An algorithm for calculating D-optimal designs for trigonometric regression through given points in terms of the discrete modified KdV equation

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An algorithm for calculating D-optimal designs for trigonometric regression through given points in terms of the discrete modified KdV equation

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Abstract. Optimal designs are required to make efficient statistical experiments. Calculation of D-optimal designs is considerably simplified by using canonical moments or trigonometric canonical moments. On the other hand, integrable systems are dynamical systems whose solutions can be written down concretely. In the previous paper, Sekido 2011, a method for calculating D-optimal designs for polynomial regression through a fix point is presented. In this paper, trigonometric regression models through given points are discussed. In order to calculate the D-optimal designs for these models, a useful relationship between trigonometric canonical moments and a class of discrete integrable systems is found. By using trigonometric canonical moments and a discrete integrable system, a new algorithm for calculating D-optimal designs for these models is proposed.

Keywords. D-optimal design, trigonometric canonical moment, trigonometric regression model, integrable system, discrete modified Korteweg-de Vries equation

1. Introduction

In this paper, we consider the D-optimal designs for trigonometric regression models. Optimal designs minimize a variance of estimator in some sense, when a statistical model is estimated. D-optimal designs correspond to an objective function of determinant form.

D-optimal designs for various models have been calculated [2, 3, 4, 5, 6, 8, 9, 10, 11, 12, 13, 14, 19, 20, 21, 24]. One of the methods for calculating or analyzing D-optimal designs is to use canonical moments or trigonometric canonical moments. However, in most cases, an explicit form of the D-optimal design is unknown. For example, D-optimal designs for this kind of models have been studied. The D-optimal designs for polynomial regression models with only odd (or even) degree terms is calculated in [3]. Polynomial regression models without intercept are considered in [11]. Polynomial regression models through origin are considered in [8].

On the other hand, the term *integrable system* is used for nonlinear dynamical systems whose solutions can be written down concretely. For Hamiltonian systems with finite degree of freedom, their integrability is defined in the Liouville-Arnold theorem [1]. However, even now, there is no mathematical definition of integrability for nonlinear systems with infinite degree of freedom. Integrable systems have been applied to numerical analysis. Typical examples are matrix eigenvalue algorithms [17, 22] in terms of the finite nonperiodic Toda equation, and algorithms for computing matrix singular values [23] in terms of the discrete Lotka-Volterra equation.

An intimate relationship between canonical moments and integrable systems is considered, and then an algorithm for calculating D-optimal designs for polynomial regression through a given point is proposed in [18]. In this paper, we consider *trigonometric regression* models with some prior information. An algorithm for calculating D-optimal designs for trigonometric regression through given points is proposed. Here, we begin with a new relationship between trigonometric canonical moments and determinant solutions of a certain discrete integrable system.

In Section 2, we give a brief review of trigonometric regression and its D-optimal designs. Section 2 enlightens that the D-optimal designs are characterized by their trigonometric canonical moments. In Section 3, an unexpected relationship between trigonometric canonical moments and a discrete integrable system is revealed, at first. Then, we formulate trigonometric regression through given points, and we propose an algorithm for calculating D-optimal designs for such trigonometric regression. A relationship between trigonometric canonical moments and discrete integrable systems plays an important role in the algorithm. Section 5 is devoted to conclusions.

2. Trigonometric regression and its D-optimal designs: A preliminary

This section explains the definition of trigonometric regression and its D-optimal designs. After that we give an introduction to trigonometric canonical moments.

Consider the common mth degree trigonometric regression models

$$Y = \sum_{k=0}^{m} c_k \cos(kx) + \sum_{k=1}^{m} s_k \sin(kx) + \varepsilon,$$

where c_k and s_k are unknown parameters, and ε is a random error term.

Let $\mathcal{P}_{[-\pi,\pi)}$ denote the set of all probability measures on the Borel sets of the interval $[-\pi, \pi)$. For given $\mu \in \mathcal{P}_{[-\pi,\pi)}$, let γ_k be the kth trigonometric moment given by

$$\gamma_k = \int_{-\pi}^{\pi} e^{-ikx} d\mu(x), \quad k = 0, \pm 1, \pm 2, \ldots.$$

The D-optimal designs are defined as probability measures in $\mathcal{P}_{[-\pi,\pi)}$ which maximize the determinant of the Fisher information matrix. It can be shown that the D-optimal designs $\mu \in \mathcal{P}_{[-\pi,\pi)}$ for trigonometric regression models are defined as the optimal solution of the optimization problem

$$\begin{aligned} &\text{maximize } T_{2m+1}(\mu) \\ &\text{subject to } \mu \in \mathcal{P}_{[-\pi,\pi)}, \end{aligned} \tag{1}$$

where $T_k(\mu)$ is the Toeplitz determinants of trigonometric moments such as

$$T_k(\mu) = |\gamma_{j-i}|_{i,j=0}^{k-1}. \tag{2}$$

A derivation of the optimization problem (1) is written in the book [7, Section 9] by Dette and Studden.

