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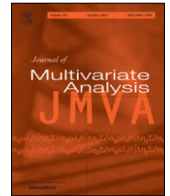
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D-optimal design for the heteroscedastic Berman model on an arc

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ABSTRACT

There are various methods for fitting data to circles or ellipses in many different types of applied problems. However, the design of such studies is rarely discussed and for the few that do, model errors are commonly assumed to be homoscedastic and uncorrelated. This paper provides an analytic description of the *D*-optimal designs for estimating parameters in the bivariate Berman model on an arc when errors are correlated and heteroscedastic. We evaluate *D*-efficiencies and relative efficiencies of the commonly used equidistant sampling methods and show that such designs can be inefficient.

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1. Introduction

Circle fitting is one of the most fundamental tasks in computer graphics, image processing, microwave engineering, industry and mechanical engineering, with many more applications in other fields; see, e.g., [1,3,6,7,26]. In particular, SenGupta and Ugwuowon [20] provided interesting applications of circular models in solar energy radiation and wind energy experiments. Various methods of fitting circular data were proposed in [11,15,21,22], among others, and inferential issues have been quite extensively studied. For example, bias issues in using least squares estimators to fit circular data when the sample is large were studied in [2] and [14]. Most recently, Fernández-Durán and Gregorio-Domínguez [9] noted that the statistical analysis of circular, multivariate circular, and spherical data is very important in different areas, such as paleomagnetism, astronomy and biology, and they developed an R package for analyzing circular data. Further references and discussion on data analysis for circular data are available in book length monographs; see [4,10,13,16].

One of the most frequently used models for fitting circular data is Berman's circular model. The model assumes that the angular differences between sample points are known in advance, either from the special structure of the problem or through experimental design. Chernov and Sapirstein [5] and Kasa [15] noted that there are situations where the common assumptions of homoscedasticity and uncorrelated observations for Berman's model may fail. For example, in microwave engineering, the different characters of the two channels and non-stationary features of a measurement system lead to unequal variances of the coordinates. Likewise, correlations may be introduced in the process of digitizing archeological field data and motivated [5] to incorporate correlated noise when fitting data to circles. Early attempts to address such concerns in the analysis phase include [23], where the problem of fitting the Berman model with heteroscedastic error variances was investigated.

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Our aim is to construct analytical D -optimal designs for the bivariate Berman model on a circle or a circular arc when errors are heteroscedastic and correlated. Our theoretical contributions are thus new because all previous design work for Berman's model assumes homoscedasticity and uncorrelated responses in this model. In addition, we study robustness properties of some aspects of the D -optimal designs to model violations, namely, whether the optimal design found under the homoscedastic assumption remains efficient when heteroscedasticity is present or to mis-specification of the nominal value of the correlation coefficient in the model.

The rest of the paper is organized as follows. Section 2 introduces Berman's model with correlated errors and heteroscedastic variances, along with a brief literature review of design work for the model. In Section 3, we construct an essentially complete class of designs for an easier search of the optimal design within this smaller class of designs. It is shown that designs in this class have a very simple structure and this information facilitates our search for D -optimal designs for Berman's model with heteroscedastic and correlated errors. Section 4 derives the D -optimal designs explicitly and we show that the commonly used equidistant sampling method is generally inefficient for estimating the model parameters. Section 5 contains a summary and all proofs are in the [Appendix](#).

2. Berman's model

Berman's bivariate linear regression model on a circle or a circular arc has two responses y_1 and y_2 observed with corresponding errors ε_1 and ε_2 . The mean responses are functions of the univariate design variable t and are given by

$$\begin{cases} y_1 = \theta_1 + \theta_3 \cos t - \theta_4 \sin t + \varepsilon_1, \\ y_2 = \theta_2 + \theta_3 \sin t + \theta_4 \cos t + \varepsilon_2, \end{cases} \quad (1)$$

where $\theta_1, \theta_2, \theta_3, \theta_4 \in \mathbb{R}$ are unknown parameters. The experimental domain or design space is $\mathcal{X} = [-\alpha/2, \alpha/2]$ and consists of all possible values of t . In practice, the value of α is user-selected and $\alpha \in (0, 2\pi]$ is the length of the arc. This model is the same as that discussed in [24] except that we do not assume $\sigma_1^2 = \sigma_2^2$ and $\rho = 0$. The variance-covariance matrix of $\varepsilon = (\varepsilon_1, \varepsilon_2)^\top$ is assumed to be

$$\Sigma = \begin{pmatrix} \sigma_1^2 & \rho\sigma_1\sigma_2 \\ \rho\sigma_1\sigma_2 & \sigma_2^2 \end{pmatrix}, \quad |\rho| < 1. \quad (2)$$

The model was proposed by Berman [1] with two particular applications in mind: (i) the calibration of an impedance measuring apparatus in microwave engineering, and (ii) the analysis of megalithic sites in Britain, in which archaeologists need to fit circles to stone rings. Let (y_{1k}, y_{2k}) be the k th coordinated measurement of the k th measurement point on the arc and t_k be the corresponding angular difference. Model (1) assumes the information that the differences t_k between the angular coordinates of successive data points are known in advance, either from the special structure of the problem or through the experimental design. Further extensions of model (1) were then considered. For example, Wang and Lam [22] extended Berman's model to simultaneous fitting of several circles, where one tests the hypothesis that several round objects have the same size. Such problems arise in quality control of manufactured mechanical parts.

Statistical inference for this model is mostly based on the likelihood approach. Following convention, the worth of a design is measured by its Fisher information matrix, which is obtained by taking the expectation of the second derivatives of the total log likelihood function with respect to the model parameters and multiplied by -1 . Maximum likelihood estimates for the model parameters are then obtained by maximizing the total likelihood function.

It is instructive to write the model in matrix form as $Y(t) = F(t)\theta + \varepsilon$, where

$$Y(t) = \begin{pmatrix} y_1(t) \\ y_2(t) \end{pmatrix}, \quad F(t) = (I_2, A(t)), \quad I_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{and} \quad A(t) = \begin{pmatrix} \cos t & -\sin t \\ \sin t & \cos t \end{pmatrix}.$$

The parameter vector for the regression model is $\theta = (\theta_1, \theta_2, \theta_3, \theta_4)^\top$, where $(\theta_1, \theta_2)^\top$ is the center and $r = (\theta_3^2 + \theta_4^2)^{1/2}$ is the radius of the circular arc. This form is helpful in the next section for finding the D -optimal designs analytically.

Design issues are an important component in many scientific studies. A poorly designed study wastes resources and provides unreliable inference sought for the study. There already exists some design work for Berman's model. Wu [24] used the Φ -optimality design criterion and provided a thorough discussion on the construction of optimal exact designs for Berman's model on a circle or a circular arc. Harman [12] developed the convex Schur optimality criterion and obtained optimal approximate designs for Berman's model using the equivalence theorem, which is applicable for any convex design criterion. Liu et al. [17] introduced the I_L^∞ -optimality criterion and found analytical descriptions of the I_L^1 - and I_L^∞ -optimal approximate designs for Berman's model.

