\ \beta_8\}$ are the same. On the other hand, when $m = 5$ the D-optimal design support points for estimating pairs of $\{\beta_0,\ \beta_4\}$, $\{\beta_0,\ \beta_8\}$, and $\{\beta_4,\ \beta_8\}$ are the same, so do those for all the pairs involving β_0. The D-optimal design support points for estimating pairs of $\{\beta_1,\ \beta_3\}$ and $\{\beta_3,\ \beta_5\}$, and those for $\{\beta_1,\ \beta_7\}$ and $\{\beta_5,\ \beta_7\}$ are the same for both $m = 4$ and 5.

From Tables 1, 2, and 3, we can observe that the patterns of the design support points for $m > 3$ are very similar to those for $m \leq 3$ indicated by our remarks (a)–(c) in Sect. 3.2. We also note that, for all cases, the designs are more uniform whenever the pairs involve β_0.

Table 3 The design support points for estimating $\{\beta_{2k},\ \beta_{2l}\}$ and $\{\beta_{2k-1},\ \beta_{2l-1}\}$ when $m = 5$

Pairs	t_1	t_2	t_3	t_4	t_5	Pairs	t_1	t_2	t_3	t_4	t_5
$\{\beta_0, \beta_2\}$	0.15π	0.35π	0.60π	0.80π	0.95π	$\{\beta_1, \beta_3\}$	0.0625π	0.25π	0.50π	0.75π	π
$\{\beta_0, \beta_4\}$	0.25π	0.45π	0.55π	0.75π	π	$\{\beta_1, \beta_5\}$	0.1875π	0.375π	0.50π	0.625π	0.8125π
$\{\beta_0, \beta_6\}$	0.30π	0.35π	0.65π	0.70π	π	$\{\beta_1, \beta_7\}$	0.125π	0.375π	0.5625π	0.6875π	0.875π
$\{\beta_0, \beta_{10}\}$	0.20π	0.40π	0.60π	0.80π	π	$\{\beta_3, \beta_5\}$	0.1875π	0.25π	0.4375π	0.625π	0.8125π
$\{\beta_2, \beta_4\}$	0.15π	0.35π	0.55π	0.80π	0.95π	$\{\beta_3, \beta_7\}$	0.125π	0.375π	0.625π	0.75π	0.875π
$\{\beta_2, \beta_6\}$	0.15π	0.35π	0.65π	0.80π	π	$\{\beta_3, \beta_9\}$	0.125π	0.3125π	0.50π	0.6875π	0.875π
$\{\beta_2, \beta_8\}$	0.20π	0.30π	0.50π	0.75π	π	$\{\beta_5, \beta_7\}$	0.1875π	0.375π	0.50π	0.625π	0.8125π
$\{\beta_4, \beta_6\}$	0.30π	0.45π	0.60π	0.70π	π	$\{\beta_5, \beta_9\}$	0.125π	0.3125π	0.50π	0.6875π	0.875π
$\{\beta_4, \beta_8\}$	0.25π	0.45π	0.55π	0.75π	π	$\{\beta_7, \beta_9\}$	0.125π	0.3125π	0.50π	0.6875π	0.875π
$\{\beta_6, \beta_8\}$	0.25π	0.40π	0.60π	0.75π	π						

Table 4 Relative efficiencies

$m = 2$		$m = 3$			$m = 4$			$m = 5$		
$\{\beta_0, \beta_2\}$	$\{\beta_1, \beta_3\}$	$\{\beta_0, \beta_2\}$	$\{\beta_4, \beta_6\}$	$\{\beta_3, \beta_5\}$	$\{\beta_0, \beta_4\}$	$\{\beta_4, \beta_8\}$	$\{\beta_5, \beta_7\}$	$\{\beta_0, \beta_4\}$	$\{\beta_4, \beta_8\}$	$\{\beta_3, \beta_7\}$
1.0418	1.5598	1.0210	1.1079	1.1975	1.0292	1.1631	1.3616	1.1184	1.1057	1.5841

In order to access the performance of our resulting designs obtained for estimating coefficient pairs, we carry out a comparison study by taking $n = 55$ as an example. The efficiencies of our designs relative to the D-optimal designs obtained by DMP for estimating all coefficients in the model are provided in Table 4. For all the cases we have considered, the efficiencies of our resulting designs are at an average of 20 % higher than their competitors. We notice that when $2m + 1$ is not a divisor of n we arrange the design allocations so that the designs appear to be as symmetric as possible.