Now, we introduce trigonometric canonical moments. Trigonometric canonical moments $\{a_k\}_{k=1}^{N}$ is a finite or infinite sequence of complex numbers defined as normalized trigonometric moments. The kth trigonometric canonical moment is defined as the normalized kth trigonometric moment γ_k. In the finite case where $N < \infty$, trigonometric canonical moments satisfy

$$\begin{cases} |a_k| < 1, & k = 1, 2, \ldots, N-1, \\ |a_N| = 1. \end{cases} \tag{3}$$

Conversely, for a given arbitrary sequence $\{a_k\}_{k=1}^{N}$ which satisfies (3), there is a unique measure $\mu \in \mathcal{P}_{[-\pi,\pi)}$ which has the trigonometric canonical moments $\{a_k\}_{k=1}^{N}$.

It is to be noted that trigonometric canonical moments have a Toeplitz determinant expression

$$a_k = (-1)^{k-1} \frac{\tilde{T}_k}{T_k}, \tag{4}$$

where

$$\tilde{T}_k = |\gamma_{j-i+1}|_{i,j=0}^{k-1}.$$

Conversely, the Toeplitz determinant T_k can be expressed by using trigonometric canonical moments as

$$T_k = \prod_{j=1}^{k-1} (1 - |a_j|^2)^{k-j} \tag{5}$$

where $k = 1, 2, \ldots, N-1$.

The D-optimal designs for trigonometric regression models are characterized by the trigonometric canonical moments such that

$$a_k = 0, \quad k = 1, 2, \ldots, 2m.$$

It can be proved easily by using (5). Hence the trigonometric canonical moments help us to calculate the D-optimal designs.

See [7, Section 9], for more details about the definition and properties of trigonometric canonical moments.

3. D-optimal designs for the trigonometric regression through given points

In this section, we consider trigonometric regression models through given points. At first, we reveal a relationship between trigonometric canonical moments and a discrete integrable system in Subsection 3.1. Then we give the definition of the models and formulate their D-optimal designs in Subsection 3.2. Finally, we propose an algorithm for calculating the D-optimal designs by using trigonometric canonical moments and the discrete integrable system in Subsection 3.3.

3.1. Trigonometric canonical moments and discrete integrable system

We indicate a relationship between trigonometric canonical moments and a discrete integrable system, before considering trigonometric regression models through given points. Toeplitz determinants are related to both the integrable system and D-optimal designs. Furthermore, in some sense, generalized trigonometric canonical moments satisfy a class of discrete integrable system.

At first, we define a sequence of a linear combination of trigonometric moments. For given trigonometric moments γ_k, $k = 0, \pm 1, \pm 2, \ldots$ and an arbitrary real sequence $\lambda^{(t)}$, $t = 0, 1, 2, \ldots$, we define $\gamma_k^{(t)}$ by the recurrence formula

$$\begin{aligned} \gamma_k^{(0)} &= \gamma_k, \\ \gamma_k^{(t+1)} &= \gamma_{k+1}^{(t)} - 2\lambda^{(t)} + \gamma_{k-1}^{(t)}, \end{aligned} \tag{6}$$

where $k = 0, \pm 1, \pm 2, \ldots$, $t = 0, 1, 2, \ldots$. Let $T_k^{(t)}$ and $\tilde{T}_k^{(t)}$ be the Toeplitz determinant of $\gamma_k^{(t)}$, that is,

$$T_k^{(t)} = |\gamma_{j-i}^{(t)}|_{i,j=0}^{k-1}, \quad \tilde{T}_k^{(t)} = |\gamma_{j-i+1}^{(t)}|_{i,j=0}^{k-1}. \tag{7}$$

Then, we can prove the following proposition.

Proposition 1. Let $a_k^{(t)}$ be defined as

$$a_k^{(t)} = (-1)^{k-1} \frac{\tilde{T}_k^{(t)}}{T_k^{(t)}}. \tag{8}$$

Then $a_k^{(t)}$ satisfy the discrete modified Korteweg-de Vries (dmKdV, for short) equation

$$a_k^{(t+1)} = a_k^{(t)} - \frac{a_{k-1}^{(t+1)} - a_{k+1}^{(t)}}{a_1^{(t)} + 2\lambda^{(t)} + \overline{a}_1^{(t)}} \frac{\prod_{j=1}^{k}(1-|a_j^{(t)}|)^2}{\prod_{j=1}^{k-1}(1-|a_j^{(t+1)}|)^2} \quad (9)$$

where $k = 0, \pm 1, \pm 2, \ldots,\ \ t = 0, 1, 2, \ldots$.

Here, the dmKdV equation is one of discrete time integrable systems derived by [15] which is derived from the modified KdV equation through an integrable discritization. It it to be noted that Ref. [15] considers only the case where $\lambda^{(t)} = 0$. The value $\gamma_k^{(t)}$ defined by (6) is considered by [16] in terms of the discrete Schur flow. This proposition can be proved by a similar way to the case where $\lambda^{(t)} = 0$. We omit the details of the proof.

