D-optimal designs based on the second-order least squares estimator

Lucy L. Gao and Julie Zhou

May 2015 (online)

D-optimal designs based on the second-order least squares estimator

Lucy L. Gao and Julie Zhou[1]

Department of Mathematics and Statistics

University of Victoria

Victoria, BC, Canada V8W 2Y2

Key words and phrases: Asymmetric distribution, convex optimization, moment theory, optimal design, polynomial regression, trigonometric regression.

MSC 2010: 62K05, 62K20.

ABSTRACT

When the error distribution in a regression model is asymmetric, the second-order least squares estimator (SLSE) is more efficient than the ordinary least squares estimator. This result motivated the research in Gao and Zhou (2014), where A-optimal and D-optimal design criteria based on the SLSE were proposed and various design properties were studied. In this paper, we continue to investigate the optimal designs based on the SLSE and derive new results for the D-optimal designs. Using convex optimization techniques and moment theories, we can construct D-optimal designs for univariate polynomial and trigonometric regression models on any closed interval. Several theoretical results are obtained. The methodology is quite general. It can be applied to reduced polynomial models, reduced trigonometric models, and other regression models. It can also be extended to A-optimal designs based on the SLSE.

[1]Corresponding author, email: jzhou@uvic.ca, phone: 250-721-7470.

1 Introduction

Consider a regression model,

$$y_i = g(\mathbf{x}_i; \boldsymbol{\theta}) + \epsilon_i, \quad i = 1, \cdots, n, \tag{1}$$

where y is a response variable, $\mathbf{x} \in R^p$ is a vector of independent variables, $g(\mathbf{x}; \boldsymbol{\theta})$ can be a linear or nonlinear function of $\boldsymbol{\theta} \in R^q$, and the errors ϵ_i's are independent and identically distributed having mean $E(\epsilon_i \mid \mathbf{x}) = 0$ and $E(\epsilon_i^2 \mid \mathbf{x}) = \sigma^2$. Note that homoscedasticity of the errors is assumed in this paper. Observations $y_1, \cdots, y_n$ are obtained by performing an experiment where the input values of the independent variables are $\mathbf{x}_1, \cdots, \mathbf{x}_n$ from a design space S. Optimal regression design of experiments aims to find the optimal points $\mathbf{x}_1, \cdots, \mathbf{x}_n$ such that we can get the most information about the unknown parameter vector $\boldsymbol{\theta}$ after fitting model (1). Optimal design theories have been developed for various design criteria and regression models based on the ordinary least squares estimator (OLSE). For example, see Fedorov (1972), Pukelsheim (1993), and Dette and Studden (1997). Design of experiments has been a very active research area in the last two decades, as optimal designs are increasingly applied in experiments in many research fields to save time, cost and resources. Berger and Wong (2009) gave many examples in the biomedical and social sciences.

If the third moment of the errors is nonzero, *i.e.*, the error distribution is asymmetric, then the second-order least squares estimator (SLSE) in Wang and Leblanc (2008) is more efficient than the OLSE. To make the paper self contained, a brief description of the SLSE is given here. Define parameter vector, $\boldsymbol{\gamma} = (\boldsymbol{\theta}^\top, \sigma^2)^\top$. Assume that $\mathbf{y}$ and $\boldsymbol{\epsilon}$ have finite fourth moments, where $\mathbf{y} = (y_1, \cdots, y_n)^\top$ and $\boldsymbol{\epsilon} = (\epsilon_1, \cdots, \epsilon_n)^\top$. The SLSE $\hat{\boldsymbol{\gamma}}_{SLS}$ of $\boldsymbol{\gamma}$ is defined as the measurable function that minimizes the following function,

$$Q_n(\boldsymbol{\gamma}) = \sum_{i=1}^{n} \boldsymbol{\rho}_i^\top(\boldsymbol{\gamma}) \boldsymbol{W}_i \boldsymbol{\rho}_i(\boldsymbol{\gamma}),$$

where $\boldsymbol{\rho}_i(\boldsymbol{\gamma}) = (y_i - g(\mathbf{x}_i; \boldsymbol{\theta}), y_i^2 - g^2(\mathbf{x}_i, \boldsymbol{\theta}) - \sigma^2)^\top$, and $\boldsymbol{W}_i = \boldsymbol{W}(\mathbf{x}_i)$ is a 2×2 positive semidefinite matrix which may depend on $\mathbf{x}_i$. The matrix $\boldsymbol{W}_i$ can be chosen to minimize the asymptotic variance of $\hat{\boldsymbol{\gamma}}_{SLS}$ and obtain the most efficient SLSE. The optimal matrix $\boldsymbol{W}_i$ is given in Wang and Leblanc (2008). In the rest of the paper, the SLSE refers to the most efficient SLSE. Based on the SLSE, Gao and Zhou (2014) proposed A-optimal and D-optimal design criteria and obtained several interesting theoretical results. In particular, sufficient conditions were derived to check for transformation invariance and symmetric properties of the D-optimal designs. Theoretical D-optimal designs have been constructed for the first-order trigonometric regression model with design space $[-\pi, \pi]$ and the first-order and second-order polynomial regression models with design spaces $[-1, 1]$ and $[0, 1]$. In fact, with the new design criteria, many new optimal designs can be constructed for various regression models and design spaces, and new design theories can be derived.

It is usually hard to find optimal designs analytically, because we need to minimize complicated objective functions with constraints. Recently, numerical algorithms have received a lot of attention for computing optimal designs, and several effective algorithms have been developed, including Dette *et al.* (2008), Yu (2010, 2011), Papp (2012), Lu and Pong (2013), Duarte and Wong (2014a, b), and Duarte *et al.* (2014). Duarte and Wong (2014a) and Pronzato and Pázman (2013, Chapter 9) provided a good review of the numerical algorithms. Using numerical algorithms, optimal designs can be constructed quickly for practical applications.

In this paper, we use convex optimization techniques to investigate D-optimal designs based on the SLSE. First we show that this design problem corresponds to a convex optimization problem. Then we develop numerical algorithms to compute D-optimal designs for various linear models. The main idea is to construct D-optimal designs in two steps. In step 1 we obtain the moments of D-optimal designs, and in step 2 we find the distributions of the D-optimal designs in terms of support points and corresponding probabilities. The moment theories in Curto and Fialkow (1991), Dette and Studden (1997), as well as the convex optimization techniques in Boyd and Vandenberghe (2004) are very useful for developing the numerical algorithms. A CVX program in MATLAB for solving convex optimization problems (Grant and Boyd, 2013) is effective to implement these algorithms to compute the D-optimal designs. Our algorithms have two different features from other algorithms: (i) the new design criterion based on the SLSE is used, and (ii) the D-optimal designs are computed through the optimal moments, without assuming fixed design points. In addition, the numerical computations of the D-optimal designs lead to the development of several theoretical results.

The rest of the paper is organized as follows. In Section 2, we discuss and characterize the D-optimal design criterion for the SLSE. Convex optimization problems and the CVX program are briefly introduced. In Section 3, we propose an algorithm to construct D-optimal designs for univariate polynomial regression models and several results are presented. In Section 4, we consider trigonometric regression models and another algorithm is proposed to compute D-optimal designs. Concluding remarks are in Section 5. All proofs are given in the Appendix.

2 D-optimal designs based on the SLSE

Let ξ be the distribution of $\mathbf{x}$ on a design space $S \subset R^p$, and design points, $\mathbf{x}_1, \cdots, \mathbf{x}_n$, are randomly selected from ξ. Suppose the true parameter value of $\boldsymbol{\theta}$ in model (1) is $\boldsymbol{\theta}^*$. Define

$$\boldsymbol{g}_1 = E\left[\frac{\partial g(\mathbf{x};\boldsymbol{\theta}^*)}{\partial \boldsymbol{\theta}}\right], \ \boldsymbol{G}_2 = E\left[\frac{\partial g(\mathbf{x};\boldsymbol{\theta}^*)}{\partial \boldsymbol{\theta}}\frac{\partial g(\mathbf{x};\boldsymbol{\theta}^*)}{\partial \boldsymbol{\theta}^\top}\right], \tag{2}$$

where the expectation is taken with respect to the distribution ξ of $\mathbf{x}$. Let $\hat{\boldsymbol{\theta}}_{OLS}$ and $\hat{\boldsymbol{\theta}}_{SLS}$ be the OLSE and SLSE of $\boldsymbol{\theta}$, respectively. Under some regularity conditions, both $\hat{\boldsymbol{\theta}}_{OLS}$ and $\hat{\boldsymbol{\theta}}_{SLS}$ are asymptotically normally distributed (Wang and Leblanc, 2008). Suppose their asymptotic covariance matrices are, respectively, $V(\hat{\boldsymbol{\theta}}_{OLS})$ and $V(\hat{\boldsymbol{\theta}}_{SLS})$.