4 Optimal designs for reduced Fourier regression models

4.1 Introduction

The sawtooth wave (or saw wave) is one special type of non-sinusoidal waveform. It is named sawtooth based on its resemblance to the teeth on the blade of a saw. The sawtooth wave is capable of producing sound, and it often forms the foundation for music synthesizers; please see Bracewell (1986) for examples of its application.

A sawtooth wave on the interval $0 \le t \le \pi$ can be expressed by a piecewise linear function:

$$S(t) = \begin{cases} t & \text{if } 0 \le t \le \pi/2, \\ \pi - t & \text{if } \pi/2 < t \le \pi, \end{cases}$$

and extended to the interval $-\pi \le t \le 0$ as an even function. Its smoothed version can be approximated by a Fourier function which can be used for the audio frequency analysis.

For a simulation study, we generate a data set with sample size of 1000 from the model:

$$y(t) = S(t) + \varepsilon,$$

where t is generated from uniform distribution within $[-\pi,\ \pi]$, and $\varepsilon \sim N(0,\ 0.1)$.

Table 5 F-test results ($\alpha = 0.05,\ n = 1000$)

$df_1 = m$	$df_2 = n - 2m - 1$	Critical values	Average F-values	Average P-values	% <Critical values
2	995	3.00477	0.9275	0.395883	97
3	993	2.61387	0.8103	0.488231	99
6	987	2.10775	1.0193	0.411062	96
9	981	1.88941	0.9895	0.446845	98

Taking the symmetry of the data into account, it may be better to fit a simpler model which only contains cosine terms ($\beta_{2i-1} = 0$). Thus, we carry out an F-test: $\mathbf{H}_0$: $\beta_{2i-1} = 0$ for all $i = 1, \ldots, m$ versus $\mathbf{H}_a$: $\beta_{2i-1} \neq 0$ for some i. We use a full-and-reduced-model approach by first considering the full Model (1). However, under $\mathbf{H}_0$ being true, the model reduces to

$$y_j = \beta_0 + \sum_{k=1}^{m} \beta_k \cos(kt) + \varepsilon_j. \tag{7}$$

By Rencher (2000), we have

$$\frac{(SSR(\text{full}) - SSR(\text{reduced}))/m}{SSE/(n-2m-1)} \sim F(m,\ n-2m-1),$$

where SSR and SSE are the sum of squares due to regression and the sum of squares of errors, respectively. Then we obtain the following table by performing 100 tests for each of the different values of m. The test results are listed in Table 5.

Taking $m = 2$ as an example, by fitting Models (1) and (7), the least squares estimators are $\hat{\boldsymbol{\beta}}_{\mathbf{Full}} = (0.7497,\ 0.0021,\ -0.0987,\ 0.0005,\ -0.6617)^T$, and $\hat{\boldsymbol{\beta}}_{\mathrm{Re}} = (0.7493,\ -0.0938,\ -0.6553)^T$, respectively. These two fitted curves are shown in Fig. 1a together with the true sawtooth wave. It is observed that these two fitted curves are very much overlapped and both are not a good of fit. This is consistent with the result of $\mathbf{H}_0$ being accepted. Therefore, we will consider the reduced model in later discussion.

To illustrate the accuracy of the approximation, we plot the fitting curves using (7) for both $m = 2$ and 6 in Fig. 1b. We observe that the reduced Fourier approximation using $m = 6$ gives a much more accurate approximation of the sawtooth wave than using $m = 2$.

Our simulation results also reveal that the model fitting has not been improved by adding more terms to the full Fourier model. Therefore, the optimal design for the reduced model is desirable.