The key difference between optimal exact designs and optimal approximate designs is that the latter are much easier to construct than optimal exact designs because there is no general approach to determine an optimal exact design. The mathematical derivation of an exact optimal design is invariably complex and depends crucially on every aspect of the model assumptions, the design criterion and the number of observations available for the study. Further, a given methodology may no longer apply if the model is slightly changed. In contrast, there is a unified approach and theory for finding optimal approximate designs under a convex design criterion. For example, there are algorithms for finding optimal approximate designs regardless of the models and theory to confirm optimality of a design.

For these reasons, we focus on approximate designs in this paper and gauge their worth using the normalized information matrix, which measures their worth per observation. In the literature, approximate designs are sometimes referred to as continuous designs and may be regarded as large-sample designs because they are limits of exact optimal designs when the sample size becomes large.

3. Complete classes

Let ξ be an approximate design on a user-selected compact design space $\mathcal{X}$ and given by

$$\xi = \begin{pmatrix} t_1 & \cdots & t_n \\ w_1 & \cdots & w_n \end{pmatrix}.$$

Here $t_1, \dots, t_n$ are distinct points from the design space $\mathcal{X}$ and are called support points of the design ξ when all the weights $w_1, \dots, w_n$ are positive and sum to unity. If there are resources to take N observations for the study, then each Nw_i is rounded to a positive integer and Nw_i observations are taken at $t_1, \dots, t_n$ and subject to $Nw_1 + \cdots + Nw_n = N$.

Following Section 1.7 in [8], the normalized Fisher information matrix of an approximate design ξ under multiresponse linear models is defined by

$$M(\xi) = \int_{\mathcal{X}} F^T(t) \Sigma^{-1} F(t) d\xi(t).$$

A direct calculation shows the normalized Fisher information matrix of an approximate design ξ under model (1) is

$$M(\xi) = \begin{pmatrix} \Sigma^{-1} & \Sigma^{-1} A(\xi) \\ A^T(\xi) \Sigma^{-1} & B(\xi) \end{pmatrix},$$

where, as before, $\mathcal{X} = [-\alpha/2, \alpha/2]$,

$$A(\xi) = \int_{\mathcal{X}} A(t) d\xi = \begin{pmatrix} c_1(\xi) & -s_1(\xi) \\ s_1(\xi) & c_1(\xi) \end{pmatrix}, \quad c_1(\xi) = \sum_{k=1}^n w_k \cos t_k, \quad s_1(\xi) = \sum_{k=1}^n w_k \sin t_k,$$

$$B(\xi) = \int_{\mathcal{X}} A^T(t) \Sigma^{-1} A(t) d\xi = \frac{1}{\det(\Sigma)} \left\{ \frac{\sigma_1^2 + \sigma_2^2}{2} I_2 - \frac{c_2(\xi)}{2} P + \frac{s_2(\xi)}{2} QP \right\},$$

$$c_2(\xi) = \sum_{k=1}^n w_k \cos 2t_k, \quad s_2(\xi) = \sum_{k=1}^n w_k \sin 2t_k, \quad P = \begin{pmatrix} \sigma_1^2 - \sigma_2^2 & 2\rho\sigma_1\sigma_2 \\ 2\rho\sigma_1\sigma_2 & \sigma_2^2 - \sigma_1^2 \end{pmatrix} \quad \text{and} \quad Q = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.$$

D -optimal designs are undoubtedly the most sought after designs in the literature. A D -optimal design maximizes the logarithm of the determinant of the information matrix, which is a concave functional over the set of all designs on $\mathcal{X}$. When errors are normally distributed, a D -optimal design minimizes the generalized variance of the estimated model parameters and so provides the smallest confidence ellipsoid for the model parameters. Consequently, such optimal designs provide the most accurate inference for the model parameters. Another reason for their popularity is that they tend to be easier to construct analytically compared with other optimal designs.

In what is to follow, we exploit the symmetry of a design to simplify the search for an optimal design. In particular, for each approximate design ξ , let $\tilde{\xi}$ be its reflection across the midpoint of the arc, i.e., $\tilde{\xi}(t) = \xi(-t)$ for all $t \in \mathcal{X}$. As we will show, such an approach typically leads to an essentially complete class theorem that allows us to find the optimal design within a substantially smaller subset of designs on $\mathcal{X}$. The following lemmas are helpful for deriving the desired results.

Lemma 1. *The information matrix $M(\tilde{\xi})$ of $\tilde{\xi}$ is similar to the information matrix $M(\xi)$ of ξ . If ξ is D -optimal, then $\tilde{\xi}$ is also D -optimal, and so is the symmetrized design $\xi^* = (\xi + \tilde{\xi})/2$.*

The implication of Lemma 1 is that it is sufficient to search for the optimal design among symmetric designs on $\mathcal{X} = [-\alpha/2, \alpha/2]$. For such a symmetric design measure, say $\tilde{\xi}$, its moment matrix under model (1) is given by

$$M(\tilde{\xi}) = \begin{pmatrix} \Sigma^{-1} & c_1(\tilde{\xi}) \Sigma^{-1} \\ c_1(\tilde{\xi}) \Sigma^{-1} & B(\tilde{\xi}) \end{pmatrix}, \tag{3}$$

where

$$B(\tilde{\xi}) = \frac{1}{\det(\Sigma)} \left\{ \frac{\sigma_1^2 + \sigma_2^2}{2} I_2 - \frac{c_2(\tilde{\xi})}{2} P \right\}.$$

Lemma 2. *For every design measure ξ on the experimental domain $\mathcal{X} = [-\alpha/2, \alpha/2]$, the following statements hold.*

- (i) $\cos(\alpha/2) \leq c_1(\xi) \leq 1$.

- (ii) $2c_1^2(\xi) - 1 \leq c_2(\xi) \leq 2\{\cos(\alpha/2) + 1\}\{c_1(\xi) - 1\} + 1$.
 (iii) If the design $\bar{\xi}_S$ is symmetric and $c_2(\bar{\xi}_S) = 2\{\cos(\alpha/2) + 1\}\{c_1(\bar{\xi}_S) - 1\} + 1$, the design $\bar{\xi}_S$ has the following form for some $w \in (0, 1]$:

$$\bar{\xi}_S = \begin{pmatrix} -\alpha/2 & 0 & \alpha/2 \\ w/2 & 1-w & w/2 \end{pmatrix}. \quad (4)$$

Let $\mathcal{E}_S$ be the set of symmetric designs of the form (4).

Theorem 1. Let ξ^* be a D -optimal design for model (1) on the experimental domain $\mathcal{X} = [-\alpha/2, \alpha/2]$.

- (i) The set $\mathcal{E}_S$ is an essentially complete class of D -optimal designs for model (1) if $\alpha \in (0, 4\pi/3)$.
 (ii) The moments $(c_1(\xi^*), c_2(\xi^*))$ of ξ^* are $(0, 0)$ if $\alpha \in [4\pi/3, 2\pi]$.

Theorem 1 simplifies the design problem by identifying a complete subclass, $\mathcal{E}_S$, which is composed of relatively simple designs and small enough, such that for any design ξ not belonging to this class, there is a design in the class that has an information matrix dominating that of ξ in the Loewner ordering. Then the search is narrowed down. In view of Theorem 1, we consider hereafter only design measures in the set $\mathcal{E}_S$.