From Wang and Leblanc (2008) and Gao and Zhou (2014), we have

$$\det(V(\hat{\boldsymbol{\theta}}_{OLS})) = \sigma^{2q}\det\left(\boldsymbol{G}_2^{-1}\right), \tag{3}$$

$$\det(V(\hat{\boldsymbol{\theta}}_{SLS})) = \frac{\sigma^{2q}(1-t)^q\det\left(\boldsymbol{G}_2^{-1}\right)}{1-t\boldsymbol{g}_1^\top\boldsymbol{G}_2^{-1}\boldsymbol{g}_1}, \tag{4}$$

where $t = \frac{\alpha_3^2}{\sigma^2(\alpha_4-\sigma^4)}$, with $\alpha_3 = E(\epsilon_i^3 \mid \mathbf{x})$ and $\alpha_4 = E(\epsilon_i^4 \mid \mathbf{x})$. For any distribution, $0 \le t < 1$ from Gao and Zhou (2014). For symmetric distributions, it is obvious that $t = 0$ and $\det(V(\hat{\boldsymbol{\theta}}_{SLS})) = \det(V(\hat{\boldsymbol{\theta}}_{OLS}))$. For asymmetric distributions, we have $0 < t < 1$, and $\det(V(\hat{\boldsymbol{\theta}}_{SLS})) \le \det(V(\hat{\boldsymbol{\theta}}_{OLS}))$.

The D-optimal design based on the OLSE (denoted by ξ_D^{OLS}) minimizes $\det(V(\hat{\boldsymbol{\theta}}_{OLS}))$, while the D-optimal design based on the SLSE (denoted by ξ_D^{SLS}) minimizes $\det(V(\hat{\boldsymbol{\theta}}_{SLS}))$. From Wang and Leblanc (2008) and Gao and Zhou (2014), if a linear model contains an intercept term, then $\boldsymbol{g}_1^\top \boldsymbol{G}_2^{-1} \boldsymbol{g}_1 = 1$ for any distribution of $\mathbf{x}$. Thus, from (3) and (4), the D-optimal designs based on the SLSE are the same as those based on the OLSE. However, if $\boldsymbol{g}_1^\top \boldsymbol{G}_2^{-1} \boldsymbol{g}_1 \neq 1$, in general the D-optimal designs differ. Linear models without the intercept term and nonlinear models usually do not have $\boldsymbol{g}_1^\top \boldsymbol{G}_2^{-1} \boldsymbol{g}_1 = 1$.

The following result characterizes $\det(V(\hat{\boldsymbol{\theta}}_{SLS}))$. This is helpful when examining the convexity of $\det(V(\hat{\boldsymbol{\theta}}_{SLS}))$ and developing numerical algorithms to construct D-optimal designs.

Theorem 1. *The $det(V(\hat{\boldsymbol{\theta}}_{SLS}))$ in (4) can be expressed as*

$$det(V(\hat{\boldsymbol{\theta}}_{SLS})) = \frac{\sigma^{2q}(1-t)^q}{det(\mathbf{A})}, \quad with \quad \mathbf{A} = \begin{pmatrix} 1 & \sqrt{t}\, \boldsymbol{g}_1^\top \\ \sqrt{t}\, \boldsymbol{g}_1 & \boldsymbol{G}_2 \end{pmatrix}. \tag{5}$$

The proof of Theorem 1 is in the Appendix. Denote the elements of $\mathbf{A}$ by a_{ij}, $i, j = 1, \cdots, q+1$. Next we consider the convexity of $\det(\mathbf{A})$.

Lemma 1. *Suppose $\mathbf{A}$ is a $(q+1)\times(q+1)$ positive definite matrix. If each element a_{ij} of $\mathbf{A}$ is a linear function of variable u, then $-(\det(\mathbf{A}))^{1/(q+1)}$ is a convex function of u.*

Lemma 1 is a result from Boyd and Vandenberghe (2004, page 74), for when matrix $\mathbf{A}$ is a function of one variable only. Note that the result is also true for $-\log(\det(\mathbf{A}))$. For simplicity, we focus on function $-(\det(\mathbf{A}))^{1/(q+1)}$ in this paper, but all the results can be applied to $-\log(\det(\mathbf{A}))$. Lemma 1 can be also extended to the multivariable case as follows.

Theorem 2. *Suppose $\mathbf{A}$ is a $(q+1)\times(q+1)$ positive definite matrix. If each element a_{ij} of $\mathbf{A}$ is a linear function of variables $\mu_1, \cdots, \mu_m$ $(m > 1)$, then $-(\det(\mathbf{A}))^{1/(q+1)}$ is a convex function of $\mu_1, \cdots, \mu_m$.*

This is similar to results in Pukelsheim (1993, p151) and Lu and Pong (2013), so the proof is omitted. This result is the key to using convex optimization techniques to find the optimal designs ξ_D^{SLS}. Let

$$\phi_1(\xi) = -\left(\det\left(\mathbf{A}\right)\right)^{1/(q+1)}, \tag{6}$$

where $\mathbf{A}$ is defined in (5). If all the elements of $\mathbf{A}$ are linear functions of the moments of ξ, then the ξ_D^{SLS} minimizes a convex objective function $\phi_1(\xi)$.

A convex optimization problem is an optimization problem with a convex objective function over a convex set. Often it is a constrained optimization problem with inequality constraints which define the convex set. The inequality constraints may include linear and/or convex nonlinear inequalities. Problems with linear objective functions subject to linear matrix inequality constraints are a special class of convex optimization problems called semidefinite programming (SDP) problems. Boyd and Vandenberghe (2004) discusses various convex optimization techniques and applications. In the past two decades, several numerical programs have been developed to solve convex optimization problems. One is the CVX program in MATLAB (Grant and Boyd, 2013), which is very powerful and widely used. Recently, Papp (2012) discussed and applied the CVX program for computing optimal designs using the (weighted) least squares estimator. Lu and Pong (2013) proposed an interior point method for solving convex optimization problems in optimal design, and this method is compared with the multiplicative algorithm introduced in Silvey *et al.* (1978).

In the next two sections, we apply the CVX program to construct D-optimal designs ξ_D^{SLS} for polynomial and trigonometric regression models. The D-optimal design problems are transformed into convex optimization problems and SDP problems. Two algorithms are developed for computing the D-optimal designs for any continuous design space. Our algorithms are different from those in Papp (2012) and Lu and Pong (2013). Lu and Pong (2013) use an interior point method, and not a linear matrix inequality that yields a SDP program. In addition, Lu and Pong (2013) only computes the optimal weights as the design points $\mathbf{x}_1, \cdots, \mathbf{x}_n$ are assumed to be known and fixed.

3 D-optimal designs for polynomial regression

Consider the qth order polynomial regression model without the intercept,

$$y_i = \theta_1 x_i + \cdots + \theta_q x_i^q + \epsilon_i, \quad i = 1, \cdots, n, \tag{7}$$

where design points $x_1, \cdots, x_n$ are selected randomly from a distribution ξ of x on a design space S. This is a linear regression model with $g(x; \boldsymbol{\theta}) = \mathbf{f}^\top(x)\boldsymbol{\theta}$, where $\boldsymbol{\theta} = (\theta_1, \cdots, \theta_q)^\top$ and $\mathbf{f}(x) = (x, \cdots, x^q)^\top$. From Gao and Zhou (2014), the ξ_D^{SLS} for this model is scale invariant, so we can assume the design space $S = [b, c] \subset [-1, 1]$, without loss of generality. Define the moments of distribution ξ on S as

$$\mu_j = \int_S x^j d\xi(x), \quad j = 0, 1, 2, \cdots$$

From (2), we have

$$\boldsymbol{g}_1 = E(\mathbf{f}(x)) = (\mu_1, \cdots, \mu_q)^\top, \quad \boldsymbol{G}_2 = E(\mathbf{f}(x)\mathbf{f}^\top(x)) = \begin{pmatrix} \mu_2 & \mu_3 & \cdots & \mu_{q+1} \\ \mu_3 & \mu_4 & \cdots & \mu_{q+2} \\ \vdots & \vdots & \vdots & \vdots \\ \mu_{q+1} & \mu_{q+2} & \cdots & \mu_{2q} \end{pmatrix}.$$

