OPTIMAL EXACT DESIGNS ON A CIRCLE OR A CIRCULAR ARC¹

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Fitting a circle to a set of data points on a plane is very common in engineering and science. An important practical problem is how to choose the locations of measurement on a circular feature. So far little attention has been paid to this design issue and only some simulation results are available. In this paper, for Berman's bivariate four-parameter model, Φ -optimality is defined and shown to be equivalent to all ϕ_p -criteria with $p \in [-\infty, 1)$. Then Φ -optimal exact designs on a circle or a circular arc are derived for any sample size and sampling range. As a by-product, Φ -optimal approximate designs are also obtained. These optimal designs are used to evaluate the efficiency of the equidistant sampling method widely used in practice. These results also provide guidelines for users on sampling method and sample size selection.

1. Introduction. The circle is one of the most common features occurring in engineering, computer science, physics and optics. The problem of fitting a circle to a set of data points on a plane has become very common in many areas such as engineering design and manufacturing [Dowling, Griffin, Tsui and Zhou (1997), computer graphics and computer vision [Moura and Kitney (1991)], microwave engineering [Berman (1983)] and high energy physics [Karimäki (1991)]. Since measurement is time consuming and costly, an important practical problem is how to choose the locations of measurement on a circular feature so that the estimates are most precise for a given sample size [Dowling, Griffin, Tsui and Zhou (1997)]. So far almost all papers on circle fitting deal with estimation of the center and radius of the circle [Chan (1965), Anderson (1981), Berman (1983), Berman and Culpin (1986), Chan and Mak (1994)]. Little attention has been paid to the design issue, and only some simulation results comparing the performance of some commonly used sampling methods are available [Dowling, Griffin, Tsui and Zhou (1997)]. A theoretical investigation is needed to provide guidelines for users on sampling method selection.

In this paper we will concentrate on the design aspects of the problem for Berman's (1983) circular model, which assumes that the angular differences

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between sample points are known in advance, either from the special structure of the problem or through experimental design. Since a circular feature can have an arbitrary angle with respect to the coordinate system of a measuring machine, the determination of the locations of sample points is equivalent to the determination of the angular differences between these points. It is therefore reasonable to use Berman's model for the search of optimal designs of the sample points. Furthermore, Berman's model is technically tractable. After some transformation of parameters, Berman's model becomes a bivariate four-parameter linear model $Y = X\theta + \varepsilon$, where X = $[f(t_1), \ldots, f(t_n)]'$ is the model matrix and t_1, \ldots, t_n are the *n* support points on the design region \mathcal{T} , that is, the circular arc to be measured. See Section 2 for details. Classical linear optimal design theory mostly focuses on the so-called approximate theory [Silvey (1980), Pukelsheim (1993)] which works on the information matrix $\int_{\mathcal{T}} f(t) f(t)' d\tau$ and chooses a probability measure (an approximate design) τ on the design region \mathcal{T} . The purpose of this paper is to find optimal *exact* designs by choosing the model matrix X, which is the more important and interesting problem in practice. Related works for optimal approximate designs on balls and cubes can be found in Galil and Kiefer (1977a, b).

The remainder of this paper proceeds as follows. Section 2 briefly reviews Berman's model and formulates the design problem using the notation close to Pukelsheim (1993). In Section 3 orthogonal designs are obtained. When orthogonality cannot be achieved, Φ -optimality is defined in Section 4 and shown to be equivalent to all ϕ_p -criteria with $p \in [-\infty, 1)$ and minimizing the common variance of the estimators of the parameters. Section 5 then derives all Φ -optimal exact designs on a circle or a circular arc for any sample size and sampling range. As a by-product, Φ -optimal approximate designs are also obtained. Finally, in Section 6 we compare the efficiency of Φ -optimal exact designs and equidistant sampling with that of Φ -optimal approximate designs. These results also provide guidelines for users on sampling method and sample size selection.