We call $a_k^{(t)}$ the generalized trigonometric canonical moments in this paper, since $a_k^{(0)} = a_k$. Here, Proposition 1 indicates that the trigonometric canonical moments a_k can be given from the determinant solution of the dmKdV equation (7) through $a_k = a_k^{(0)}$.

3.2. Formulation of trigonometric regression through given points

Here, let us consider trigonometric regression models through given points. Throughout this paper, given points means that we know values of $E(Y|x = \beta_k)$ as prior information, for some points $x = \beta_k$. Moreover, we consider the case where we know values of differential of $E(Y|x)$ additionally at the given points. The definition of the model is

$$Y = \sum_{k=0}^{m+S} c_k \cos kx + \sum_{k=1}^{m+S} s_k \sin kx + \varepsilon \quad (10)$$

with known values as prior information

$$\begin{aligned}
&h(\beta_0), \frac{dh}{dx}(\beta_0), \cdots, \frac{d^{b_0-1}h}{dx^{b_0-1}}(\beta_0),\\
&h(-\beta_0), \frac{dh}{dx}(-\beta_0), \cdots, \frac{d^{b_0-1}h}{dx^{b_0-1}}(-\beta_0),\\
&h(\beta_1), \frac{dh}{dx}(\beta_1), \cdots, \frac{d^{b_1-1}h}{dx^{b_1-1}}(\beta_1),\\
&h(-\beta_1), \frac{dh}{dx}(-\beta_1), \cdots, \frac{d^{b_1-1}h}{dx^{b_1-1}}(-\beta_1),\\
&\vdots,\\
&h(\beta_{l-1}), \frac{dh}{dx}(\beta_{l-1}), \cdots, \frac{d^{b_{l-1}-1}h}{dx^{b_{l-1}-1}}(\beta_{l-1}),\\
&h(-\beta_{l-1}), \frac{dh}{dx}(-\beta_{l-1}), \cdots, \frac{d^{b_{l-1}-1}h}{dx^{b_{l-1}-1}}(-\beta_{l-1}),
\end{aligned}$$

where

$\beta_0, \beta_1, \ldots, \beta_{l-1}$ are distinct positive numbers less than π,

$S = b_0 + b_1 + \cdots + b_{l-1}$ is a number of known values,

$$h(x) = E(Y|x) = \sum_{k=0}^{m+S} c_k \cos kx + \sum_{k=1}^{m+S} s_k \sin kx.$$

We denote the above trigonometric regression model as $\mathrm{TRM}_m(\beta, b)$, for short, where $\beta = (\beta_0, \beta_1, \ldots, \beta_{l-1}), b = (b_0, b_1, \ldots, b_{l-1})$. Note that we only consider the case where the given prior information is symmetric with respect to $x = 0$. We also note that some cases where the given prior information is not symmetric can be reduced to the above symmetric case by the transformation $y = x + \alpha$. For example, the case with given prior information $h(x)$ at $x = \beta_0, \beta_1$ can be reduced to $\mathrm{TRM}_m((|\beta_1 - \beta_2|/2), (1))$ by the transformation $y = x - (\beta_0 + \beta_1)/2$.

Let us formulate $\mathrm{TRM}_m(\beta, b)$ as a linear regression model. A linear regression model can be written as

$$\begin{aligned}
Y &= \theta^{\mathrm{T}} f(x) + \varepsilon\\
&= \begin{pmatrix}\theta_0 & \theta_1 & \cdots & \theta_{m-1}\end{pmatrix} \begin{pmatrix} f_0(x) \\ f_1(x) \\ \vdots \\ f_{m-1}(x) \end{pmatrix} + \varepsilon,
\end{aligned}$$

where $f(x) = (f_0(x), f_1(x), \ldots, f_{m-1}(x))^{\mathrm{T}}$ is a known vector of basis functions, and θ_k are unknown parameters. A trigonometric regression model through given points does not correspond to a linear regression model uniquely. However, we can define D-optimal designs for $\mathrm{TRM}_m(\beta, b)$ uniquely, since D-optimal designs depend only on the linear space spanned by the basis functions. (See [7, Theorem 5.5.1].) Therefore, we can consider that the linear regression model with a vector $Af(x)$ of basis functions is essentially the same as that with $f(x)$, if A is a real nonsingular matrix.

As the result of a formulation, we obtain the following theorem. A proof of this theorem is given in Appendix.