4. D -optimal designs

The following theorem gives the approximate D -optimal designs on an arc. It shows that the D -optimal design on the domain $\mathcal{X} = [-\alpha/2, \alpha/2]$ for model (1) depends on the covariance structure of Σ given in (2) only through the ratio $\lambda_\sigma = \sigma_1^2/\sigma_2^2$ of the two variances and the absolute value of the correlation coefficient $|\rho|$.

Theorem 2. Let $\mathcal{X} = [-\alpha/2, \alpha/2]$ be the experimental domain for model (1). Let also $\lambda_\sigma = \sigma_1^2/\sigma_2^2$ and $\tau = \{\cos(\alpha/2) - 1\}(1 + \lambda_\sigma)^2 + 4\lambda_\sigma(1 - \rho^2)$.

- (i) Suppose $\alpha \in (0, \pi]$ and $\tau \geq 0$. The design $\bar{\xi}_S$ in (4) is D -optimal if $w = 1$.
 (ii) Suppose $\alpha \in (0, \pi]$ and $\tau < 0$, or $\alpha \in (\pi, 4\pi/3)$. The design $\bar{\xi}_S$ in (4) is D -optimal if

$$w = \frac{-3b - \sqrt{9b^2 - 32ac}}{8a}, \quad (5)$$

where

$$a = \lambda_\sigma \{(\cos(\alpha/2) - 1)^2(1 - \rho^2)\}, \quad (6)$$

$$b = \{\cos(\alpha/2) - 1\}\{[1 + \cos(\alpha/2)](1 - \lambda_\sigma)^2 + 4\lambda_\sigma\{1 + \rho^2 \cos(\alpha/2)\}\}, \quad (7)$$

$$c = \{1 - \cos^2(\alpha/2)\}(1 - \lambda_\sigma)^2 + 4\lambda_\sigma\{1 - \rho^2 \cos^2(\alpha/2)\}. \quad (8)$$

- (iii) Suppose $\alpha \in [4\pi/3, 2\pi]$. The following design $\bar{\xi}_D$ is D -optimal:

$$\bar{\xi}_D = \begin{pmatrix} -2\pi/3 & 0 & 2\pi/3 \\ 1/3 & 1/3 & 1/3 \end{pmatrix}.$$

We denote such a D -optimal design by $\xi_D(\lambda_\sigma, \rho, \alpha)$ and by Theorem 2, it suffices to consider only the case where $\rho \geq 0$. Accordingly, $\xi_D(1, \rho, \alpha)$ is the D -optimal design for the model with homoscedastic responses and $\xi_D(\lambda_\sigma, 0, \alpha)$ is the D -optimal design for the model with uncorrelated responses.

Fig. 1 displays the equal weight at each of the endpoints $\pm\alpha/2$ of the two D -designs, $\xi_D(\lambda_\sigma, 0, \alpha)$ and $\xi_D(1, \rho, \alpha)$ as the design domain $\mathcal{X} = [-\alpha/2, \alpha/2]$ varies from $\alpha = 0$ to $\alpha = 4\pi/3$. The left panel shows $\rho = 0$ and $\lambda_\sigma \in (0, 10]$ and the right panel assumes $\rho \in [0, 1)$ and $\lambda_\sigma = 1$. We observe from Fig. 1 that there exists a certain region of (λ_σ, α) or (ρ, α) for which the D -optimal design $\xi_D(\lambda_\sigma, 0, \alpha)$ or $\xi_D(1, \rho, \alpha)$ is equally supported at two extreme points $\pm\alpha/2$ of the design domain. In fact, it can be verified from Theorem 2(i) and (4) that over the region $\alpha \in (0, \pi]$ and $\tau \geq 0$, $\xi_D(\lambda_\sigma, 0, \alpha)$ is equally supported at the two endpoints if $(\lambda_\sigma + 1)^2\{\cos(\alpha/2) - 1\} + 4\lambda_\sigma \geq 0$ and $\xi_D(1, \rho, \alpha)$ is equally supported at the two endpoints if $\cos(\alpha/2) - \rho^2 \geq 0$.

Table 1 displays the equal weight at each of the two endpoints $\pm\alpha/2$ of the D -optimal designs $\xi_D(\lambda_\sigma, \rho, \alpha)$ for various combinations of $\alpha \in \{\pi/3, \pi/2, \pi\}$, $\lambda_\sigma \in \{2, 5, 10, 100\}$, and $\rho \in \{0.1, 0.3, 0.5, 0.7, 0.9\}$. The D -optimal design has two support points at $\pm\alpha/2$ when the values of λ_σ , ρ and α are small, and has three support points at 0 and at $\pm\alpha/2$ when λ_σ or ρ or α becomes large.

McCool [18] and Wu [24] both observed that equidistant sampling is widely used in practice for sampling circular measure data because of its simplicity and intuitive appeal. Motivated by [24], we investigate the efficiencies of equidistant sampling schemes here. To this end, we use the determinant of the information matrix near (10) in the Appendix, and write the optimality criterion as

$$\Phi_D\{c_1(\xi), c_2(\xi)\} = \{1 - c_1^2(\xi)\}^2(1 + \lambda_\sigma)^2 - \{(\lambda_\sigma - 1)^2 + 4\rho^2\lambda_\sigma\}\{c_2(\xi) - c_1^2(\xi)\}^2.$$

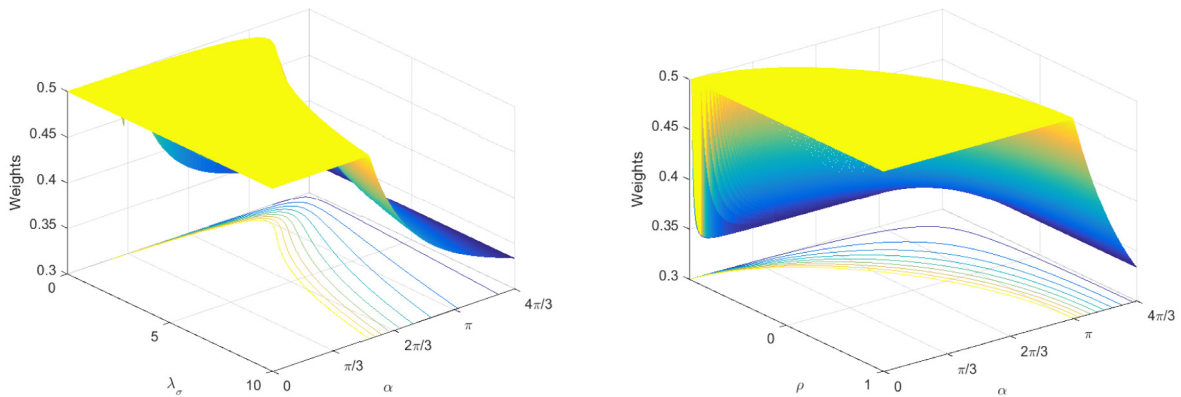


Fig. 1. The equal weight at each of the endpoints $\pm\alpha/2$ of the two D -designs, $\xi_D(\lambda_\sigma, 0, \alpha)$ and $\xi_D(1, \rho, \alpha)$, as the design domain $\mathcal{X} = [-\alpha/2, \alpha/2]$ varies from $\alpha = 0$ to $\alpha = 4\pi/3$. The left figure assumes that $\rho = 0$ and $\lambda_\sigma \in (0, 10]$ and the right figure assumes that $\rho \in [0, 1)$ and $\lambda_\sigma = 1$.