4.2 D-optimal designs for reduced models

In this subsection, we consider (7) which only contains cosine term regressors. According to the general equivalence theorem (Kiefer 1961), the variance function (as defined in Pukelsheim 1993) for a D-optimal design ξ^* should satisfy:

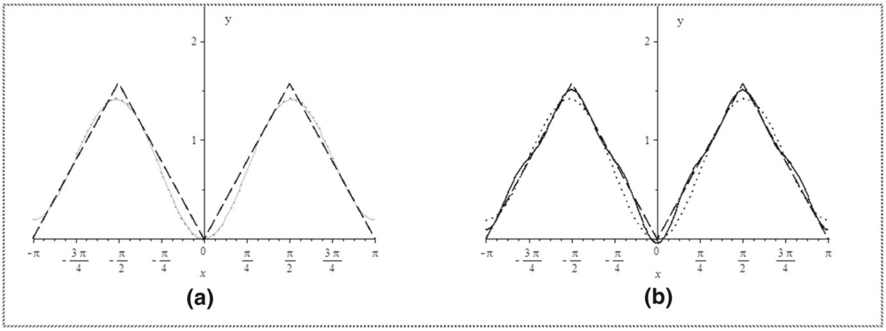

Fig. 1 Fitted curves using full and reduced models. For both **a** and **b**, *dash line* is used for the true sawtooth wave and *dotted line* is used for the reduced model fitting without sine terms, $m = 2$. **a** *Light solid line* is used for the full model fitting, and **b** *solid line* is the reduced model fitting without sine terms, $m = 6$

$$d(t, \xi^*) = \mathbf{f}^T(t)\mathbf{M}^{-1}\mathbf{f}(t) - (m+1) \leq 0,$$

with equality at the design support points. On the other hand, the importance of the reduced model can be perceived in its practical use for approximating an even function or a set of symmetric data. Thus, we now discuss the D-optimal design problem for (7).

Consider (7), with $t \in [-a, a]$, $0 < a \leq \pi$, where ε_i is under the same assumption as indicated in Sect. 1. Define $\boldsymbol{\beta}_c = (\beta_0, \beta_1, \ldots, \beta_m)^T$ as the vector of parameters in (7), and define

$$\mathbf{f}_c(t) = (1, \cos t, \cos(2t), \ldots, \cos(mt))^T,$$

as the regressor vector. For uncorrelated observations, the covariance matrix of the least squares estimator for $\boldsymbol{\beta}_c$ is proportional to the inverse of the information matrix

$$\mathbf{M}_c(\xi) = \left(\int_{-a}^{a} \cos(it)\cos(jt)dF_\xi(t)\right)_{i,j=0}^{m} \in \mathbb{R}^{(m+1)\times(m+1)}.$$

Since $\cos(it)$ is an even function, it is reasonable to only consider symmetric designs on a symmetric design space $[-a, a]$. DMP has also indicated that all allocations of a D-optimal design for a Fourier regression model have to be equal, so we search for D-optimal designs for (7) with the form

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

where $0 = t_0 < t_1 < \cdots < t_m = a$.

For the design

$$\xi_\eta = \begin{pmatrix} x_0 & x_1 & \cdots & x_m \\ \frac{1}{2m+1} & \frac{2}{2m+1} & \cdots & \frac{2}{2m+1} \end{pmatrix},$$

with $x_i = \cos t_i$, the corresponding information matrix has been derived by Dette and Haller (1998) as

$$\mathbf{M}_c\left(\xi_\eta\right) = \left(\int_{-1}^{1} T_i(x)T_j(x)dF_{\xi_\eta}(x)\right)_{i,j=0}^{m} \in \mathbb{R}^{(m+1)\times(m+1)},$$

where $T_i(x)$ are the Chebyshev polynomials of the first kind, defined by $T_i(x) = \cos(i \arccos x)$. Then, we have

$$\det\left(\mathbf{M}_c\left(\xi_\eta\right)\right) = \frac{2^{m^2}}{(2m+1)^{m+1}} \prod_{i=1}^{m}(1-x_i)^2 \prod_{1\le i<j\le m}\left(x_j - x_i\right)^2.$$