Theorem 1. The D-optimal design $\mu \in \mathcal{P}_{[-\pi,\pi)}$ for $\mathrm{TRM}_m(\beta, b)$, where $\beta = (\beta_0, \beta_1, \ldots, \beta_{l-1})$ denotes the given points, is described as the optimal solution of the optimization problem

$$\begin{aligned}
&\text{maximize } T_{2m+1}^{(2S)}(\mu)\\
&\text{subject to } \mu \in \mathcal{P}_{[-\pi,\pi)},
\end{aligned} \quad (11)$$

where the parameters $\lambda^{(t)}$ of (6) are chosen satisfying

$$\begin{aligned}
&\lambda^{(0)} = \lambda^{(1)} = \cdots = \lambda^{(2b_0-1)} = \cos\beta_0,\\
&\lambda^{(2b_0)} = \lambda^{(2b_0+1)} = \cdots = \lambda^{(2b_0+2b_1-1)} = \cos\beta_1,\\
&\vdots\\
&\lambda^{(2b_1+2b_2+\cdots+2b_{l-2})} = \lambda^{(2b_1+2b_2+\cdots+2b_{l-2}+1)} =\\
&\cdots = \lambda^{(2b_1+2b_2+\cdots+2b_{l-1}-1)} = \cos\beta_{l-1}.
\end{aligned}$$

3.3. Construction of the D-optimal designs for trigonometric regression through given points

As indicated in [13], D-optimal designs can be characterized by their trigonometric canonical moments. Moreover, considering trigonometric canonical moments, instead of trigonometric moments, simplify the set $\mathcal{P}_{[-\pi,\pi)}$ of feasible solutions of (11). Therefore, we propose a method for calculating an expression of the objective function $T_{2m+1}^{(2S)}(\mu)$ in terms of trigonometric canonical moments a_k. The following three formulas among the generalized trigonometric canonical moments $a_k^{(t)}$ and trigonometric moments γ_k can be used for our aims. The first formula is the dmKdV equation (9). The second formula is

$$T_k^{(t)} = \left(\gamma_0^{(t)}\right)^k \prod_{j=1}^{k-1} \left(1 - |a_j^{(t)}|\right)^{k-j}. \qquad (12)$$

This formula (12) can be derived from the definition (8) of the generalized trigonometric canonical moments. The third formula is

$$\gamma_0^{(t+1)} = \gamma_0^{(t)} \frac{(1 - |a_1^{(t)}|^2)(1 + a_2^{(t)})}{a_1^{(t+1)} - a_1^{(t)}}, \quad \gamma_0^{(0)} = 1. \qquad (13)$$

The second formula (12) and the third formula (13) are proved in Appendix.

The objective function $T_{2m+1}^{(2S)}(\mu)$ can be rephrased in terms of the generalized trigonometric canonical moments by using the second formula (12) and the third formula (13). Therefore, the generalized trigonometric canonical moments are rephrased in terms of trigonometric canonical moments through the dmKdV equation (9).

By putting it all together, it turns out that an expression of the objective function $T_{2m+1}^{(2S)}(\mu)$ in terms of trigonometric canonical moments can be obtained, for example, by using a computer algebra system. After obtaining the expression, we can calculate trigonometric canonical moments which maximize the objective function $T_{2m+1}^{(2S)}(\mu)$ numerically.

Note that trigonometric canonical moments can be a sequence of arbitrary complex numbers which satisfy $|a_k| \leq 1$. It is a bit complicated, however, there exists at least one D-optimal designs for $\mathrm{TRM}_m(\beta, b)$ whose all trigonometric canonical moments are real. This fact can be shown by using a convexity of the optimization problem, and using symmetricity of the model $\mathrm{TRM}_m(\beta, b)$. The D-optimal designs can be obtained by using Theorem 3.4.1 in the book [7] after trigonometric canonical moments are given, if trigonometric canonical moments are real.

By putting it all together, the algorithm for calculating D-optimal designs for $\mathrm{TRM}_m(\beta, b)$ is described as follows.

The algorithm for calculating D-optimal designs for $\mathrm{TRM}_m(\beta, b)$

Step 1. By using Theorem 1, describe the objective function $T_{2m+1}^{(2S)}$ in terms of $a_k^{(t)}$ and $\gamma_0^{(t)}$.

Step 2. By using the formulas (9), (12) and (13), describe the objective function $T_{2m+1}^{(2S)}$ in terms of trigonometric canonical moments a_k.

Step 3. Find trigonometric canonical moments which maximize the objective function $T_{2m+1}^{(2S)}$.

4. Examples

Let us consider the case where $m = 1, \beta = (\beta_0), b = (1)$, that is, we consider the model

$$Y = c_0 + c_1 \cos x + c_2 \cos 2x + s_1 \sin x + s_2 \sin 2x,$$

with two known values as prior information

$$c_0 + c_1 \cos \beta_0 + c_2 \cos 2\beta_0 + s_1 \sin \beta_0 + s_2 \sin \beta_0,$$
$$c_0 + c_1 \cos \beta_0 + c_2 \cos 2\beta_0 - s_1 \sin \beta_0 - s_2 \sin \beta_0.$$

The objective function corresponding to D-optimal designs for this model can be expressed in terms of trigonometric canonical moments by using the proposed algorithm, then we can find the trigonometric canonical moments numerically which maximize the objective function. The results for some β_0 are shown in Table 1.