Table 1

The equal weight at each of the endpoints $\pm\alpha/2$ of the D -optimal designs for model (1) on the domain $\mathcal{X} = [-\alpha/2, \alpha/2]$ for various values of α , ρ and λ_σ .

α	λ_σ	ρ				
		0.1	0.3	0.5	0.7	0.9
$\pi/3$	2	0.5000	0.5000	0.5000	0.5000	0.5000
	5	0.5000	0.5000	0.5000	0.5000	0.4626
	10	0.5000	0.5000	0.5000	0.5000	0.4086
	100	0.3793	0.3755	0.3620	0.3568	0.3420
$\pi/2$	2	0.5000	0.5000	0.5000	0.5000	0.4226
	5	0.5000	0.5000	0.5000	0.4936	0.3873
	10	0.5000	0.5000	0.4706	0.4225	0.3647
	100	0.3525	0.3509	0.3478	0.3431	0.3370
π	2	0.4545	0.4357	0.4069	0.3761	0.3469
	5	0.3887	0.3827	0.3717	0.3575	0.3415
	10	0.3619	0.3592	0.3541	0.3469	0.3381
	100	0.3363	0.3360	0.3355	0.3348	0.3339

Because the model has four unknown parameters, we define the D -efficiency of a symmetric sampling scheme $\bar{\xi}$ by

$$\text{Eff}_D(\bar{\xi}) = \left[\frac{\Phi_D\{c_1(\bar{\xi}), c_2(\bar{\xi})\}}{\Phi_D\{c_1(\xi_D^*), c_2(\xi_D^*)\}} \right]^{1/4},$$

where ξ_D^* is the D -optimal design in Theorem 2. If the D -efficiency of the design $\bar{\xi}$ is one half, this means that the design $\bar{\xi}$ would need to be replicated twice to perform as well as the D -optimal design.

Let $\xi_{n,\alpha}$ be the equidistant sampling with sample size n on $\mathcal{X} = [-\alpha/2, \alpha/2]$ and its n support points are $t_j = -\alpha/2 + (j-1)\alpha/(n-1)$ for all $j \in \{1, \dots, n\}$. By [24], if $\alpha \in [2\pi(n-1)/n, 2\pi]$, then $\xi_{n,2\pi(n-1)/n}$ is an equidistant sampling on a complete cycle, which is D -optimal by Theorem 1 (ii). In this case, we use $\xi_{n,2\pi(n-1)/n}$ instead of $\xi_{n,\alpha}$. Fig. 2 displays the D -efficiencies of the equidistant sampling designs $\xi_{n,\alpha}$ for $\alpha \in (0, 2\pi]$, $n = 5$ and $n = 10$ for the model (1) with $\rho = 0$ and $\lambda_\sigma = 1$, respectively. We observe that when $\alpha \in (0, 4\pi/3]$, most of the D -efficiencies are less than 0.8, suggesting that there is some room for improvement in the efficiency of the designs.

Next, we present a simulation study to compare the D -optimal design ξ_D and the equidistant sampling design $\xi_{n,\alpha}$ on $[-\alpha/2, \alpha/2]$. Denoted by $\hat{\theta}_D$ and $\hat{\theta}_E$ the best linear unbiased estimates (BLUEs) of θ , which are obtained from the data sets generated at the n experimental settings determined by ξ_D and $\xi_{n,\alpha}$, respectively. The mean squared errors of the estimators are given, for $C \in \{D, E\}$, by

$$\text{MSE}(\hat{\theta}_C) = \frac{1}{N} \sum_{k=1}^N (\hat{\theta}_{C,k} - \theta)^\top (\hat{\theta}_{C,k} - \theta), \quad (9)$$

where $\hat{\theta}_{C,k}$ is the estimate computed from each of the two designs in the k th simulation run and N is the total number of simulation runs. We define the relative efficiency of these two estimates by

$$\text{RE}(\hat{\theta}_E, \hat{\theta}_D) = \frac{\text{MSE}(\hat{\theta}_D)}{\text{MSE}(\hat{\theta}_E)}.$$

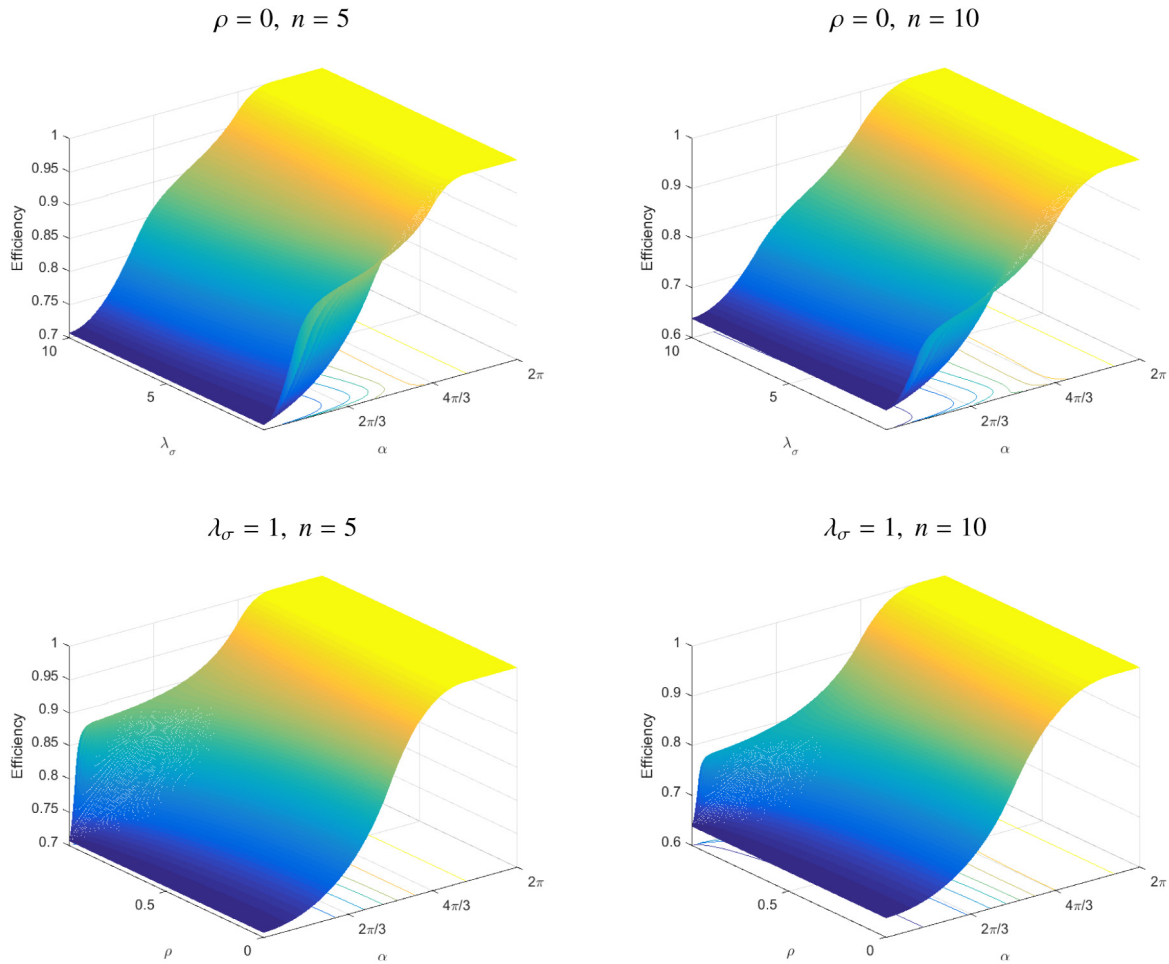


Fig. 2. The D -efficiencies of the equidistant sampling designs $\xi_{n,\alpha}$ on $[-\alpha/2, \alpha/2]$ with $n = 5$ and $n = 10$ for model (1) with $\rho = 0$ and $\lambda_\sigma = 1$, respectively.