We let $\boldsymbol{\tau} = (\tau_1,\ldots,\tau_{m-1})^T$, $\mathbf{x} = (x_1,\ldots,x_{m-1})^T$, $\varphi(\mathbf{x}, a) = \prod_{i=1}^{m}(1 - x_i)^2 \prod_{1\le i<j\le m}(x_j - x_i)^2$, $T = \{\tau|0 < \tau_1 < \cdots < \tau_{m-1} < 1\}$, and $\chi = \{\mathbf{x}|x_i = \cos(a\tau_i),\ i = 1,\ldots,m-1,\ (\tau_1,\ldots,\tau_{m-1})^T \in T\}$. We notice that $x_m = \cos a$. By the transformation $t_i = a\tau_i = \arccos x_i$, $i = 1,\ldots,m-1$, $t_0 = 0$ and $t_m = a$, a design ξ can be uniquely determined by $\boldsymbol{\tau}$ or $\mathbf{x}$. Since $\varphi(\mathbf{x}, a)$ is a strictly concave function of $\mathbf{x} \in \chi$ for fixed a, it has a unique maximum $\mathbf{x}^*(a)$ in χ. We define a real function

$$\boldsymbol{\tau}^*\colon \begin{cases} [-\pi,\ \pi]\backslash\{0\} \to T, \\ a \to \boldsymbol{\tau}^*(a) = \left(\dfrac{\arccos x_1^*(a)}{a},\ldots,\dfrac{\arccos x_{m-1}^*(a)}{a}\right)^T, \end{cases} \tag{8}$$

for all $a \neq 0$. This definition of $\boldsymbol{\tau}^*$ can be extended to $a = 0$ by continuity.

Lemma 1 *The elements in $\boldsymbol{\tau}^*$, $\boldsymbol{\tau}_1^* < \cdots < \boldsymbol{\tau}_{m-1}^*$, are the positive roots of the polynomial*

$$P_{m-1}^{(1,1)}\left(1-2x^2\right) = \frac{2}{m+1}P_m'\left(1-2x^2\right),$$

where $P_{m-1}^{(1,1)}(x)$ is the $(m-1)$th Jacobi polynomial, and $P_m(x)$ is the mth Legendre polynomial.

The proof of Lemma 1 is provided in Appendix.

Remark 1 The result of Lemma 1 for Model (7) is an extension to the corresponding result for the full model, Model (1), stated in Lemma 3.2 in DMP.

Since $\mathbf{x}^*(a)$ is the unique solution of maximizing the strictly concave function $\varphi(\mathbf{x}, a)$, $\mathbf{x}^*(a)$ can be obtained by solving the equations

$$\frac{\partial\varphi(\mathbf{x},\ a)}{\partial x_i} = 0, \quad i = 1,\ldots,m-1.$$

Then, the following theorem can be attained.

Theorem 1 *Consider the regression Model (7) with $t \in [-a, a]$, $0 < a \le \pi$, the D-optimal design is given by*

$$\xi^*(a) = \begin{pmatrix} -a & -a\tau^*_{m-1}(a) & \cdots & -a\tau^*_1(a) & 0 & a\tau^*_1(a) & \cdots & a\tau^*_{m-1}(a) & a \\ \frac{1}{2m+1} & \frac{1}{2m+1} & \cdots & \frac{1}{2m+1} & \frac{1}{2m+1} & \frac{1}{2m+1} & \cdots & \frac{1}{2m+1} & \frac{1}{2m+1} \end{pmatrix}, \tag{9}$$

where τ^* is defined by (8), and $x^*_k(a)$ in (8) has a recursive formula:

$$x^*_k(a) = \frac{1}{2}\left(\cos(a) + 1 - \frac{2}{\sum_{i=1,i\neq k}^{m-1} \frac{1}{x^*_k - x_i}} + \sqrt{\cos^2(a) - 2\cos(a) + 1 + \frac{4}{\sum_{i=1,i\neq k}^{m-1} \frac{1}{x^*_k - x_i}}}\right). \tag{10}$$

We note that the expression in (10) can be explained further in Step (ii) of the computation algorithm provided in Sect. 4.3.

4.3 Algorithm and result

For a fixed value of a, we search for x_k ($k = 1, 2, \ldots, m-1$) within interval $[\cos a, 1]$, so that (10) can be satisfied for all k. The following steps can be taken:

(i) Initialize a starting design with $\mathbf{x} = \mathbf{x}^{(0)} = (x_1^{(0)}, x_2^{(0)}, \ldots, x_{m-1}^{(0)})^T$. For example, a uniform design can serve as a starting point.