5. Conclusions

In this paper, we first indicate a relationship between trigonometric canonical moments and a discrete integrable system. By using this relationship, we propose a new algorithm for calculating an expression of the Toeplitz determinant $T_k^{(2S)}$ in terms of trigonometric canonical moments a_k, where $T_k^{(2S)}$ is the objective function of the optimization problem (11). This algorithm enable us to calculate D-optimal designs for trigonometric regression models through given points.

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A. Appendix

A.1. The proof of Theorem 1

The optimization problem (1) corresponding to ordinary trigonometric regression is derived through a linear regression model with the vector of basis functions

$$f(x) = (e^{-imx}, e^{-i(m-1)x}, \ldots, e^{imx})^{\mathrm{T}}$$

or

$$f(x) = (1, \cos x, \ldots, \cos mx, \sin x, \sin 2x, \ldots, \sin mx)^{\mathrm{T}}.$$

On the other hand, it can turn out that the optimization problem (11) corresponding to $\mathrm{TRM}_m(\beta, b)$ corresponds to a vector of basis functions

$$f(x) = \prod_{j=0}^{l-1} (e^{-ix} - 2\cos\beta_j + e^{ix})^{b_j}$$
$$(e^{-imx}, e^{-i(m-1)x}, \ldots, e^{imx})^{\mathrm{T}}$$

β_0	a_k	D-optimal design
$\beta_0 = 0.451$ $\cos\beta_0 = 0.900$	$a_1 = 0.520$ $a_2 = -0.684$ $a_3 = 1.000$	$P(-1.287) = 0.333$ $P(0.000) = 0.333$ $P(1.287) = 0.333$
$\beta_0 = 0.644$ $\cos\beta_0 = 0.800$	$a_1 = 0.541$ $a_2 = -0.702$ $a_3 = 1.000$	$P(-1.225) = 0.333$ $P(0.000) = 0.333$ $P(1.225) = 0.333$
$\beta_0 = 0.795$ $\cos\beta_0 = 0.700$	$a_1 = 0.562$ $a_2 = -0.720$ $a_3 = 1.000$	$P(-1.219) = 0.333$ $P(0.000) = 0.333$ $P(1.219) = 0.333$
$\beta_0 = 0.927$ $\cos\beta_0 = 0.600$	$a_1 = 0.421$ $a_2 = -0.009$ $a_3 = -0.521$ $a_4 = 1.000$	$P(-3.141) = 0.136$ $P(-1.085) = 0.287$ $P(0.000) = 0.289$ $P(1.085) = 0.287$
$\beta_0 = 1.047$ $\cos\beta_0 = 0.500$	$a_1 = 0.194$ $a_2 = 0.480$ $a_3 = -1.000$	$P(-3.141) = 0.333$ $P(-0.659) = 0.333$ $P(0.659) = 0.333$
$\beta_0 = 1.159$ $\cos\beta_0 = 0.400$	$a_1 = 0.200$ $a_2 = 0.500$ $a_3 = -1.000$	$P(-3.141) = 0.333$ $P(-0.644) = 0.333$ $P(0.644) = 0.333$
$\beta_0 = 1.266$ $\cos\beta_0 = 0.300$	$a_1 = 0.267$ $a_2 = 0.521$ $a_3 = -1.000$	$P(-3.141) = 0.333$ $P(-0.626) = 0.333$ $P(0.626) = 0.333$
$\beta_0 = 1.369$ $\cos\beta_0 = 0.200$	$a_1 = 0.214$ $a_2 = 0.543$ $a_3 = -1.000$	$P(-3.141) = 0.333$ $P(-0.609) = 0.333$ $P(0.609) = 0.333$
$\beta_0 = 1.471$ $\cos\beta_0 = 0.100$	$a_1 = 0.221$ $a_2 = 0.567$ $a_3 = -1.000$	$P(-3.141) = 0.333$ $P(-0.589) = 0.333$ $P(0.589) = 0.333$
$\beta_0 = 1.521$ $\cos\beta_0 = 0.050$	$a_1 = 0.143$ $a_2 = 0.589$ $a_3 = -0.629$ $a_4 = -1.000$	$P(-2.834) = 0.197$ $P(-0.549) = 0.303$ $P(0.549) = 0.303$ $P(2.834) = 0.197$
$\beta_0 = 1.571$ $\cos\beta_0 = 0.000$	$a_1 = 0.000$ $a_2 = 0.600$ $a_3 = 0.000$ $a_4 = -1.000$	$P(-2.678) = 0.250$ $P(-0.464) = 0.250$ $P(0.464) = 0.250$ $P(2.678) = 0.250$
$\beta_0 = 1.621$ $\cos\beta_0 = -0.050$	$a_1 = -0.143$ $a_2 = 0.589$ $a_3 = 0.629$ $a_4 = -1.000$	$P(-2.592) = 0.303$ $P(-0.308) = 0.197$ $P(0.308) = 0.197$ $P(2.592) = 0.303$