Notice that both $\boldsymbol{g}_1$ and $\boldsymbol{G}_2$ do not depend on the true parameter value $\boldsymbol{\theta}^*$, which implies that the ξ_D^{SLS} does not depend on $\boldsymbol{\theta}^*$. In fact, this is true for all linear models. From (5), we get

$$\mathbf{A} = \mathbf{A}(t, \mu_1, \cdots, \mu_{2q}) = \begin{pmatrix} 1 & \sqrt{t}\,\mu_1 & \sqrt{t}\,\mu_2 & \cdots & \sqrt{t}\,\mu_q \\ \sqrt{t}\,\mu_1 & \mu_2 & \mu_3 & \cdots & \mu_{q+1} \\ \sqrt{t}\,\mu_2 & \mu_3 & \mu_4 & \cdots & \mu_{q+2} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \sqrt{t}\,\mu_q & \mu_{q+1} & \mu_{q+2} & \cdots & \mu_{2q} \end{pmatrix}. \tag{8}$$

For given $t \in [0, 1)$, all the elements of $\mathbf{A}$ are linear functions of $\mu_1, \cdots, \mu_{2q}$. By Theorem 2, $\phi_1(\xi)$ in (6) is a convex function of $\mu_1, \cdots, \mu_{2q}$. Therefore, the D-optimal design problem is a convex optimization problem.

3.1 Convex optimization and Algorithm I

The D-optimal design ξ_D^{SLS} is constructed in two steps for the polynomial regression model.

Algorithm I

Step (1): Find the optimal moments $\mu_1^*, \cdots, \mu_{2q}^*$ that minimize

$$\phi(\mu_1, \cdots, \mu_{2q}) = \phi_1(\xi),$$

over moments $\mu_1, \cdots, \mu_{2q}$ of all possible distributions ξ on S.

Step (2): From the optimal moments $\mu_1^*, \cdots, \mu_{2q}^*$, we construct the support points, say $x_1^*, \cdots, x_N^*$, and their probabilities, $p_1, \cdots, p_N$, for some $N \geq q$. These support points and probabilities must satisfy

$$\sum_{i=1}^{N} p_i = 1, \quad \sum_{i=1}^{N} p_i \cdot (x_i^*)^j = \mu_j^*, \quad j = 1, \cdots, 2q. \tag{9}$$

Then the D-optimal design ξ_D^{SLS} is a discrete distribution that is represented as

$$\xi_D^{SLS} = \begin{pmatrix} x_1^* & x_2^* & \cdots & x_N^* \\ p_1 & p_2 & \cdots & p_N \end{pmatrix}.$$

We now detail how to find a solution for each step. To minimize $\phi(\mu_1, \cdots, \mu_{2q})$ over $\mu_1, \cdots, \mu_{2q}$ in Step (1), we first find the constraints for the moments. For a given sequence $a_0, a_1, \cdots, a_{2q}$, define a $(q+1) \times (q+1)$ Hankel matrix as

$$\mathbf{H}(a_0, a_1, \cdots, a_{2q}) = (a_{i+j-2}) = \begin{pmatrix} a_0 & a_1 & a_2 & \cdots & a_q \\ a_1 & a_2 & a_3 & \cdots & a_{q+1} \\ a_2 & a_3 & a_4 & \cdots & a_{q+2} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ a_q & a_{q+1} & a_{q+2} & \cdots & a_{2q} \end{pmatrix}.$$

For any $x \in S = [b, c]$, it is clear that $(c - x)(x - b) = -bc + (b + c)x - x^2 \geq 0$. Thus, for any ξ on S, the following matrix is always positive semidefinite,

$$
\begin{aligned}
&\mathbf{B}(b,c,\mu_0,\mu_1,\cdots,\mu_{2q}) \\
&= \int_S [-bc + (b+c)x - x^2] \begin{pmatrix} 1 \\ x \\ \vdots \\ x^{q-1} \end{pmatrix} \begin{pmatrix} 1 & x & \cdots & x^{q-1} \end{pmatrix} d\xi(x) \\
&= -bc\,\mathbf{H}(\mu_0,\mu_1,\cdots,\mu_{2q-2}) + (b+c)\mathbf{H}(\mu_1,\mu_2,\cdots,\mu_{2q-1}) - \mathbf{H}(\mu_2,\mu_3,\cdots,\mu_{2q}),
\end{aligned}
\tag{10}
$$

and we write $\mathbf{B}(b,c,\mu_0,\mu_1,\cdots,\mu_{2q}) \succeq 0$. Similarly, we have $\mathbf{H}(\mu_0,\mu_1,\cdots,\mu_{2q}) \succeq 0$. These moment constraints can be found in Dette and Studden (1997, page 19) for design space $[b,c] = [0,1]$. These moment constraints are also necessary and sufficient conditions for $\mu_1,\cdots,\mu_{2q}$ to be moments of a probability distribution from Laurent (2010, Theorem 5.39). By Theorem 2, $\phi(\mu_1,\cdots,\mu_{2q})$ is a convex function of $\mu_1,\cdots,\mu_{2q}$. Both $\mathbf{B}(b,c,\mu_0,\mu_1,\cdots,\mu_{2q}) \succeq 0$ and $\mathbf{H}(\mu_0,\mu_1,\cdots,\mu_{2q}) \succeq 0$ are linear matrix inequality constraints. Thus in Step (1), we solve a convex optimization problem,

$$
(P1) \quad \begin{cases} \min_{\mu_1,\cdots,\mu_{2q}} \phi(\mu_1,\cdots,\mu_{2q}) \\ \textit{subject to}: \quad \mathbf{B}(b,c,\mu_0,\mu_1,\cdots,\mu_{2q}) \succeq 0, \\ \qquad\qquad\qquad \mathbf{H}(\mu_0,\mu_1,\cdots,\mu_{2q}) \succeq 0. \end{cases}
\tag{11}
$$

The CVX program is applied to solve $(P1)$. Denote the solution by $\mu_1^*,\cdots,\mu_{2q}^*$. It is shown in the Appendix (Proof of Theorem 3) that there must be at least q support points in the optimal distribution with moments $\mu_1^*,\cdots,\mu_{2q}^*$.

In Step (2), using the results in Curto and Fialkow (1991), we find the support points $x_1^*,\cdots,x_N^* \in S$ and their associated weights $p_1,\cdots,p_N$ satisfying the equations in (9). The following procedure provides an answer with the smallest N, *i.e.*, the distribution has the minimum number of support points. Step (2) has four parts: (i), (ii), (iii) and (iv).

Step (2 - i): If $\det\big(\mathbf{H}(\mu_0,\mu_1^*,\cdots,\mu_{2q}^*)\big) = 0$, let $N = q$ and go to Step (2 - ii). If $\det\big(\mathbf{H}(\mu_0,\mu_1^*,\cdots,\mu_{2q}^*)\big) > 0$, we solve the following SDP problem to find two more moments μ^*_{2q+1} and μ^*_{2q+2} of the distribution ξ_D^{SLS},

$$(P2) \quad \begin{cases} \min_{\mu_{2q+1},\mu_{2q+2}} \ \mu_{2q+2} \\ \textit{subject to}: \quad \mathbf{B}(b,c,\mu_0,\mu_1^*,\cdots,\mu_{2q}^*,\mu_{2q+1},\mu_{2q+2}) \succeq 0, \\ \qquad\qquad\qquad \mathbf{H}(\mu_0,\mu_1^*,\cdots,\mu_{2q}^*,\mu_{2q+1},\mu_{2q+2}) \succeq 0. \end{cases} \tag{12}$$

There are only two variables μ_{2q+1} and μ_{2q+2} in $(P2)$. The two constraints in (12) are needed such that $\mu_1^*,\cdots,\mu_{2q}^*,\mu_{2q+1}^*,\mu_{2q+2}^*$ are moments of a distribution on $[b,c]$. Minimizing μ_{2q+2} gives the minimum number of support points for ξ_D^{SLS} with $N=q+1$. From Curto and Fialkow (1991), we have

$$\det\left(\mathbf{H}(\mu_0,\mu_1^*,\cdots,\mu_{2q}^*,\mu_{2q+1}^*,\mu_{2q+2}^*)\right) = 0. \tag{13}$$

Problem $(P2)$ can also be solved by the CVX program.

Step (2 - ii): We find a vector $\mathbf{v} = (v_0, v_1, \cdots, v_N)^\top$ satisfying

$$\mathbf{H}(\mu_0,\mu_1^*,\cdots,\mu_{2N}^*)\ \mathbf{v} = \mathbf{0}.$$

From $\det\left(\mathbf{H}(\mu_0,\mu_1^*,\cdots,\mu_{2N}^*)\right)=0$ and $\det\left(\mathbf{H}(\mu_0,\mu_1^*,\cdots,\mu_{2N-2}^*)\right)>0$, we must have $v_N \neq 0$.