2. The bivariate, four-parameter Berman model. The Berman (1983) model uses the regression function $f: \mathscr{T} \to \mathscr{R}^{4 \times 2}$ given by

(1)
$$f(t) = \begin{pmatrix} I_2 \\ A(t)' \end{pmatrix}, \text{ where } A(t) = \begin{pmatrix} \cos t & -\sin t \\ \sin t & \cos t \end{pmatrix}$$

is the 2 × 2 matrix of a plane rotation by the angle $t \in [0, 2\pi)$, \mathcal{T} is a circular arc and $\mathscr{R}^{4\times 2}$ is the set of all real 4 × 2 matrices. The parameter vector for the regression model is $\theta = (\theta_1, \theta_2, \theta_3, \theta_4)$, where (θ_1, θ_2) is the center and $\rho = \sqrt{\theta_3^2 + \theta_4^2}$ is the radius of the circular arc. The bivariate observations at t_1, \ldots, t_n are assumed to have independent and identically distributed errors

 ε_{ij} with mean zero and variance σ^2 . Thus, the model is represented by

(2)

$$\begin{pmatrix} Y_{1j} \\ Y_{2j} \end{pmatrix} = f(t_j)' \theta + \begin{pmatrix} \varepsilon_{1j} \\ \varepsilon_{2j} \end{pmatrix}$$

$$= \begin{pmatrix} \theta_1 + \theta_3 \cos t_j - \theta_4 \sin t_j + \varepsilon_{1j} \\ \theta_2 + \theta_3 \sin t_j + \theta_4 \cos t_j + \varepsilon_{2j} \end{pmatrix} \text{ for } j = 1, \dots, n,$$

or simply denoted by $Y = X\theta + \varepsilon$. This is a linear model with $(2n) \times 4$ model matrix

(3)
$$X = \begin{pmatrix} I_2 & A(t_1) \\ \vdots & \vdots \\ I_2 & A(t_n) \end{pmatrix}$$

and dispersion matrix $\sigma^2 I_{2n}$. Hence the design with one bivariate observation at each of the support points t_1, \ldots, t_n has the moment matrix

(4)
$$M(\tau) = \frac{1}{n} X' X = \begin{pmatrix} I_2 & A(\tau) \\ A(\tau)' & I_2 \end{pmatrix},$$

where the design quantities of interest are

(5)

$$A(\tau) = \int A(t) d\tau = \frac{1}{n} \sum_{j \le n} A(t_j) = \begin{pmatrix} c(\tau) & -s(\tau) \\ s(\tau) & c(\tau) \end{pmatrix},$$

$$c(\tau) = \int \cos(t) d\tau = \frac{1}{n} \sum_{j \le n} \cos(t_j),$$

$$s(\tau) = \int \sin(t) d\tau = \frac{1}{n} \sum_{j \le n} \sin(t_j),$$

$$d(\tau) = \det A(\tau) = (c(\tau))^2 + (s(\tau))^2 \ge 0.$$

The quantity $d(\tau)$ turns out to play a key role. By definition, $d(\tau)$ is nonnegative. The Cauchy–Schwarz inequality gives its upper bound

(6)
$$d(\tau) = \left(\frac{1}{n}\sum_{j\leq n}\cos(t_j)\right)^2 + \left(\frac{1}{n}\sum_{j\leq n}\sin(t_j)\right)^2$$
$$\leq \frac{1}{n}\sum_{j\leq n}\left(\cos t_j\right)^2 + \frac{1}{n}\sum_{j\leq n}\left(\sin t_j\right)^2 = 1.$$

The maximum value 1 of $d(\tau)$ is obtained if and only if $t_1 = \cdots = t_n$, that is, τ is a one-point design. Then its moment matrix $M(\tau)$ is of rank 2 and singular. If a design τ has two or more distinct support points, then $M(\tau)$ is positive definite and the parameter θ is estimable. The minimum value 0 of $d(\tau)$ leads to $M(\tau) = I_4$. Then the dispersion matrix of the least squares estimator $\hat{\theta}$ of θ becomes proportional to the identity matrix. Such designs are called *orthogonal*.

3. Experimental domain and orthogonality. We first point out that the location of a (single, connected) proper circular arc \mathscr{T} in the complete circle $[0, 2\pi)$ does not matter. To show this, assume that the support points t_1, \ldots, t_n are all rotated by an angle $r \in (0, 2\pi)$. Then the off-diagonal blocks of the moment matrix $M(\tau)$ in (4) change into $A(\tau)A(r)$ and $(A(\tau)A(r))^{\prime}$, respectively. Since det A(r) = 1, $d(\tau)$ is unchanged. Therefore, for all analyses based on $d(\tau)$, such as those in this paper, a circular arc \mathscr{T} may be placed anywhere in the complete circle $[0, 2\pi)$. Thus we can standardize \mathscr{T} to make 0 its midpoint, that is, $\mathscr{T} = [-\alpha/2, \alpha/2]$ for an arc of length $\alpha \in (0, 2\pi)$. When $\alpha = 2\pi$, we take $\mathscr{T} = [-\pi, \pi)$.