Table 1: D-optimal designs for $\mathrm{TRM}_1((\beta_0),(1))$. The second column contains trigonometric canonical moments maximizing the objective function. The third column contains the support points and its weights of D-optimal designs, where $P(s) = w$ means the D-optimal design has support s whose weight is w.

or

$$f(x) = \prod_{j=0}^{l-1}(e^{-ix} - 2\cos\beta_j + e^{ix})^{b_j} \\ (1, \cos x, \ldots, \cos mx, \sin x, \sin 2x, \ldots, \sin mx)^{\mathrm{T}} \tag{14}$$

by simple calculation. See [7, Section 9] for detail.

Let $g_k(x)$ be the vector of functions

$$g_k(x) = (1, \cos x, \ldots, \cos kx, \sin x, \sin 2x, \ldots, \sin kx)^{\mathrm{T}}.$$

To prove Theorem 1, it suffices to show that $\mathrm{TRM}_m(\beta, b)$ corresponds to the vector of the basis functions (14). Moreover, according to the symmetricity of β and b, we should prove by the principle of induction only that $\mathrm{TRM}_m((\beta_0, \beta_1, \ldots, \beta_{l-1}), (b_0, b_1, \ldots, b_{l-1}))$ corresponds to the vector of the basis functions (14), under the assumption that $\mathrm{TRM}_{m+1}((\beta_0, \beta_1, \ldots, \beta_{l-1}), (b_0 - 1, b_1, \ldots, b_{l-1}))$ corresponds to the vector of the basis functions

$$f(x) = (e^{-ix} - 2\cos\beta_0 + e^{ix})^{b_0 - 1} \\ \left(\prod_{j=1}^{l-1}(e^{-ix} + 2\cos\beta_j + e^{ix})^{2b_j}\right) g_{m+1}(x). \tag{15}$$

Let $M(x) = \prod_{j=1}^{l-1}(e^{-ix} + 2\cos\beta_j + e^{ix})^{b_j}$, and let the linear regression model corresponding to $\mathrm{TRM}_{m+1}((\beta_0, \beta_1, \ldots, \beta_{l-1}), (b_0 - 1, b_1, \ldots, b_{l-1}))$ be

$$Y = (e^{-ix} - 2\cos\beta_0 + e^{ix})^{b_0 - 1} M(x) \\ \left(\sum_{k=0}^{m+1} c_k \cos kx + \sum_{k=1}^{m+1} s_k \sin kx\right) + \varepsilon. \tag{16}$$

When $\mathrm{TRM}_m((\beta_0, \beta_1, \ldots, \beta_{l-1}), (b_0, b_1, \ldots, b_{l-1}))$ is considered, we know the two more values

$$\frac{d^{b_0-1}}{dx^{b_0-1}}\Bigg((e^{-ix} - 2\cos\beta_0 + e^{ix})^{b_0-1} M(x) \\ \left(\sum_{k=0}^{m+1} c_k \cos kx + \sum_{k=1}^{m+1} s_k \sin kx\right)\Bigg)\Bigg|_{x=\beta_0}, \\ \frac{d^{b_0-1}}{dx^{b_0-1}}\Bigg((e^{-ix} - 2\cos\beta_0 + e^{ix})^{b_0-1} M(x) \\ \left(\sum_{k=0}^{m+1} c_k \cos kx + \sum_{k=1}^{m+1} s_k \sin kx\right)\Bigg)\Bigg|_{x=-\beta_0} \tag{17}$$

as prior information. Since

$$\frac{d^k}{dx^k}\left(e^{-ix} - 2\cos\beta_0 + e^{ix}\right)^{b_0-1}\Big|_{x=\beta_0} = 0, \\ k = 0, 1, \ldots, b_0 - 2,$$

the prior information (17) becomes

$$\begin{aligned}
&-2(b_0-1)!(\sin\beta_0)M(\beta_0)\\
&\quad\left(\sum_{k=0}^{m+1} c_k\cos k\beta_0+\sum_{k=1}^{m+1} s_k\sin k\beta_0\right),\\
&2(b_0-1)!(\sin\beta_0)M(\beta_0)\\
&\quad\left(\sum_{k=0}^{m+1} c_k\cos k\beta_0-\sum_{k=1}^{m+1} s_k\sin k\beta_0\right),
\end{aligned}\tag{18}$$

respectively, by using the general Leibniz rule. Note that $(\sin\beta_0)M(\beta_0)\neq 0$, since $\beta_0,\beta_1,\ldots,\beta_{l-1}$ are distinct positive numbers less than π. We can here obtain the two values

$$\alpha_1=\sum_{k=0}^{m+1} c_k\cos k\beta_0,\quad \alpha_2=\sum_{k=1}^{m+1} s_k\sin k\beta_0 \tag{19}$$

from the prior information (18).