Step (2 - iii): Since $\mathbf{H}(\mu_0,\mu_1^*,\cdots,\mu_{2N}^*) = \sum_{i=1}^N p_i (1\ x_i^*\ \cdots\ (x_i^*)^N)^\top (1\ x_i^*\ \cdots\ (x_i^*)^N)$ and $\mathbf{H}(\mu_0,\mu_1^*,\cdots,\mu_{2N}^*)\ \mathbf{v} = \mathbf{0}$ from Step (2 - ii), we have $\mathbf{v}^\top\mathbf{H}(\mu_0,\mu_1^*,\cdots,\mu_{2N}^*)\ \mathbf{v} = 0$, which implies that $(1\ x_i^*\ \cdots\ (x_i^*)^N)\mathbf{v} = 0$ for all $i=1,\cdots,N$. Thus, the N support points, $x_1^*,\cdots,x_N^*$, are the roots of a polynomial equation

$$v_0 + v_1 x + \cdots + v_N x^N = 0.$$

Since $v_N \neq 0$, there exists N roots.

Step (2 - iv): Using any N equations in (9), we can solve for probabilities $p_1,\cdots,p_N$. Notice that given the support points $x_1^*,\cdots,x_N^*$ and the moments $\mu_1^*,\cdots,\mu_{2q}^*$, these are all linear equations about $p_1,\cdots,p_N$.

3.2 Results

D-optimal designs are constructed for model (7) using Algorithm I. A MATLAB program applying the CVX program to solve problems ($P1$) and ($P2$) is available on request. Table 1 presents some representative results for $S_1 = [-1, 1]$ and various values of t, and Table 2 gives the results for $S_2 = [0, 1]$. In these tables, the optimal designs ξ_D^{OLS} for the OLSE correspond to the special case $t = 0$. For $t > 0$, the results give the optimal designs ξ_D^{SLS} for the SLSE.

Tables 1 and 2 here

When $q = 2$ with S_1, Gao and Zhou (2014) derived the theoretical designs for any $t \in [0, 1)$, which are consistent with the results in Table 1. For any q on design space $[a, 1]$ with $-1 \leq a \leq 1$, it is shown in Huang *et al.* (1995) that theoretical and numerically computed designs for $t = 0$ are also consistent with the results in Tables 1 and 2. On S_1 with $t = 0$, it is shown that the minimum number of support points is q when q is even and $q+1$ when q is odd. Furthermore, theoretical designs are derived for even q and numerically computed designs are given for odd q. On S_2 with $t = 0$, it is shown that the minimum number of support points is q, and theoretical designs are derived.

From the numerical results, design ξ_D^{SLS} has either q or $q + 1$ support points on both S_1 and S_2. When t is close to 0, ξ_D^{SLS} has the same number of support points as ξ_D^{OLS} has. For large t, ξ_D^{SLS} tends to have $q+1$ support points on both S_1 and S_2. For the symmetric design space S_1, ξ_D^{SLS} is also symmetric for any q, which is consistent with the theoretical result in Gao and Zhou (2014). Algorithm I is effective to compute the D-optimal designs for model (7) with any design space.

After studying the numerical results, we are able to establish several properties of the D-optimal designs ξ_D^{SLS} for polynomial regression models with design space $S = [b, c]$.

Theorem 3. *For model (7) with design space $S = [b, c] \subset [-1, 1]$, the D-optimal designs ξ_D^{SLS} with the minimum number of support points have the following properties.*

(i) The minimum number of support points in ξ_D^{SLS} is either q or $q+1$.

(ii) For a symmetric design space $S=[-c,c]$, there exists a symmetric D-optimal design ξ_D^{SLS}. In addition, the support points of the ξ_D^{SLS} must include the two boundary points $-c$ and c.

(iii) For a design space $S=[b,c]$ with $0 \le b < c$, the support points of ξ_D^{SLS} must include the boundary point c.

(iv) For a design space $S=[b,c]$ with $b < 0 < c$, the support points of ξ_D^{SLS} must include at least one of the two boundary points b and c.

The proof of Theorem 3 is in the Appendix. Some D-optimal designs ξ_D^{SLS} also include the support point 0, which can provide information for the SLSE. In particular, when $x_i = 0$, the model becomes $y_i = \epsilon_i$. The observations at $x_i = 0$ provide information on σ^2 which is estimated together with $\boldsymbol{\theta}$ in the SLSE.

4 D-optimal designs for trigonometric regression

Optimal designs for trigonometric regression models have been studied by many authors, since it is hard to derive optimal designs on partial circles. For example, Dette *et al.* (2002) and Chang *et al.* (2013) constructed D-optimal designs on partial circles using the OLSE. Recently, Xu and Shang (2014) gave a good review of various optimal designs and also studied robust designs. In this section, we develop an algorithm for computing the D-optimal designs, using the OLSE or SLSE. The algorithm is effective to find D-optimal designs for any partial circle.

Consider a trigonometric regression model without the intercept,

$$y_i = \sum_{j=1}^{q} \theta_{1j} \cos(j\ x_i) + \sum_{j=1}^{q} \theta_{2j} \sin(j\ x_i) + \epsilon_i, \quad i = 1, \cdots, n, \tag{14}$$

where $x_i \in S_x = [-a, a]$ with $0 < a \le \pi$. This is a linear model with $g(x;\boldsymbol{\theta}) = \mathbf{f}^\top(x)\boldsymbol{\theta}$, where $\boldsymbol{\theta} = (\theta_{11}, \cdots, \theta_{1q}, \theta_{21}, \cdots, \theta_{2q})^\top$ and $\mathbf{f}(x) = (\cos(x), \cdots, \cos(qx), \sin(x), \cdots, \sin(qx))^\top$. If the model includes an intercept, then the D-optimal designs using the OLSE and SLSE are the same. However, the D-optimal designs ξ_D^{SLS} and ξ_D^{OLS} may be different for model (14). The discussion below is for model (14), but it can be easily applied to the model with an intercept.

From Gao and Zhou (2014), the D-optimal design ξ_D^{SLS} is shift invariant, so the design space S_x can be assumed to be symmetric about 0. Since $\cos(jx)$ and $\sin(jx)$ are periodic functions, we will study the optimal design for $a \le \pi$. Gao and Zhou (2014) also showed that the ξ_D^{SLS} is symmetric about 0. Thus we only consider symmetric distributions of x to find the ξ_D^{SLS} below.

Since some elements of matrix $\mathbf{A}$ are not linear functions of the moments of the distribution of x, we work on a transformation of x. Let $z = \cos(x)$. Then $\cos(kx)$ is a kth order polynomial function of z, since

$$\begin{aligned} \cos(2x) &= 2\cos^2(x) - 1 = 2z^2 - 1, \\ \cos(kx) &= 2\cos(x)\cos((k-1)x) - \cos((k-2)x), \quad k = 3, 4, \cdots \end{aligned}$$

In addition, $\sin^2(kx) = 1 - \cos^2(kx)$ and $\sin(kx)\sin(lx) = 0.5(\cos((k-l)x) - \cos((k+l)x))$, so they are all polynomial functions of z, for $k, l = 1, \cdots, q$. Now define the following moments to present $\boldsymbol{g}_1$ and $\boldsymbol{G}_2$ in (2),

$$u_j = E(z^j), \quad j = 0, 1, 2, \cdots$$

For symmetric distributions of x on S_x, we have

$$\begin{aligned} & E(\sin(jx)) = 0, \quad j = 1, \cdots, q, \\ & \boldsymbol{g}_1 = E(\mathbf{f}(x)) = (d_1, \cdots, d_q, 0, \cdots, 0)^\top, \\ & \boldsymbol{G}_2 = E(\mathbf{f}(x)\mathbf{f}^\top(x)) = \mathbf{A}_1 \oplus \mathbf{A}_2, \\ & \mathbf{A}(t, u_1, \ldots, u_{2q}) = \begin{pmatrix} 1 & \sqrt{t}\, \boldsymbol{g}_1^\top \\ \sqrt{t}\, \boldsymbol{g}_1 & \boldsymbol{G}_2 \end{pmatrix}, \end{aligned} \tag{15}$$

where $d_j = E(\cos(jx))$, and $\mathbf{A}_1$ and $\mathbf{A}_2$ are $q \times q$ matrices. For instance, when $q = 2$,