(ii) Use the recursive formula (10) by substituting $x_2^{(0)}, \ldots, x_{m-1}^{(0)}$ in $\mathbf{x}^{(0)}$ to find $x_1^{(1)}$ and replace $x_1^{(0)}$ with $x_1^{(1)}$. Then use $x_1^{(1)}, x_3^{(0)}, \ldots, x_{m-1}^{(0)}$ to calculate $x_2^{(1)}$. Repeat this procedure to obtain $x_3^{(1)}, \ldots, x_{m-1}^{(1)}$ and then replace $x_3^{(0)}, \ldots, x_{m-1}^{(0)}$ with them. Finally we get the first round updated design point $\mathbf{x}^{(1)} = (x_1^{(1)}, x_2^{(1)}, \ldots, x_{m-1}^{(0)})^T$.

(iii) After the sth round ($s = 1, 2, \ldots$), we stop this process if $\max_k(|x_k^{(s)} - x_k^{(s-1)}|) < \delta$, for a predefined constant δ, is satisfied. Then, $\mathbf{x}^{(s)}$ is the final result. Otherwise, we repeat Steps (ii) and (iii).

Using the above algorithm, the D-optimal designs $\xi^*(a)$ for Model (7) can be obtained by (9) with $x^*_k(a)$ being the kth element of $x^{(s)}$. The Matlab code that generates D-optimal designs using this algorithm is also available upon request. The D-optimal designs for Model (7) are with equal allocations at their support points $-a, -a\tau^*_{m-1}(a), \ldots, -a\tau^*_1(a), 0, a\tau^*_1(a), \ldots, a\tau^*_{m-1}(a)$, and a. The resulting values of τ^*_i ($i = 1, \ldots, m-1$) attained for our D-optimal designs are listed in Table 6 for $m = 2$, 3, and 4 with various values of a. The design support points are plotted in Fig. 2. It seems that our D-optimal designs for the reduced model do not have the same form as the D-optimal designs obtained from Theorem 3.1 in DMP. We uncover that D-optimal designs for the reduced model are uniform only on the full circle (when $a = \pi$) and for all other cases the optimal support points are no longer uniformly scattered on its design space $[-a, a]$ when $a < \pi$.

Table 6 The resulting values of τ_i^* $(i = 1, \ldots, m-1)$ for our D-optimal designs

	$a = 1$	$a = \frac{1}{2}\pi$	$a = \frac{2}{3}\pi$	$a = \frac{4}{5}\pi$	$a = \pi$
$m = 2$	0.6917	$\pi/3$	0.4196π	0.4695π	$\pi/2$
$m = 3$	0.5092	0.2424π	0.3009π	0.3335π	0.3524π
	0.8404	0.4108π	0.5271π	0.6000π	0.6475π
$m = 4$	0.4010	0.1897π	0.2342π	0.2587π	0.2728π
	0.6919	0.3332π	0.4194π	0.4696π	0.5002π
	0.9026	0.4448π	0.5775π	0.6652π	0.7275π

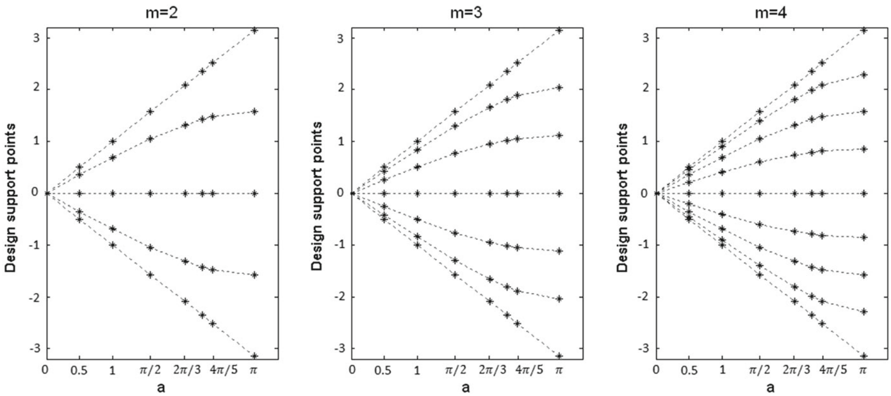

Fig. 2 Support points of our D-optimal designs for Model (7) for $m = 2$, 3, and 4 versus a, the half length of the design space $[-a, a]$