Substitute $c_0=\alpha_1-\sum_{k=1}^{m+1}c_k\cos k\beta_0$ and $s_1=(\alpha_2-\sum_{k=2}^{m+1}s_k\sin k\beta_0)/\sin\beta_0$ into (16), we obtain

$$\begin{aligned}
Y=&(e^{-ix}-2\cos\beta_0+e^{ix})^{b_0-1}M(x)\\
&\left(\sum_{k=1}^{m+1} c_k(\cos kx-\cos k\beta_0)\right.\\
&\quad+\sum_{k=2}^{m+1} s_k\left(\sin kx-\sin x\frac{\sin k\beta_0}{\sin\beta_0}\right)\\
&\quad\left.+\alpha_1+\frac{\alpha_2}{\sin\beta_0}\right)+\varepsilon.
\end{aligned}\tag{20}$$

When we obtain a response y_k by observation at the experimental condition x_k, we can calculate the value $y_k-(e^{-ix_k}-2\cos\beta_0+e^{ix_k})^{b_0-1}M(x_k)(\alpha_1+\alpha_2/\sin\beta_0)$ easily. Therefore, we ignore the $\alpha_1+\alpha_2/\sin\beta_0$ in the model (20). Then, we here obtain the vector of the basis functions

$$(e^{-ix}-2\cos\beta_0+e^{ix})^{b_0-1}M(x)
\begin{pmatrix}
\cos x-\cos\beta_0\\
\cos 2x-\cos 2\beta_0\\
\vdots\\
\cos(m+1)x-\cos(m+1)\beta_0\\
\sin 2x-\sin x\sin 2\beta_0/\sin\beta_0\\
\sin 3x-\sin x\sin 3\beta_0/\sin\beta_0\\
\vdots\\
\sin(m+1)x-\sin x\sin(m+1)\beta_0/\sin\beta_0
\end{pmatrix}. \tag{21}$$

Let the nonsingular real matrix A be

$$A=\begin{pmatrix} A_1 & 0\\ 0 & A_2\end{pmatrix}\in\mathbb{R}^{(2m+1)\times(2m+1)},$$

where

$$A_1=\begin{pmatrix}
2 & 0 & 0 & \cdots & 0 & 0\\
1-2\cos\beta_0 & 1 & 0 & \cdots & 0 & 0\\
1 & -2\cos\beta_0 & 1 & \cdots & 0 & 0\\
\vdots & & & \ddots & \ddots & \\
1 & 0 & 0 & \cdots & 1 & 0\\
1 & 0 & 0 & \cdots & -2\cos\beta_0 & 1
\end{pmatrix}
\in\mathbb{R}^{(m+1)\times(m+1)},$$

$$A_2=\begin{pmatrix}
1 & 0 & 0 & \cdots & 0 & 0\\
-1 & 1 & 0 & \cdots & 0 & 0\\
0 & -1 & 1 & \cdots & 0 & 0\\
\vdots & & & \ddots & & \vdots\\
0 & 0 & 0 & \cdots & 1 & 0\\
0 & 0 & 0 & \cdots & -1 & 1
\end{pmatrix}\in\mathbb{R}^{m\times m}.$$

Then, by multiplying A to the vector (21) of basis functions from the left, we obtain (14).

A.2. The proof of formula (12)

From the definition (8) of generalized trigonometric canonical moments, we obtain

$$(T_k^{(t)})^2|a_k^{(t)}|^2=\tilde{T}_k^{(t)}\overline{\tilde{T}_k^{(t)}},$$

where the bar indicates the complex conjugate. Note that $\gamma_k^{(t)}=\overline{\gamma_{-k}^{(t)}}$, and that $T_k^{(t)}$ is real. By using Sylvester's determinant identity

$$T_{k+1}^{(t)}T_{k-1}^{(t)}=(T_k^{(t)})^2-\tilde{T}_k^{(t)}\overline{\tilde{T}_k^{(t)}},$$

we obtain

$$\frac{T_{k+1}^{(t)}/T_k^{(t)}}{T_k^{(t)}/T_{k-1}^{(t)}}=1-|a_k|^2,$$

and it indicates

$$\begin{aligned}
\frac{T_k^{(t)}}{T_{k-1}^{(t)}}&=\frac{T_{k-1}^{(t)}}{T_{k-2}^{(t)}}(1-|a_{k-1}|^2)\\
&=\frac{T_{k-2}^{(t)}}{T_{k-3}^{(t)}}(1-|a_{k-2}|^2)(1-|a_{k-1}|^2)\\
&=\frac{T_1^{(t)}}{T_0^{(t)}}\prod_{j=1}^{k-1}(1-|a_j|^2)\\
&=\gamma_0^{(t)}\prod_{j=1}^{k-1}(1-|a_j|^2).
\end{aligned}$$

Therefore, the formula (12)

$$\begin{aligned}
T_k^{(t)}&=T_{k-1}^{(t)}\gamma_0^{(t)}\prod_{j=1}^{k-1}(1-|a_j|^2)\\
&=\left(\gamma_0^{(t)}\right)^k\prod_{j=1}^{k-1}\left(1-|a_j^{(t)}|\right)^{k-j}
\end{aligned}$$

is shown.