$$d_1 = E(\cos(x)) = u_1, \quad d_2 = E(\cos(2x)) = 2u_2 - 1,$$
$$\mathbf{A}_1 = \begin{pmatrix} E(\cos^2(x)) & E(\cos(x)\cos(2x)) \\ E(\cos(x)\cos(2x)) & E(\cos^2(2x)) \end{pmatrix} = \begin{pmatrix} u_2 & 2u_3 - u_1 \\ 2u_3 - u_1 & 4u_4 - 4u_2 + 1 \end{pmatrix},$$
$$\mathbf{A}_2 = \begin{pmatrix} E(\sin^2(x)) & E(\sin(x)\sin(2x)) \\ E(\sin(x)\sin(2x)) & E(\sin^2(2x)) \end{pmatrix} = \begin{pmatrix} 1 - u_2 & 2u_1 - 2u_3 \\ 2u_1 - 2u_3 & 4u_2 - 4u_4 \end{pmatrix},$$

and,

$$\mathbf{A}(t, u_1, \ldots, u_4) = \begin{pmatrix} 1 & \sqrt{t}\ u_1 & \sqrt{t}\ (2u_2 - 1) & 0 & 0 \\ \sqrt{t}\ u_1 & u_2 & 2u_3 - u_1 & 0 & 0 \\ \sqrt{t}\ (2u_2 - 1) & 2u_3 - u_1 & 4u_4 - 4u_2 + 1 & 0 & 0 \\ 0 & 0 & 0 & 1 - u_2 & 2u_1 - 2u_3 \\ 0 & 0 & 0 & 2u_1 - 2u_3 & 4u_2 - 4u_4 \end{pmatrix}.$$

Notice that $d_1, \cdots, d_q$ and all the elements of $\mathbf{A}_1$ and $\mathbf{A}_2$ are linear functions of moments $u_1, \cdots, u_{2q}$. Thus all the elements of $\mathbf{A}$ are linear functions of $u_1, \cdots, u_{2q}$.

4.1 Algorithm II

For $x \in S_x = [-a, a]$ with $0 < a \leq \pi$, we have $z = \cos(x) \in S_z = [\cos(a), 1]$. The D-optimal design ξ_D^{SLS} can be constructed in three steps for model (14). Let $\phi(u_1, \cdots, u_{2q}) = \phi_1(\xi)$, where $\phi_1(\xi)$ is defined in (6), and matrix $\mathbf{A}$ is given in (15). Since all the elements of $\mathbf{A}$ are linear functions of $u_1, \cdots, u_{2q}$, $\phi(u_1, \cdots, u_{2q})$ is a convex function of $u_1, \cdots, u_{2q}$.

Algorithm II

Step (1): Find the optimal moments $u_1^*, \cdots, u_{2q}^*$ that minimize $\phi(u_1, \cdots, u_{2q})$ over moments $u_1, \cdots, u_{2q}$ of all possible distributions ξ on S_z.

Step (2): From the optimal moments $u_1^*, \cdots, u_{2q}^*$, we construct the support points, say $z_1^*, \cdots, z_N^*$, and their probabilities, $p_1, \cdots, p_N$, for some $N \geq q$. These support points and probabilities must satisfy

$$\sum_{i=1}^{N} p_i = 1, \quad \sum_{i=1}^{N} p_i \cdot (z_i^*)^j = u_j^*, \quad j = 1, \cdots, 2q.$$

Step (3): Let $x_i^* = \cos^{-1}(z_i^*) \in [0, a],\ i = 1, \cdots, N$. Then the symmetric D-optimal design is given by

$$\xi_D^{SLS}(x) = \begin{pmatrix} x_1^* & \cdots & x_N^* & -x_1^* & \cdots & -x_N^* \\ \frac{p_1}{2} & \cdots & \frac{p_N}{2} & \frac{p_1}{2} & \cdots & \frac{p_N}{2} \end{pmatrix}. \tag{16}$$

In the first two steps we compute the optimal design in terms of z on design space S_z, and in the third step we find the optimal design in terms of x on design space S_x. Steps (1) and (2) are similar to those in Algorithm I, and the differences are the objective function and the design space. In particular, problems $(P1)$ and $(P2)$ become $(P1')$ and $(P2')$, respectively, as follows:

$$(P1') \quad \begin{cases} \min_{u_1,\cdots,u_{2q}} \phi(u_1, \cdots, u_{2q}) \\ \textit{subject to}: \quad \mathbf{B}(\cos(a), 1, u_0, u_1, \cdots, u_{2q}) \succeq 0, \\ \qquad\qquad\qquad \mathbf{H}(u_0, u_1, \cdots, u_{2q}) \succeq 0, \end{cases}$$

and

$$(P2') \quad \begin{cases} \min_{u_{2q+1},u_{2q+2}} \ u_{2q+2} \\ \textit{subject to}: \quad \mathbf{B}(\cos(a), 1, u_0, u_1^*, \cdots, u_{2q}^*, u_{2q+1}, u_{2q+2}) \succeq 0, \\ \qquad\qquad\qquad \mathbf{H}(u_0, u_1^*, \cdots, u_{2q}^*, u_{2q+1}, u_{2q+2}) \succeq 0. \end{cases}$$

The CVX program can be applied to solve $(P1')$ and $(P2')$. After we get the support points $z_1^*, \cdots, z_N^*$ in Step (2), Step (3) can be easily implemented to compute $x_1^*, \cdots, x_N^*$. Since $\cos(jx)$ and $\sin(jx)$ are periodic functions, the D-optimal designs are usually not unique. Algorithm II only gives a symmetric D-optimal design, and the number of support points for the distribution of x may not be the minimum.

4.2 Results

Using Algorithm II, we can find a symmetric D-optimal design in (16) for model (14) for any $q \geq 1$ and S_x with $a \leq \pi$. Tables 3, 4 and 5 give some representative results for design spaces $[-\pi, \pi]$, $[-3\pi/4, 3\pi/4]$ and $[-2\pi/3, 2\pi/3]$, respectively.

Tables 3, 4, and 5 here.

Our numerical results indicate that the optimal distributions of z have either q or $q+1$ support points. For small t, ξ_D^{SLS} and ξ_D^{OLS} have the same number of support points. For large t, ξ_D^{SLS} usually has $q+1$ support points. On the full circle, ξ_D^{SLS} and ξ_D^{OLS} are the same in Table 3, and they do not depend on t. On partial circles, ξ_D^{SLS} and ξ_D^{OLS} are often different, even if they have the same number of support points. See Table 4 for $q = 4$. Sometimes when the support points are the same for ξ_D^{SLS} and ξ_D^{OLS}, their probabilities are different. See Table 5 for $q = 2$.

5 Discussion

D-optimal designs based on the SLSE are investigated. Since we can show that the D-optimal design problem is convex, convex optimization techniques and the CVX program in MATLAB can be applied to construct D-optimal designs. Two algorithms are developed for polynomial and trigonometric regression models, which are very powerful and can be used to compute D-optimal designs on any closed interval.

If all the regressors of a regression model are linear functions of $x, x^2, \cdots, x^q$, we call it a generalized polynomial regression model (GPRM). The trigonometric regression models in Section 4 are transformed into GPRMs through variable transformation $z = \cos(x)$. There are other models that can be transformed into GPRMs, such as $y_i = \theta_0 + \theta_1 \exp(x_i) + \cdots + \theta_q \exp(qx_i) + \epsilon_i$, $y_i = \theta_0 \exp(\theta_1 x_i)\epsilon_i$, reduced polynomial regression models, and trigonometric regression models with only cosine terms or sine terms (Zhang, 2007). The methodology discussed in this paper can be easily applied to any regression model that can be transformed into a GPRM.

In addition, the methodology in this paper can be extended to A-optimal designs for polynomial and trigonometric regression models, since it can be shown that trace $\left(V(\hat{\boldsymbol{\theta}}_{SLS})\right)$

is also a convex function of the moments $\mu_1, \cdots, \mu_{2q}$ and the linear matrix inequalities are the same as those in the D-optimal design problem.