4.4 Comparisons

We compare our resulting D-optimal designs constructed for the reduced model with both D-optimal design obtained for the full model by DMP and uniform designs which has demonstrated to be optimal in Dette and Melas (2003). The loss function used here is the inverse of $\det(n\mathbf{M}_c)$. We denote L_O as the loss when our D-optimal design is adopted, and L_F and L_U as the losses when the optimal design for the full model and the uniform design (as in Wiens 1991) are adopted, respectively. Now, we use $eff_U = \frac{L_U}{L_O}$ representing the relative efficiency of our design relative to the uniform design, and $eff_F = \frac{L_F}{L_O}$ representing the relative efficiency of our design relative to the optimal design for the full model. The relative efficiencies are listed in Table 7 for various m and a.

We notice that the optimal designs constructed for a full Fourier regression model are not optimal any more for its reduced form. From Table 7, we can confirm that our designs have higher efficiency for all discussed cases compared to both uniform designs and D-optimal designs for the full form. For some cases, the efficiency gains are tremendous. Therefore, once the experimenter doubts (for instance, via proper testing such as the one indicated in Sect. 4.1 using previous data) the fitted model not

Table 7 Comparison among our designs, the uniform designs,and the DMP designs

	$a=1$	$a=\frac{1}{2}\pi$	$a=\frac{2}{3}\pi$	$a=\frac{4}{5}\pi$
$m=2$				
eff_U	1.6372	1.4571	1.26562	1.1216
eff_F	1.0537	1.0363	1.0119	1.0003
$m=3$				
eff_U	3.8854	2.8388	1.9341	1.3856
eff_F	1.0905	4.2814	518.723	26.6244
$m=4$				
eff_U	13.4236	7.4675	3.5992	1.8919
eff_F	1.1201	11.463	1.1807	1.2415

being the full model, the optimal designs for a reduced model should be considered. From our comparison analysis, we suspect that there also exists a " turning" point like the "a" in the way of Theorem 3.1 in DMP. This turning point should also be the threshold to determine whether or not our resulting designs have much higher efficiency. Further investigation on this turning point deserves future attention.

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Appendix: Proof of Lemma 1

Let $\mathbf{x}_\tau = (\cos(a\tau_1), \ldots, \cos(a\tau_{m-1}))^T$. The following expansion

$$\cos(t) = 1 - \frac{t^2}{2} + o\left(t^2\right),$$

implies that as $a \to 0$,

$$\varphi\left(\mathbf{x}_\tau,\ a\right) = \frac{a^{2m(m+1)}}{2^{m(m+1)}} \prod_{i=1}^{m} \left(\tau_i^2\right)^2 \prod_{1\le i<j\le m} \left(\tau_j^2 - \tau_i^2\right)^2 (1 + o(a));$$

then, $\lim_{a\to 0} \tau^*(a)$ exists and can be obtained by maximizing

$$\tilde{\varphi}(\tau) = \prod_{i=1}^{m-1} \left(\tau_i^2\right)^2 \left(1 - \tau_i^2\right)^2 \prod_{1\le i<j\le m-1} \left(\tau_j^2 - \tau_i^2\right)^2$$

over T defined in Sect. 4.2. Let $y_i = \tau_i^2 \in (0,\ 1)$. In order to maximize the following quantity,

$$\hat{\varphi}(y) = \prod_{i=1}^{m-1} y_i^2 \left(1 - y_i\right)^2 \prod_{1\le i<j\le m-1} \left(y_j - y_i\right)^2,$$

the conditions in (11)

$$\frac{\partial \log \hat{\varphi}(y)}{\partial y_i} = \frac{4}{y_i} + \sum_{j=1, j \neq i}^{m-1} \frac{4}{y_i - y_j} = 0, \quad i = 1, \ldots, m-1, \tag{11}$$

must be satisfied. Similar arguments as given in Fedorov (1972) show that the polynomial $\phi(y) = (y - y_1)(y - y_2), \ldots, (y - y_{m-1})$ satisfies the differential equation

$$y(1-y)\phi''(y)(2-4y)\phi'(y) + (m-1)(m+2)\phi(y) = 0. \tag{12}$$

It is well known that Eq. (12) has a unique solution given by the Jacobi polynomial $P_{m-1}^{(1,1)}(1-2y)$, and the lemma is now proved by transformation $y = \tau^2$. $\square$

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