For convenience in the ensuing discussion, we define the following concepts.

DEFINITION 1. Two support points t_1 and t_2 $(-\alpha/2 \le t_1, t_2 \le \alpha/2)$ are called a *diametrical pair* if $|t_1 - t_2| = \pi$, and an *endpoint pair* if $|t_1 - t_2| = \alpha$. A support point t_1 is called a *midpoint* if $t_1 = 0$, and an *endpoint* if $t_1 = \pm \alpha/2$.

For any design $\tau = \{t_1, \ldots, t_n\}$, let

(7)
$$g_n(t_1,\ldots,t_n) \equiv n^2 d(\tau) = \left(\sum_{j \le n} \cos t_j\right)^2 + \left(\sum_{j \le n} \sin t_j\right)^2.$$

Then orthogonality is equivalent to $g_n = 0$. If n = 2m and $\pi \le \alpha \le 2\pi$, we can take *m* points at $-\pi/2$ and the remaining *m* points at $\pi/2$, so that orthogonality is achieved. If n = 2m + 1, then in order to obtain an orthogonal design, we consider the design with *m* pairs at $(-\beta/2, \beta/2)$ and a midpoint, where $0 < \beta \le \alpha$. Then

(8)
$$g_{2m+1}(t_1,\ldots,t_{2m+1}) = (2m\cos(\beta/2)+1)^2.$$

Let β_m be such that

 1.161π

 $\frac{4}{3}\pi$

 β_m

 1.107π

(9) $2m\cos(\beta_m/2) + 1 = 0$, that is, $\beta_m = 2\pi - 2\arccos(1/2m)$.

Then, for any $\beta_m \leq \alpha \leq 2\pi$, the design with *m* pairs at $(-\beta_m/2, \beta_m/2)$ and a midpoint is orthogonal. Some selected values of β_m , given in Table 1, indicate

 1.032π

 1.016π

 1.006π

 ∞

 π

 1.003π

 TABLE 1

 Some selected values of βm

 m
 1
 2
 3
 5
 10
 20
 50
 100

 1.064π

that β_m is quite close to π for $m \ge 10$. Later we will see that, if n = 2m and $0 < \alpha < \pi$, or if n = 2m + 1 and $0 < \alpha < \beta_m$, then orthogonal designs do not exist.

The above orthogonal designs only contain two or three distinct points and do not provide much opportunity for model verification. More interesting orthogonal designs with more distinct points will be constructed based on the following lemma, where the design consisting of designs $\tau_1 = \{t_1, \ldots, t_{n_1}\}$ and $\tau_2 = \{t_{n_1+1}, \ldots, t_{n_1+n_2}\}$ is denoted by $\tau = \tau_1 \cup \tau_2$.

LEMMA 1. The following designs are all orthogonal: (a) equidistant sampling on a complete circle; (b) designs consisting of any diametrical pairs and (c) designs consisting of any orthogonal designs.

PROOF. (a) For equidistant sampling on $[-\alpha/2, \alpha/2]$, the *n* support points are $t_i = -\alpha/2 + (j-1)\alpha/(n-1)$, for j = 1, ..., n. Then

(10)
$$g_{n}(t_{1},...,t_{n}) = \left|\sum_{j \leq n} \cos t_{j} + \mathbf{i} \sum_{j \leq n} \sin t_{j}\right|^{2}$$
$$= \left|\sum_{j \leq n} \exp(\mathbf{i}[-\alpha/2 + (j-1)\alpha/(n-1)])\right|^{2}$$
$$= \left|\frac{1 - \exp(\mathbf{i}(n\alpha/(n-1)))}{1 - \exp(\mathbf{i}(\alpha/(n-1)))}\right|^{2}$$
$$= \frac{1 - \cos(n\alpha/(n-1))}{1 - \cos(\alpha/(n-1))},$$

where **i** is the imaginary unit. Hence $d(\tau) = 0$ if and only if $\alpha = ((n - 1)/n)2\pi$. Then $t_j = -\pi + (2\pi/n)(j + \frac{1}{2})$, j = 1, ..., n. Hence the angle between t_1 and t_n is $2\pi/n$, which is the same as the angles between any other neighboring pairs $(t_1, t_2), ..., (t_{n-1}, t_n)$. This indicates that the design τ is an equidistant sampling on a complete circle.