Appendix: Proofs

Proof of Theorem 1: From (4), we have

$$\begin{aligned}\det(V(\hat{\boldsymbol{\theta}}_{SLS})) &= \frac{\sigma^{2q}(1-t)^q}{1-t\ \boldsymbol{g}_1^\top \boldsymbol{G}_2^{-1}\boldsymbol{g}_1}\det\left(\boldsymbol{G}_2^{-1}\right) \\ &= \frac{\sigma^{2q}(1-t)^q}{\left(1-t\ \boldsymbol{g}_1^\top \boldsymbol{G}_2^{-1}\boldsymbol{g}_1\right)\det\left(\boldsymbol{G}_2\right)} \\ &= \frac{\sigma^{2q}(1-t)^q}{\det\left(\mathbf{A}\right)}.\end{aligned}$$

□

Proof of Theorem 3: (i) For the ξ_D^{SLS}, it is clear that $\phi(\mu_1^*, \cdots, \mu_{2q}^*) < \infty$, which implies that $\det\left(\mathbf{A}(t, \mu_1^*, \cdots, \mu_{2q}^*)\right) > 0$. By (5), we have $\det\left(\boldsymbol{G}_2\right) > 0$, so the rank of $\boldsymbol{G}_2$ is q. For model (7), since $\boldsymbol{G}_2 = \sum_{i=1}^N p_i \mathbf{f}(x_i^*)\mathbf{f}^\top(x_i^*)$, we must have $N \geq q$, which means that there must be at least q support points. From Curto and Fialkow (1991) and Step (2 - i) in Algorithm I, there are at most $q+1$ support points. Thus the number of support points is either q or $q+1$.

(ii) For a symmetric design space $S = [-c, c]$, Gao and Zhou (2014) have proved that there exists a symmetric D-optimal design ξ_D^{SLS}. We prove by contradiction that the support points include the two boundary points. Suppose the ordered support points of a symmetric ξ_D^{SLS} are $x_1^* < x_2^* < \cdots < x_N^*$, and $|x_1^*| = x_N^* < c$. Define $\nu = \frac{c}{x_N^*}$, then we have $\nu > 1$ and all the points $\nu x_1^*, \nu x_2^*, \cdots, \nu x_N^*$ are still in the design space. Define a distribution ξ_D^+ on $S = [-c, c]$ as

$$\xi_D^+ = \left(\begin{array}{cccc} \nu x_1^* & \nu x_2^* & \cdots & \nu x_N^* \\ p_1 & p_2 & \cdots & p_N \end{array}\right),$$

and its moments are $\mu_j^+ = \nu^j \mu_j^*$, $j = 1, \cdots, 2q$. By (8), it is easy to verify that

$$\det\left(\mathbf{A}(t, \mu_1^+, \cdots, \mu_{2q}^+)\right) = \nu^{q(q+1)} \det\left(\mathbf{A}(t, \mu_1^*, \cdots, \mu_{2q}^*)\right) > \det\left(\mathbf{A}(t, \mu_1^*, \cdots, \mu_{2q}^*)\right),$$

which implies that $\phi(\mu_1^+, \cdots, \mu_{2q}^+) < \phi(\mu_1^*, \cdots, \mu_{2q}^*)$. This is a contradiction to the fact that the ξ_D^{SLS} minimizes $\phi(\mu_1, \cdots, \mu_{2q})$. Therefore, the support points of ξ_D^{SLS} must include the two boundary points $-c$ and c.

The results in (iii) and (iv) can be proved similarly to the result in (ii), and the proof is omitted. □

Acknowledgements

This research work is supported by Discovery Grants from the Natural Science and Engineering Research Council of Canada. The authors thank Professor Jiawang Nie for his valuable suggestions that lead to the development of Algorithm I. The authors are also grateful to the Editor and reviewers for their helpful comments and suggestions.

References

Berger, M.P.F. and Wong, W.K. (2009). *An Introduction to Optimal Designs for Social and Biomedical Research.* Wiley, Chichester.

Boyd, S. and Vandenberghe, L. (2004). *Convex Optimization.* Cambridge University Press, New York.

Chang, F.C., Imhof, L. and Sun, Y.Y. (2013). Exact D-optimal designs for first-order trigonometric regression models on a partial circle. *Metrika*, 76, 857-872.

Curto, R.E. and Fialkow, L.A. (1991). Recursiveness, positivity, and truncated moment problems. *Houston Journal of Mathematics*, 17, 603-635.

Dette, H., Melas, V.B. and Pepelyshev, A. (2002). D-optimal designs for trigonometric regression models on a partial circle. *Annals of the Institute of Statistical Mathematics*, 54, 945-959.

Dette, H., Pepelyshev, A. and Zhigljavsky, A. (2008). Improving updating rules in multiplicative algorithms for computing D-optimal designs. *Computational Statistics and Data Analysis*, 53, 312-320.

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

Duarte, B.P.M. and Wong, W.K. (2014a). A semi-infinite programming based algorithm for finding minimax D-optimal designs for nonlinear models. *Statistics and Computing*, 24, 1063-1080.

Duarte, B.P.M. and Wong, W.K. (2014b). Finding Bayesian optimal designs for nonlinear models: A semidefinite programming-based approach. *International Statistical Review*, in press.

Duarte, B.P.M., Wong, W.K. and Atkinson, A.C. (2015). A semi-infinite programming based algorithm for determining T-optimum designs for model discrimination. *Journal of Multivariate Analysis*, 135, 11-24.

Fedorov, V.V. (1972). *Theory Of Optimal Experiments*. Academic Press, New York.

Gao, L.L. and Zhou, J. (2014). New optimal design criteria for regression models with asymmetric errors. *Journal of Statistical Planning and Inference*, 149, 140-151.

Grant, M.C. and Boyd, S.P. (2013). *The CVX Users' Guide*. Release 2.0 (beta), CVX Research, Inc. (http://cvxr.com/cvx/doc/CVX.pdf, October 14, 2013.)

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

Laurent, M. (2010). Updated version of *Sums of squares, moment matrices and optimization over polynomials*, Available at http://homepages.cwi.nl/~ monique/files/moment-ima-update-new.pdf, (February 6, 2010).

Lu, Z. and Pong, T.K. (2013). Computing optimal experimental designs via interior point method. *SIAM Journal on Matrix Analysis and Applications*, 34, 1556-1580.

Papp, D. (2012). Optimal designs for rational function regression. *Journal of the American Statistical Association*, 107, 400-411.

Pronzato, L. and Pázman, A. (2013). *Design of Experiments in Nonlinear Models - Asymptotic Normality, Optimality Criteria and Small-Sample Properties*. Springer, New York.

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

Seber, G.A.F. (2008). *A Matrix Handbook for Statisticians*. Wiley, Hoboken.

Silvey, S.D., Titterington, D.M. and Torsney, B. (1978). An algorithm for optimal designs on a finite design space. *Communications in Statistics - Theory and Methods*, 14, 1379-1389.

Wang, L. and Leblanc, A. (2008). Second-order nonlinear least squares estimation. *Annals of the Institute of Statistical Mathematics*, 60, 883-900.

Xu, X. and Shang, X. (2014). Optimal and robust designs for trigonometric regression models. *Metrika*, 77, 753-769.

Yu, Y. (2010). Monotonic convergence of a general algorithm for computing optimal designs. *Annals of Statistics*, 38, 1593-1606.

Yu, Y. (2011). D-optimal designs via a cocktail algorithm. *Statistics and Computing*, 21, 475-481.

Zhang, C. (2007). Optimal designs for trigonometric regression. *Communications in Statistics - Theory and Methods*, 36, 755-766.

Table 1: D-optimal designs for the polynomial models and $S_1 = [-1, 1]$. For all models, $\mu_i^* = 0$ if i is odd.