The value $\text{RE}(\hat{\theta}_E, \hat{\theta}_D)$ being smaller than 1 would indicate that $\hat{\theta}_D$ is preferable. Note that for any design ξ for the model (1) the BLUE can be expressed by

$$\hat{\theta} = \left\{ \int_{\mathcal{X}} F^T(t) \Sigma^{-1} F(t) d\xi(t) \right\}^{-1} \int_{\mathcal{X}} F^T(t) \Sigma^{-1} Y(t) d\xi(t) = \theta + \int_{\mathcal{X}} F^T(t) \Sigma^{-1} \varepsilon(t) d\xi(t),$$

and then in order to calculate the MSEs defined by (9) it is enough to generate the error vector ε for a given design. In the following two cases, the errors $(\varepsilon_1, \varepsilon_2)^T$ follow the Gaussian distribution $\mathcal{N}(0, \Sigma)$ and $n \in \{5, 10\}$. The number of runs is $N = 10,000$.

- (i) For model (1) with uncorrelated responses, i.e., $\rho = 0$, the variance $\sigma_2^2 = 1$ and the variance $\sigma_1^2 = \lambda_\sigma \sigma_2^2$. Table 2 is a summary of simulation results for this case, which indicates that $\hat{\theta}_D$ is always preferable, especially for small α and small λ_σ .
- (ii) For model (1) with homoscedastic responses, i.e., $\sigma_1^2 = \sigma_2^2$, the variance $\sigma_1^2 = \sigma_2^2 = 1$. The simulation results are summarized in Table 3, which still indicates that $\hat{\theta}_D$ is always preferable, especially for small α and small ρ .

Before a design is implemented, it is a good strategy to assess its robustness properties to model assumptions and when the nominal values for the model parameters are mis-specified. Our optimal designs depend on the parameters in the covariance structure, which are typically unknown in practice. One may then investigate how robust the optimal design is when nominal values of the parameters are mis-specified or when certain aspects of the model are wrongly assumed.

For example, one may wish to investigate two particular assumptions we used in the construction of the D -optimal designs for model (1). The first pertains to earlier work where responses are assumed to have equal variances. To check whether this assumption results in an inefficient design when the model is heteroscedastic, we compare the performances

Table 2The relative efficiency $RE(\hat{\theta}_E, \hat{\theta}_D)$ with $n = 5$ and $n = 10$ for model (1) with $\rho = 0$.

n	α	λ_σ				
		1	2	5	10	100
5	$\pi/3$	0.4338	0.4406	0.4513	0.5038	0.6522
	$\pi/2$	0.4610	0.4757	0.5394	0.6291	0.7320
	π	0.6890	0.7214	0.7269	0.7712	0.9582
	$4\pi/3$	0.7848	0.7735	0.8141	0.8523	0.9603
	2π	0.7975	0.8059	0.8627	0.9136	0.9593
10	$\pi/3$	0.4195	0.4306	0.4696	0.4966	0.5615
	$\pi/2$	0.4569	0.4587	0.5134	0.5996	0.6682
	π	0.6745	0.6345	0.6860	0.7372	0.9540
	$4\pi/3$	0.8512	0.8650	0.8585	0.9135	0.9718
	2π	0.9474	0.9436	0.9497	0.9710	0.9898

Table 3The relative efficiency $RE(\hat{\theta}_E, \hat{\theta}_D)$ with $n = 5$ and $n = 10$ for model (1) with $\sigma_1^2 = \sigma_2^2 = 1$.

n	α	ρ					
		0	0.1	0.3	0.5	0.7	0.9
5	$\pi/3$	0.4281	0.4272	0.4302	0.4391	0.4652	0.5962
	$\pi/2$	0.4616	0.4567	0.4782	0.4937	0.5433	0.7027
	π	0.6855	0.6868	0.7202	0.7852	0.7429	0.8515
	$4\pi/3$	0.7749	0.7613	0.7836	0.7958	0.8360	0.9040
	2π	0.7992	0.8044	0.8023	0.8287	0.8708	0.9627
10	$\pi/3$	0.4357	0.4301	0.4298	0.4372	0.4480	0.5557
	$\pi/2$	0.4727	0.4649	0.4594	0.4665	0.5262	0.6120
	π	0.6847	0.6099	0.6397	0.6884	0.7172	0.8520
	$4\pi/3$	0.8689	0.8513	0.8500	0.8701	0.8909	0.9329
	2π	0.9474	0.9528	0.9337	0.9577	0.9831	0.9982

of the two designs, $\xi_D(1, \rho, \alpha)$ and $\xi_D(\lambda_\sigma, 0, \alpha)$ for model (1) on the domain $[-\alpha/2, \alpha/2]$ for various λ_σ , ρ and α . Fig. 3 displays the D -efficiencies of $\xi_D(1, \rho, \alpha)$ with respect to the D -optimal designs $\xi_D(\lambda_\sigma, \rho, \alpha)$ for the model with $\lambda_\sigma \in (0, 10]$, $\rho \in \{0, 0.1, 0.5, 0.9\}$ and $\alpha \in (0, 2\pi]$. The figure suggests that $\xi_D(1, \rho, \alpha)$ performs very well except for the pairs of values of (λ_σ, α) in some small area, where λ_σ is much smaller than 1 and α gets smaller as its range narrows rapidly as ρ increases.

The second situation concerns the assumption of uncorrelated responses indicated by $\rho = 0$ in the model. Our question of interest is whether the D -optimal design for model (1) with $\rho = 0$ remains robust when we have correlated responses. Fig. 4 displays the D -efficiencies of $\xi_D(\lambda_\sigma, 0, \alpha)$ relative to the D -optimal designs $\xi_D(\lambda_\sigma, \rho, \alpha)$ for various values of $\lambda_\sigma \in \{1, 5, 10, 100\}$, $\rho \in [0, 1)$ and $\alpha \in (0, 2\pi]$. The figure suggests that the design $\xi_D(\lambda_\sigma, 0, \alpha)$ also performs very well except for pairs of values of (ρ, α) in some small area, where ρ is near 1 and α becomes smaller as its range narrows rapidly as λ_σ increases.