A.3. The proof of formula (13)

The equation

$$a_k^{(t+1)} - a_k^{(t)} = -\frac{T_{k-1}^{(t+1)}/T_k^{(t+1)}}{T_{k-1}^{(t)}/T_k^{(t)}}(1-|a_k^{(t)}|^2)(a_{k-1}^{(t+1)} - a_{k+1}^{(t)}) \tag{22}$$

is shown by [16]. By substituting $k = 1$, we obtain the equation (13) from (22). Note that (22) holds for arbitrary $\lambda_k^{(t)}$.

References

[1] Arnold, V. I.: *Mathematical Methods of Classical Mechanics*, Springer-Verlag, New York-Heidelberg, 1978.

[2] Biedermann, S., Dette, H., Hoffmann, P.: Constrained optimal discrimination designs for Fourier regression models, *Ann. Inst. Stat. Math.*, **61** (2009), 143–157.

[3] Dette, H.: Optimal designs for a class of polynomial regression of odd or even degree, *Ann. Stat.*, **20** (1992), 238–259.

[4] Dette, H., Franke, T.: Constrained D- and D_1-optimal designs for polynomial regression, *Ann. Stat.*, **28** (2000), 1702–1727.

[5] Dette, H., Franke, T.: Robust designs for polynomial regression by maximizing a minimum of D- and D_1-efficiencies, *Ann. Stat.*, **29** (2001), 1024–1049.

[6] Dette, H., Haines, L. M., Imhof, L. A.: Maximin and Bayesian optimal designs for regression models, *Statistica Sinica*, **17** (2007), 463–480.

[7] Dette, H., Studden, W. J.: *The Theory of Canonical Moments with Applications in Statistics, Probability and Analysis*, Wiley, New York, 1997.

[8] Fang, Z.: D-optimal designs for polynomial regression models through origin, *Stat. Prob. Lett.*, **57** (2002), 343–351.

[9] Fang, Z.: Some robust designs for polynomial regression models, *Can. J. Stat.*, **34** (2006), 623–638.

[10] Fang, Z., Wiens, D. P.: Robust regression designs for approximate polynomial models, *J. Stat. Plann. Inference*, **117** (2003), 305–321.

[11] Huang, M. N. L., Chang, F. C., Wong, W. K.: D-optimal designs for polynomial regression without intercept, *Statistica Sinica*, **5** (1995), 441–458.

[12] Lau, T. S.: D-optimal designs on the unit q-ball, *J. Stat. Plann. Inference*, **19** (1988), 299–315.

[13] Lau, T. S., Studden, W. J.: Optimal designs for trigonometric and polynomial regression using canonical moments, *Ann. Stat.*, **13** (1985), 385–394.

[14] Lim, Y. B., Studden, W. J.: Efficient D_s-optimal designs for multivariate polynomial regression on the q-cube, *Ann. Stat.*, **16** (1988), 1225–1240.

[15] Mukaihira, A., Nakamura, Y.: Integrable discretization of the modified KdV equation and applications, *Inverse Problems*, **16** (2000), 413–424.

[16] Mukaihira, A., Nakamura, Y.: Schur flow for orthogonal polynomials on the unit circle and its integrable discretization, *J. Comput. Appl. Math.*, **139** (2002), 75–94.

[17] Nakamura, Y.: A tau-function of the finite nonperiodic Toda lattice, *Phys. Lett. A.*, **195** (1988), 346–350.

[18] Sekido, H.: An algorithm for calculating D-optimal designs for polynomial regression through a fixed point, *J. Stat. Plann. Inference*, (2011), doi:10.1016/j.jspi.2011.10.014.

[19] Studden, W. J.: D_s-optimal designs for polynomial regression using continued fractions, *Ann. Stat.*, **8** (1980), 1132–1141.

[20] Studden, W. J.: Some robust-type D-optimal design in polynomial regression, *J. Amer. Stat. Assoc.*, **77** (1982), 916–1921.

[21] Studden, W. J.: Note on some Φ_p optimal design for polynomial regression, *Ann. Stat.*, **17** (1989), 618–623.

[22] Symes, W. W.: The QR algorithm and scattering for the finite nonperiodic Toda lattice, *Physica D*, **4** (1982), 275–280.

[23] Tsujimoto, S., Nakamura, Y., Iwasaki, M.: The discrete Lotka-Volterra system computes singular values, *Inverse Problems*, **17** (2001), 53–58.

[24] Zen, M. M., Tsai, M. H.: Criterion-robust optimal designs for model discrimination and parameter estimation in Fourier regression models, *J. Stat. Plann. Inference*, **124** (2004), 475–487.

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