q	t	D-optimal moments and distributions
2	0	$(\mu_2^*,\ \mu_4^*) = (1.000,\ 1.000)$
		$(x_1^*,\ x_2^*) = (-1.000,\ 1.000)$
		$(p_1,\ p_2) = (0.500,\ 0.500)$
	0.7	$(\mu_2^*,\ \mu_4^*,\ \mu_6^*) = (0.952,\ 0.952,\ 0.952)$
		$(x_1^*,\ x_2^*,\ x_3^*) = (-1.000,\ 0.000,\ 1.000)$
		$(p_1,\ p_2,\ p_3) = (0.476,\ 0.048,\ 0.476)$
3	0	$(\mu_2^*,\ \mu_4^*,\ \mu_6^*,\ \mu_8^*) = (0.773,\ 0.691,\ 0.661,\ 0.650)$
		$(x_1^*,\ x_2^*,\ x_3^*,\ x_4^*) = (-1.000, -0.602,\ 0.602,\ 1.000)$
		$(p_1,\ p_2,\ p_3,\ p_4) = (0.322,\ 0.178,\ 0.178,\ 0.322)$
	0.3	$(\mu_2^*,\ \mu_4^*,\ \mu_6^*,\ \mu_8^*) = (0.761,\ 0.678,\ 0.649,\ 0.639)$
		$(x_1^*,\ x_2^*,\ x_3^*,\ x_4^*) = (-1.000, -0.589,\ 0.589,\ 1.000)$
		$(p_1,\ p_2,\ p_3,\ p_4) = (0.317,\ 0.183,\ 0.183,\ 0.317)$
	0.7	$(\mu_2^*,\ \mu_4^*,\ \mu_6^*,\ \mu_8^*) = (0.711,\ 0.627,\ 0.603,\ 0.596)$
		$(x_1^*,\ x_2^*,\ x_3^*,\ x_4^*) = (-1.000, -0.539,\ 0.539,\ 1.000)$
		$(p_1,\ p_2,\ p_3,\ p_4) = (0.296,\ 0.204,\ 0.204,\ 0.296)$
5	0	$(\mu_2^*,\ \mu_4^*,\ \mu_6^*,\ \mu_8^*,\ \mu_{10}^*,\ \mu_{12}^*) = (0.660,\ 0.538,\ 0.479,\ 0.446,\ 0.426,\ 0.414)$
		$(x_1^*,\ x_2^*,\ x_3^*,\ x_4^*,\ x_5^*,\ x_6^*) = (-1.000, -0.781, -0.434,\ 0.434,\ 0.781,\ 1.000)$
		$(p_1,\ p_2,\ p_3,\ p_4,\ p_5,\ p_6) = (0.198,\ 0.178,\ 0.124,\ 0.124,\ 0.178,\ 0.198)$
	0.7	$(\mu_2^*,\ \mu_4^*,\ \mu_6^*,\ \mu_8^*,\ \mu_{10}^*,\ \mu_{12}^*) = (0.642,\ 0.522,\ 0.465,\ 0.433,\ 0.414,\ 0.402)$
		$(x_1^*,\ x_2^*,\ x_3^*,\ x_4^*,\ x_5^*,\ x_6^*) = (-1.000, -0.776, -0.398,\ 0.398,\ 0.776,\ 1.000)$
		$(p_1,\ p_2,\ p_3,\ p_4,\ p_5,\ p_6) = (0.193,\ 0.179,\ 0.128,\ 0.128,\ 0.179,\ 0.193)$

Table 2: D-optimal designs for the polynomial models and $S_2 = [0, 1]$.

q	t	D-optimal moments and distributions
2	0	$(\mu_1^*,\ \mu_2^*,\ \mu_3^*,\ \mu_4^*) = (0.750,\ 0.625,\ 0.563,\ 0.531)$ $(x_1^*,\ x_2^*) = (0.500,\ 1.000)$ $(p_1, p_2) = (0.500,\ 0.500)$
	0.7	$(\mu_1^*,\ \mu_2^*,\ \mu_3^*,\ \mu_4^*,\ \mu_5^*,\ \mu_6^*) = (0.714,\ 0.595,\ 0.536,\ 0.506,\ 0.491,\ 0.484)$ $(x_1^*,\ x_2^*,\ x_3^*) = (0.000,\ 0.500,\ 1.000)$ $(p_1,\ p_2,\ p_3) = (0.048,\ 0.476,\ 0.476)$
3	0	$(\mu_1^*,\ \mu_2^*,\ \mu_3^*,\ \mu_4^*,\ \mu_5^*,\ \mu_6^*) = (0.667,\ 0.533,\ 0.467,\ 0.427,\ 0.400,\ 0.381)$ $(x_1^*,\ x_2^*,\ x_3^*) = (0.276,\ 0.724,\ 1.000)$ $(p_1,\ p_2,\ p_3) = (0.333,\ 0.334,\ 0.333)$
	0.9	$(\mu_1^*,\ \mu_2^*,\ \mu_3^*,\ \mu_4^*,\ \mu_5^*,\ \mu_6^*,\ \mu_7^*,\ \mu_8^*) =$ $(0.556,\ 0.444,\ 0.389,\ 0.356,\ 0.333,\ 0.318,\ 0.307,\ 0.299)$ $(x_1^*,\ x_2^*,\ x_3^*,\ x_4^*) = (0.000,\ 0.276,\ 0.724,\ 1.000)$ $(p_1,\ p_2,\ p_3,\ p_4) = (0.166,\ 0.278,\ 0.278,\ 0.278)$
4	0	$(\mu_1^*,\ \mu_2^*,\ \mu_3^*,\ \mu_4^*,\ \mu_5^*,\ \mu_6^*,\ \mu_7^*,\ \mu_8^*) =$ $(0.625,\ 0.491,\ 0.424,\ 0.383,\ 0.355,\ 0.334,\ 0.318,\ 0.306)$ $(x_1^*,\ x_2^*,\ x_3^*,\ x_4^*) = (0.173,\ 0.500,\ 0.827,\ 1.000)$ $(p_1,\ p_2,\ p_3,\ p_4) = (0.250,\ 0.250,\ 0.250,\ 0.250)$
	0.9	$(\mu_1^*,\ \mu_2^*,\ \mu_3^*,\ \mu_4^*,\ \mu_5^*,\ \mu_6^*,\ \mu_7^*,\ \mu_8^*,\ \mu_9^*,\ \mu_{10}^*) =$ $(0.556,\ 0.437,\ 0.377,\ 0.340,\ 0.315,\ 0.297,\ 0.283,\ 0.272,\ 0.263,\ 0.256)$ $(x_1^*,\ x_2^*,\ x_3^*,\ x_4^*,\ x_5^*) = (0.000,\ 0.173,\ 0.500,\ 0.828,\ 1.000)$ $(p_1,\ p_2,\ p_3,\ p_4,\ p_5) = (0.112,\ 0.222,\ 0.222,\ 0.222,\ 0.222)$

Table 3: D-optimal designs for the trigonometric models and $S_x = [-\pi, \pi]$. For all models, $u_i^* = 0$ if i is odd. The optimal designs do not depend on parameter t.

q	D-optimal moments and distributions
2	$(u_2^*,\ u_4^*,\ u_6^*) = (0.500,\ 0.375,\ 0.281)$
	$(z_1^*,\ z_2^*,\ z_3^*) = (0.866,\ 0.000, -0.866)$
	$(p_1,\ p_2,\ p_3) = (0.333,\ 0.334,\ 0.333)$
	$(x_1^*,\ x_2^*,\ x_3^*) = (0.524,\ 1.571,\ 2.618)$
3	$(u_2^*,\ u_4^*,\ u_6^*,\ u_8^*) = (0.500,\ 0.375,\ 0.313,\ 0.266)$
	$(z_1^*,\ z_2^*,\ z_3^*,\ z_4^*) = (0.924,\ 0.383, -0.383, -0.924)$
	$(p_1,\ p_2,\ p_3,\ p_4) = (0.250,\ 0.250,\ 0.250,\ 0.250)$
	$(x_1^*,\ x_2^*,\ x_3^*,\ x_4^*) = (0.393,\ 1.178,\ 1.964,\ 2.749)$
4	$(u_2^*,\ u_4^*,\ u_6^*,\ u_8^*,\ u_{10}^*) = (0.500,\ 0.375,\ 0.313,\ 0.273,\ 0.244)$
	$(z_1^*,\ z_2^*,\ z_3^*,\ z_4^*,\ z_5^*) = (0.951,\ 0.588,\ 0.000, -0.588, -0.951)$
	$(p_1,\ p_2,\ p_3,\ p_4,\ p_5) = (0.200,\ 0.200,\ 0.200,\ 0.200,\ 0.200)$
	$(x_1^*,\ x_2^*,\ x_3^*,\ x_4^*,\ x_5^*) = (0.314,\ 0.943,\ 1.571,\ 2.200,\ 2.827)$
5	$(u_2^*,\ u_4^*,\ u_6^*,\ u_8^*,\ u_{10}^*,\ u_{12}^*) = (0.500,\ 0.375,\ 0.313,\ 0.273,\ 0.246,\ 0.225)$
	$(z_1^*,\ z_2^*,\ z_3^*,\ z_4^*,\ z_5^*,\ z_6^*) = (0.966,\ 0.707,\ 0.259, -0.259, -0.707, -0.966)$
	$(p_1,\ p_2,\ p_3,\ p_4,\ p_5,\ p_6) = (0.167,\ 0.166,\ 0.167,\ 0.167,\ 0.166,\ 0.167)$
	$(x_1^*,\ x_2^*,\ x_3^*,\ x_4^*,\ x_5^*,\ x_6^*) = (0.262,\ 0.785,\ 1.310,\ 1.833,\ 2.356,\ 2.880)$