5. Summary

Motivated by real applications, it is increasingly recognized that Berman's model for analyzing circular data can be made more realistic by incorporating heteroscedasticity and correlatedness of the observations in the model. While there is work to accommodate these additional features in the data analysis, there is no design work to date for taking account such concerns at the design stage. In this paper, we obtained closed form descriptions for the D -optimal designs, which are always helpful for investigating further robustness properties of D -optimal designs. We also show that the commonly used equidistant sampling method of taking observations for the bivariate Berman's model with correlated and heteroscedastic errors can be inefficient.

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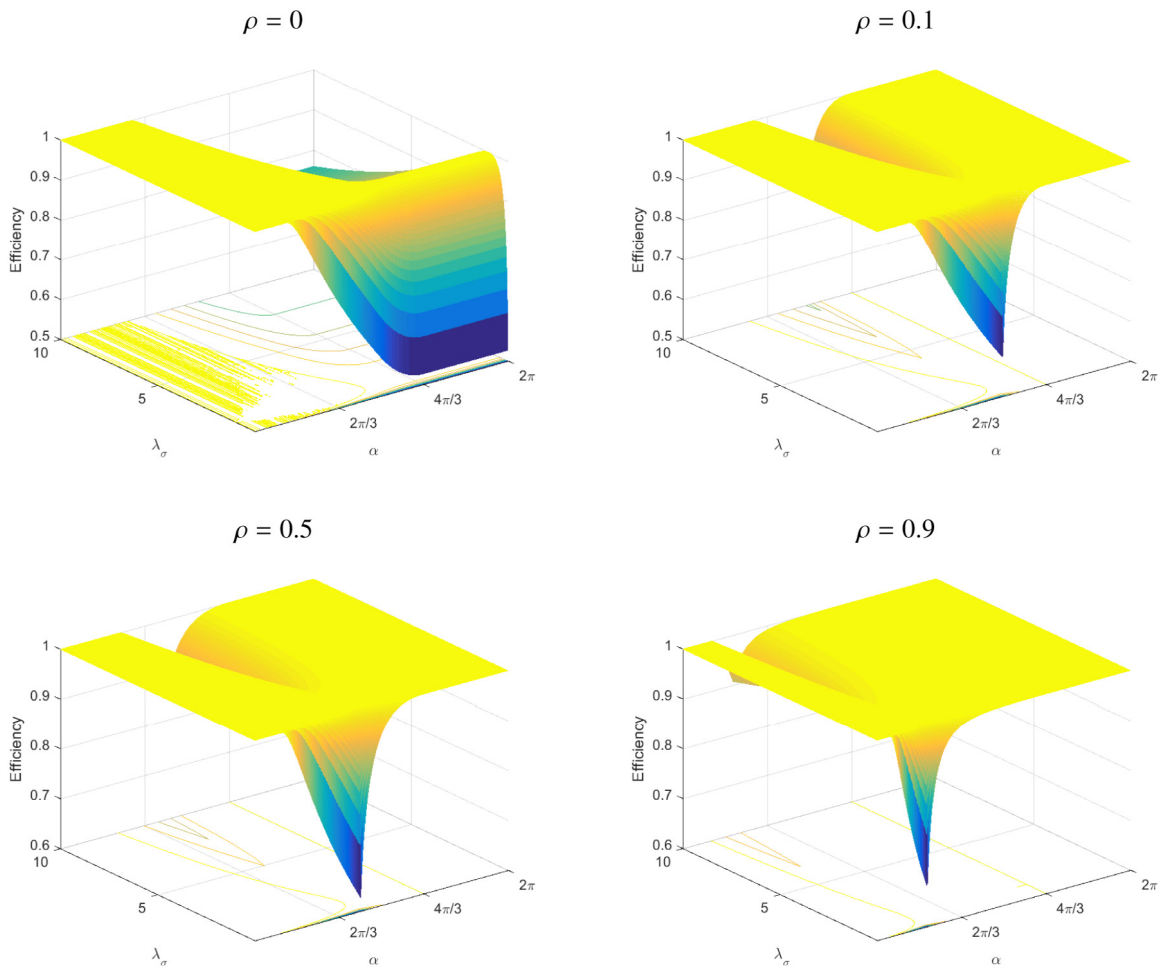


Fig. 3. The D -efficiencies of $\xi_D(1, \rho, \alpha)$ with respect to $\xi_D(\lambda_\sigma, \rho, \alpha)$ for model (1) with $\lambda_\sigma \in (0, 10]$, $\rho \in \{0, 0.1, 0.5, 0.9\}$ and $\alpha \in (0, 2\pi]$.

Appendix

We provide justifications for technical results in [Lemma 1](#), [Theorems 1](#) and [2](#) in the text using the same notation from the main text.

A.1. Proof of [Lemma 1](#)

Let ξ be an arbitrary approximate design and let $\tilde{\xi}$ be its reflected design. Since $c_1(\tilde{\xi}) = c_1(\xi)$, $s_1(\tilde{\xi}) = -s_1(\xi)$, $c_2(\tilde{\xi}) = c_2(\xi)$, $s_2(\tilde{\xi}) = -s_2(\xi)$, a direct calculation shows that the normalized information matrix of $\tilde{\xi}$ is

$$M(\tilde{\xi}) = \begin{pmatrix} \Sigma^{-1} & \Sigma^{-1}A(\tilde{\xi}) \\ A(\tilde{\xi})\Sigma^{-1} & B(\tilde{\xi}) \end{pmatrix},$$

where

$$A(\tilde{\xi}) = A^\top(\xi), \quad B(\tilde{\xi}) = \frac{1}{\det(\Sigma)} \left\{ \frac{\sigma_1^2 + \sigma_2^2}{2} I_2 - \frac{c_2(\xi)}{2} P - \frac{s_2(\xi)}{2} QP \right\}.$$