Table 4: D-optimal designs for the trigonometric models and $S_x = [-3\pi/4, 3\pi/4]$.

q	t	D-optimal moments and distributions
2	0	$(u_1^*,\ u_2^*,\ u_3^*,\ u_4^*,\ u_5^*,\ u_6^*) = (0.073,\ 0.411,\ 0.069,\ 0.277,\ 0.119,\ 0.227)$
		$(z_1^*,\ z_2^*,\ z_3^*) = (1.000,\ 0.326, -0.707)$
		$(p_1,\ p_2,\ p_3) = (0.181,\ 0.456,\ 0.363)$
		$(x_1^*,\ x_2^*,\ x_3^*) = (0.000,\ 1.239,\ 2.356)$
4	0	$(u_1^*,\ u_2^*,\ u_3^*,\ u_4^*,\ u_5^*,\ u_6^*,\ u_7^*,\ u_8^*,\ u_9^*,\ u_{10}^*) =$
		$(0.145,\ 0.414,\ 0.155,\ 0.266,\ 0.147,\ 0.198,\ 0.137,\ 0.160,\ 0.127,\ 0.136)$
		$(z_1^*,\ z_2^*,\ z_3^*,\ z_4^*,\ z_5^*) = (1.000,\ 0.828,\ 0.388, -0.258, -0.707)$
		$(p_1,\ p_2,\ p_3,\ p_4,\ p_5) = (0.093,\ 0.235,\ 0.204,\ 0.243,\ 0.225)$
		$(x_1^*,\ x_2^*,\ x_3^*,\ x_4^*,\ x_5^*) = (0.000,\ 0.595,\ 1.173,\ 1.831,\ 2.356)$
	0.6	$(u_1^*,\ u_2^*,\ u_3^*,\ u_4^*,\ u_5^*,\ u_6^*,\ u_7^*,\ u_8^*,\ u_9^*,\ u_{10}^*) =$
		$(0.141,\ 0.408,\ 0.154,\ 0.263,\ 0.148,\ 0.197,\ 0.138,\ 0.161,\ 0.129,\ 0.139)$
		$(z_1^*,\ z_2^*,\ z_3^*,\ z_4^*,\ z_5^*) = (1.000,\ 0.804,\ 0.314, -0.296, -0.707)$
		$(p_1,\ p_2,\ p_3,\ p_4,\ p_5) = (0.105,\ 0.239,\ 0.207,\ 0.234,\ 0.215)$
		$(x_1^*,\ x_2^*,\ x_3^*,\ x_4^*,\ x_5^*) = (0.000,\ 0.637,\ 1.251,\ 1.871,\ 2.356)$
5	0	$(u_1^*,\ u_2^*,\ u_3^*,\ u_4^*,\ u_5^*,\ u_6^*,\ u_7^*,\ u_8^*,\ u_9^*,\ u_{10}^*) =$
		$(0.154,\ 0.407,\ 0.161,\ 0.265,\ 0.156,\ 0.203,\ 0.148,\ 0.169,\ 0.140,\ 0.148)$
		$(z_1^*,\ z_2^*,\ z_3^*,\ z_4^*,\ z_5^*) = (0.964,\ 0.667,\ 0.196, -0.348, -0.707)$
		$(p_1,\ p_2,\ p_3,\ p_4,\ p_5) = (0.200,\ 0.200,\ 0.200,\ 0.200,\ 0.200)$
		$(x_1^*,\ x_2^*,\ x_3^*,\ x_4^*,\ x_5^*) = (0.271,\ 0.841,\ 1.373,\ 1.926,\ 2.356)$
	0.8	$(u_1^*,\ u_2^*,\ u_3^*,\ u_4^*,\ u_5^*,\ u_6^*,\ u_7^*,\ u_8^*,\ u_9^*,\ u_{10}^*,\ u_{11}^*,\ u_{12}^*) =$
		$(0.153,\ 0.405,\ 0.161,\ 0.264,\ 0.156,\ 0.202,\ 0.148,\ 0.168,\ 0.139,\ 0.147,\ 0.130,\ 0.132)$
		$(z_1^*,\ z_2^*,\ z_3^*,\ z_4^*,\ z_5^*,\ z_6^*) = (1.000,\ 0.900,\ 0.588,\ 0.135, -0.372, -0.707)$
		$(p_1,\ p_2,\ p_3,\ p_4,\ p_5,\ p_6) = (0.083,\ 0.162,\ 0.184,\ 0.184,\ 0.193,\ 0.194)$
		$(x_1^*,\ x_2^*,\ x_3^*,\ x_4^*,\ x_5^*,\ x_6^*) = (0.011,\ 0.450,\ 0.942,\ 1.436,\ 1.952,\ 2.356)$

Table 5: D-optimal designs for the trigonometric models and $S_x = [-2\pi/3, 2\pi/3]$.

q	t	D-optimal moments and distributions
2	0	$(u_1^*,\ u_2^*,\ u_3^*,\ u_4^*,\ u_5^*,\ u_6^*) = (0.206,\ 0.335,\ 0.160,\ 0.202,\ 0.162,\ 0.174)$
		$(z_1^*,\ z_2^*,\ z_3^*) = (1.000,\ 0.411, -0.500)$
		$(p_1,\ p_2,\ p_3) = (0.167,\ 0.500,\ 0.333)$
		$(x_1^*,\ x_2^*,\ x_3^*) = (0.000,\ 1.147,\ 2.094)$
	0.4	$(u_1^*,\ u_2^*,\ u_3^*,\ u_4^*,\ u_5^*,\ u_6^*) = (0.193,\ 0.345,\ 0.165,\ 0.212,\ 0.171,\ 0.185)$
		$(z_1^*,\ z_2^*,\ z_3^*) = (1.000,\ 0.411, -0.500)$
		$(p_1,\ p_2,\ p_3) = (0.177,\ 0.469,\ 0.354)$
		$(x_1^*,\ x_2^*,\ x_3^*) = (0.000,\ 1.147,\ 2.094)$
4	0	$(u_1^*,\ u_2^*,\ u_3^*,\ u_4^*,\ u_5^*,\ u_6^*,\ u_7^*,\ u_8^*) =$
		$(0.241,\ 0.365,\ 0.224,\ 0.240,\ 0.194,\ 0.189,\ 0.170,\ 0.162)$
		$(z_1^*,\ z_2^*,\ z_3^*,\ z_4^*) = (0.944,\ 0.563, -0.041, -0.500)$
		$(p_1,\ p_2,\ p_3,\ p_4) = (0.250,\ 0.250,\ 0.250,\ 0.250)$
		$(x_1^*,\ x_2^*,\ x_3^*,\ x_4^*) = (0.335,\ 0.973,\ 1.161,\ 2.094)$
	0.95	$(u_1^*,\ u_2^*,\ u_3^*,\ u_4^*,\ u_5^*,\ u_6^*,\ u_7^*,\ u_8^*,\ u_9^*,\ u_{10}^*) =$
		$(0.240,\ 0.362,\ 0.223,\ 0.238,\ 0.193,\ 0.188,\ 0.169,\ 0.161,\ 0.151,\ 0.144)$
		$(z_1^*,\ z_2^*,\ z_3^*,\ z_4^*,\ z_5^*) = (1.000,\ 0.867,\ 0.475, -0.083, -0.500)$
		$(p_1,\ p_2,\ p_3,\ p_4,\ p_5) = (0.093,\ 0.210,\ 0.220,\ 0.236,\ 0.241)$
		$(x_1^*,\ x_2^*,\ x_3^*,\ x_4^*,\ x_5^*) = (0.000,\ 0.522,\ 1.076,\ 1.654,\ 2.094)$
5	0	$(u_1^*,\ u_2^*,\ u_3^*,\ u_4^*,\ u_5^*,\ u_6^*,\ u_7^*,\ u_8^*,\ u_9^*,\ u_{10}^*) =$
		$(0.248,\ 0.358,\ 0.227,\ 0.237,\ 0.196,\ 0.190,\ 0.172,\ 0.164,\ 0.154,\ 0.147)$
		$(z_1^*,\ z_2^*,\ z_3^*,\ z_4^*,\ z_5^*) = (0.966,\ 0.703,\ 0.269, -0.200, -0.500)$
		$(p_1,\ p_2,\ p_3,\ p_4,\ p_5) = (0.200,\ 0.200,\ 0.200,\ 0.200,\ 0.200)$
		$(x_1^*,\ x_2^*,\ x_3^*,\ x_4^*,\ x_5^*) = (0.263,\ 0.791,\ 1.299,\ 1.772,\ 2.094)$