Let

$$L = \begin{pmatrix} P & 0 \\ 0 & P \end{pmatrix},$$

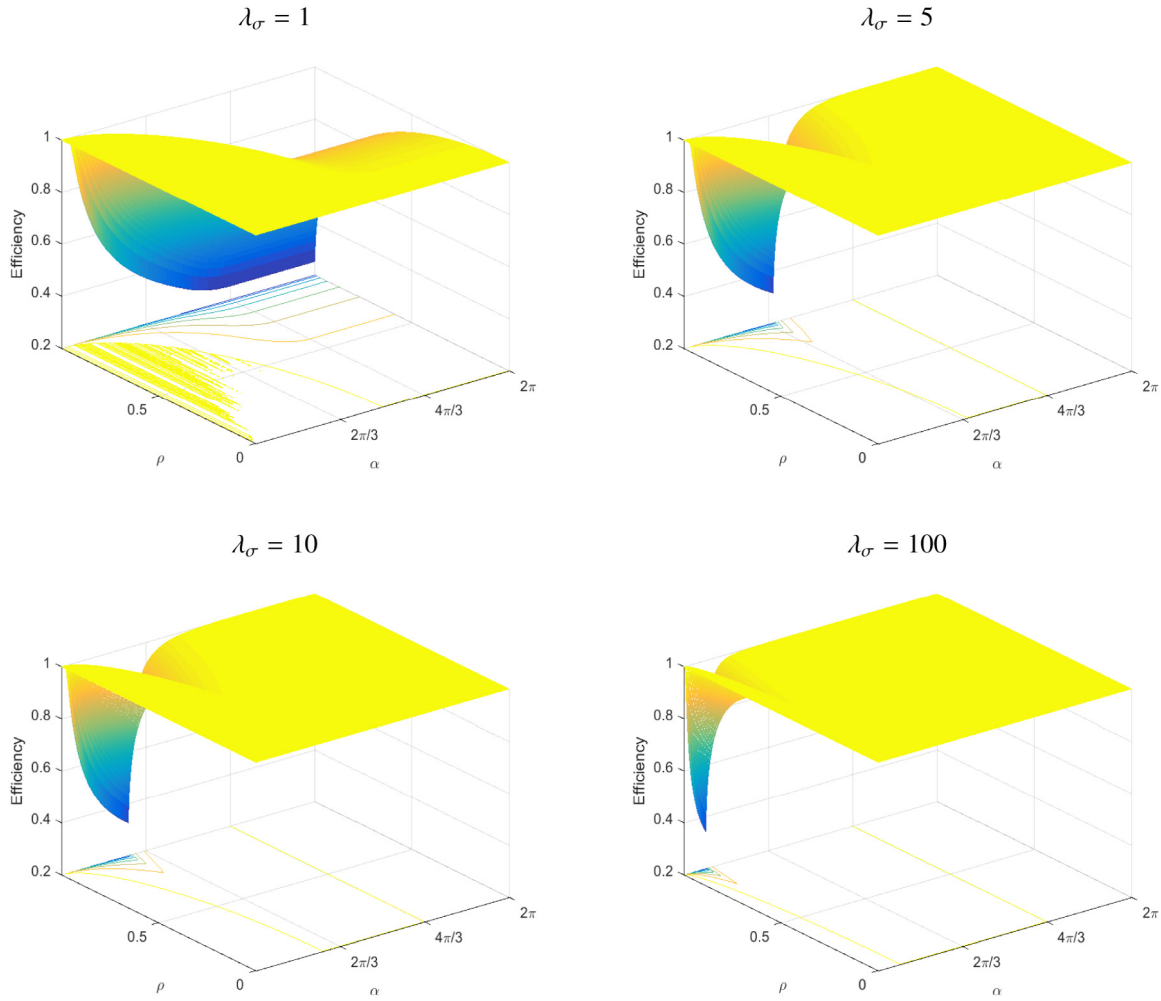


Fig. 4. The D -efficiencies of $\xi_D(\lambda_\sigma, 0, \alpha)$ with respect to the D -optimal designs $\xi_D(\lambda_\sigma, \rho, \alpha)$ for model (1) with $\lambda_\sigma \in \{1, 5, 10, 100\}$, $\rho \in [0, 1]$ and $\alpha \in (0, 2\pi]$.

and observe that

$$LM(\xi)L^{-1} = \begin{pmatrix} P\Sigma^{-1}P^{-1} & P\Sigma^{-1}A(\xi)P^{-1} \\ PA(\xi)\Sigma^{-1}P^{-1} & PB(\xi)P^{-1} \end{pmatrix} = M(\tilde{\xi}),$$

which follows directly from $\Sigma^{-1}P^{-1} = P^{-1}\Sigma^{-1}$, $P\Sigma^{-1}AP^{-1} = P\Sigma^{-1}P^{-1}PAP^{-1} = \Sigma^{-1}A^\top PP^{-1} = \Sigma^{-1}A^\top$, and $PQ = -QP$. Since L is singular if and only if $\det(P) = -(\sigma_1^2 - \sigma_2^2)^2 - 4\rho^2\sigma_1^2\sigma_2^2 = 0$, i.e., $\sigma_1^2 = \sigma_2^2$ and $\rho = 0$, this implies that $\det\{M(\tilde{\xi})\} = \det\{M(\xi)\}$. Then, by concavity of the D optimality criterion [19], we have $\det\{M(\xi^*)\} \geq \det\{M(\xi)\}/2 + \det\{M(\tilde{\xi})\}/2 = \det\{M(\xi)\}$, which proves the second part of the lemma. $\square$

A.2. Proof of Lemma 2

The result in (i) is obvious from the definition of $c_1(\xi)$. To prove (ii) and (iii), we note that

$$c_2(\xi) = \int_{\mathcal{X}} \cos 2t d\xi = 2 \int_{\mathcal{X}} \cos^2 t d\xi - 1$$

and the assertions follow directly from Lemma 1 in [25]. $\square$

Lemma 1. Let $\mu = \int_{\mathcal{X}} \cos t d\xi$, $\nu = \int_{\mathcal{X}} \cos^2 t d\xi$, $c = \cos(\alpha/2)$, and $v_m(u) = (1+c)u - c$, for $u \in [-1, 1]$. For $w \in [0, 1]$, $x \in [0, \alpha/2]$, let $\xi(w, x)$ denote the symmetric design that assigns weights $w/2$, $1-w$, and $w/2$ to $-x$, 0 , and x , respectively. Let $\xi_m(w) \equiv \xi(w, \alpha/2)$. Then,

- (i) the design $\xi_m(w)$ gives $\mu = 1 - (1 - c)w$, and $v = 1 - (1 - c^2)w = v_m(\mu)$;
- (ii) any symmetric design ξ has $v \in [\mu^2, v_m(\mu)]$;
- (iii) if a symmetric design ξ gives $v = v_m(\mu)$, the design is $\xi_m\{(1 - \mu)/(1 - c)\}$.

A.3. Proof of Theorem 1

Let $\bar{\xi}$ be a symmetric design, let $\lambda_\sigma = \sigma_1^2/\sigma_2^2$ and let

$$\Phi_D\{c_1(\bar{\xi}), c_2(\bar{\xi})\} = \{1 - c_1^2(\bar{\xi})\}^2(1 + \lambda_\sigma)^2 - \{(\lambda_\sigma - 1)^2 + 4\rho^2\lambda_\sigma\}\{c_2(\bar{\xi}) - c_1^2(\bar{\xi})\}^2.$$

From (3), the determinant of the information matrix of $\bar{\xi}$ is

$$\det(M(\bar{\xi})) = |\Sigma^{-1}| |B(\bar{\xi}) - c_1^2(\bar{\xi})\Sigma^{-1}| = |\Sigma|^{-3} \left| \frac{\sigma_1^2 + \sigma_2^2}{2} I_2 - \frac{c_2(\bar{\xi})}{2} P - c_1^2(\bar{\xi})|\Sigma|^{-1} \right| = \frac{\Phi_D\{c_1(\bar{\xi}), c_2(\bar{\xi})\}}{4\lambda_\sigma^3\sigma_2^8(1 - \rho^2)^3}. \quad (10)$$

To prove part (i) of Theorem 1, it suffices to show that the maximizer of $\Phi_D\{c_1(\bar{\xi}), c_2(\bar{\xi})\}$ over Ξ_S must occur on the straight line segment

$$\mathcal{L} = \{(c_1(\bar{\xi}), c_2(\bar{\xi})) : c_2(\bar{\xi}) = 2\{\cos(\alpha/2) + 1\}\{c_1(\bar{\xi}) - 1\} + 1, c_1(\bar{\xi}) \in [\cos(\alpha/2), 1]\}.$$

We justify this claim by considering values of α in two intervals separately, when $\alpha \in (0, \pi]$ and when $\alpha \in (\pi, 4\pi/3)$.

Case 1, $\alpha \in (0, \pi]$: Since $\cos(\alpha/2) \geq 0$, for a fixed $c_1(\bar{\xi}) \in [\cos(\alpha/2), 1]$, we have $2\{\cos(\alpha/2) + 1\}\{c_1(\bar{\xi}) - 1\} + 1 \leq 2c_1(\bar{\xi}) - 1 \leq c_1^2(\bar{\xi})$. It follows that $\Phi_D\{c_1(\bar{\xi}), c_2(\bar{\xi})\}$ is an increasing function in $c_2(\bar{\xi})$ and it attains its maximum on $\mathcal{L}$.

Case 2, $\alpha \in (\pi, 4\pi/3)$: Since $-1/2 < \cos(\alpha/2) < 0$, it is easy to check that

- (a) $2\{\cos(\alpha/2) + 1\}\{c_1(\bar{\xi}) - 1\} + 1 \leq c_1^2(\bar{\xi})$ for $c_1(\bar{\xi}) \in [\cos(\alpha/2), 2\cos(\alpha/2) + 1]$, and
- (b) $2\{\cos(\alpha/2) + 1\}\{c_1(\bar{\xi}) - 1\} + 1 \geq c_1^2(\bar{\xi}) \geq 2c_1^2(\bar{\xi}) - 1$ for $c_1(\bar{\xi}) \in [2\cos(\alpha/2) + 1, 1]$.

Under (a), $\Phi_D\{c_1(\bar{\xi}), c_2(\bar{\xi})\}$ is an increasing function in $c_2(\bar{\xi})$ and attains its maximum on

$$\mathcal{L}_1 = \{(c_1(\bar{\xi}), c_2(\bar{\xi})) : c_2(\bar{\xi}) = 2\{\cos(\alpha/2) + 1\}\{c_1(\bar{\xi}) - 1\} + 1, c_1(\bar{\xi}) \in [\cos(\alpha/2), 2\cos(\alpha/2) + 1]\}.$$

Under (b) holds, the function

$$\max_{c_2(\bar{\xi})} \Phi_D\{c_1(\bar{\xi}), c_2(\bar{\xi})\} = \Phi_D\{c_1(\bar{\xi}), c_1^2(\bar{\xi})\} = \{1 - c_1^2(\bar{\xi})\}^2(1 + \lambda_\sigma)^2$$

is a decreasing function in $c_1(\bar{\xi})$ on the interval $[2\cos(\alpha/2) + 1, 1]$ and attains its maximum on $c_1(\bar{\xi}) = 2\cos(\alpha/2) + 1$. Therefore, the maximizer of $\Phi_D\{c_1(\bar{\xi}), c_2(\bar{\xi})\}$ occurs on $\mathcal{L}_1$ (which is a subset of $\mathcal{L}$) and Part (i) of Theorem 1 holds.

For Part (ii), it is easy to see that the maximum of $\Phi_D\{c_1(\bar{\xi}), c_2(\bar{\xi})\}$ is attained at $(c_1(\bar{\xi}), c_2(\bar{\xi})) = (0, 0)$ on the set $\{(c_1(\bar{\xi}), c_2(\bar{\xi}))\}$, where both $c_1(\bar{\xi})$ and $c_2(\bar{\xi})$ satisfy the conditions in Lemma 2(i) and (ii). $\square$

A.4. Proof of Theorem 2

For a symmetric design $\bar{\xi}_S$ of the form in (4), we have $c_1(\bar{\xi}_S) = 1 - w + w\cos(\alpha/2)$, $c_2(\bar{\xi}_S) = 1 - 2w\{1 - \cos^2(\alpha/2)\}$. When $\alpha \in (0, 4\pi/3)$, we have $\cos(\alpha/2) \in (-1/2, 1)$ and by calculus, $a > 0$, $b < 0$, $c > 0$ and

$$0 < 1 - \frac{4\lambda_\sigma(1 - \rho^2)}{(1 + \lambda_\sigma)^2} < 1. \quad (11)$$

Let $\Phi_D(w) = \Phi_D\{c_1(\bar{\xi}_S), c_2(\bar{\xi}_S)\} = 4\{1 - \cos^2(\alpha/2)\}^2 w^2(aw^2 + bw + c)$, where a , b and c are given in (6) and (7) and (8), respectively. Using the above information facts and the below arguments, we now complete the proof of Part (i) of Theorem 2 by showing that $\Phi_D(w)$ is positive, its derivative with respect to w is positive on $(0, 1]$ and so $\Phi_D(w)$ is maximized at $w = 1$.

A direct calculation shows that the derivative of $\Phi_D(w)$ is $4\{1 - \cos^2(\alpha/2)\}^2 w(4aw^2 + 3bw + 2c) = wg_D(w)$, where $g_D(w) = 4aw^2 + 3bw + 2c$ is a parabola opening upward with axis of symmetry at $w = -3b/8a > 1$. This is because $a > 0$, $-1/2 \leq \cos(\alpha/2) < 1$ and

$$8a + 3b = \{\cos(\alpha/2) - 1\}[3(\lambda_\sigma - 1)^2\{1 + \cos(\alpha/2)\} + 4\lambda_\sigma\{1 + 2\cos(\alpha/2)\} + \cos(\alpha/2)\rho^2 + 2\rho^2] < 0.$$

Further, $g_D(0) = 2c > 0$ and $g_D(1) = 4a + 3b + 2c = \{\cos(\alpha/2) + 1\}[\{\cos(\alpha/2) - 1\}(1 + \lambda_\sigma)^2 + 4\lambda_\sigma(1 - \rho^2)] > 0$ if $\alpha \in (0, \pi]$ and $\{\cos(\alpha/2) - 1\}(1 + \lambda_\sigma)^2 + 4\lambda_\sigma(1 - \rho^2) \geq 0$. Consequently, we have $g_D(w) > 0$ when $w \in (0, 1]$ and the derivative of $\Phi_D(w)$ is positive, implying that $\Phi_D(w)$ is an increasing function on $w \in (0, 1]$ and has a maximum at $w = 1$. This proves Part (i).

Furthermore, we have $g_D(1) < 0$ if (a) $\alpha \in (0, \pi]$ and $\{\cos(\alpha/2) - 1\}(1 + \lambda_\sigma)^2 + 4\lambda_\sigma(1 - \rho^2) < 0$, or (b) $\pi < \alpha < 4\pi/3$ since $\cos(\alpha/2) < 0$ and (11). This implies that $g_D(w) > 0$ if $0 < w < w_D$ and $g_D(w) > 0$ if $w_D < w \leq 1$, where w_D defined in (5) is the unique root of $g_D(w)$ for $w \in (0, 1]$. Hence, $\Phi_D(w)$ increases on $w \in (0, w_D]$ and decreases on $w \in [w_D, 1]$, implying that $\Phi_D(w)$ is maximized at $w = w_D$. This proves Part (ii).

Part (iii) of Theorem 2 follows immediately from Part (ii) since $c_1(\bar{\xi}_D) = c_2(\bar{\xi}_D) = 0$. $\square$

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