(b) If t_1 and t_2 are any diametrical pair, then $\cos t_1 + \cos t_2 = \sin t_1 + \sin t_2 = 0$. Hence for any design consisting of diametrical pairs $(t_1, t_2), \ldots, (t_{2m-1}, t_{2m})$, we have $\sum_{j=1}^{2m} \cos t_j = \sum_{j=1}^{2m} \sin t_j = 0$. Then $d(\tau) = 0$ and the design is orthogonal.

(c) From (5), a design τ is orthogonal if and only if $A(\tau) = 0$. Therefore, if $\tau_j = \{t_{j1}, \ldots, t_{jn_j}\}$ $(j = 1, \ldots, k, k \ge 2)$ are orthogonal, and if $n_1 + \cdots + n_k$ is denoted by n, then we have $A(\tau_1 \cup \cdots \cup \tau_k) = \{n_1 A(\tau_1) + \cdots + n_k A(\tau_k)\}/n = 0$, which implies that the design $\tau_1 \cup \cdots \cup \tau_k$ is also orthogonal. \Box

Note that the proof of (a) shows that equidistant sampling is orthogonal if and only if its support points form an equidistant sampling on a complete circle.

The first main result then follows from Lemma 1. It gives many choices for orthogonal designs.

THEOREM 1. (a) If n = 2m and $\pi \le \alpha \le 2\pi$, them m diametrical pairs form an orthogonal design.

If n = 2m + 1, then the following designs are orthogonal:

(b) m - k diametrical pairs and 2k + 1 equidistant points on a complete circle, if $4\pi/3 \le \alpha \le 2\pi$, where $k = 1, ..., k_0$ and k_0 is given by (11);

(c) $m - k_1 - 1$ diametrical pairs, k_1 endpoint pairs, one pair at $\pm \gamma_0/2$, and a midpoint, if $\beta_n \leq \alpha < 4\pi/3$, where k_1 is determined by (14), β_m is given by (9) and γ_0 by (15).

PROOF. The results of (a) and (b) follow directly from Lemma 1. All that remains is to determine k_0 for part (b). To arrange 2k + 1 equidistant points on a circle within the experimental domain $[-\alpha/2, \alpha/2]$, we must have $2\pi/(2k + 1) \ge 2\pi - \alpha$. Hence

(11)
$$k \le k_0 \equiv \min(m, \left[\alpha/(4\pi - 2\alpha) \right])$$

where $[\alpha/(4\pi - 2\alpha)]$ denotes the integral part of $\alpha/(4\pi - 2\alpha)$. When $\alpha \ge (1 - 1/(2m + 1))2\pi$, we have $k_0 = m$, that is, all 2m + 1 points can be placed equidistantly on a circle.

(c) We need to find k_1 and γ_0 such that the design satisfies

(12)
$$g_{2m+1} = (2k_1\cos(\alpha/2) + 2\cos(\gamma_0/2) + 1)^2 = 0$$

Since $\pi < \beta_m \le \alpha < 4\pi/3$, then, by (9), we have

(13) $2\cos(\alpha/2) + 1 > 0 = 2m\cos(\beta_m/2) + 1 \ge 2m\cos(\alpha/2) + 1$.

Hence there exists a unique k_1 , $1 \le k_1 < m$, such that

(14)
$$2k_1 \cos(\alpha/2) + 1 > 0 \ge 2(k_1 + 1)\cos(\alpha/2) + 1$$

Let $v(\gamma) = 2k_1 \cos(\alpha/2) + 2\cos(\gamma/2) + 1$. Then $v(\pi) = 2k_1 \cos(\alpha/2) + 1 > 0$ and $v(\alpha) = 2(k_1 + 1)\cos(\alpha/2) + 1 \le 0$. Since $v(\gamma)$ is continuous and strictly decreases on $[\pi, \alpha]$, there exists a unique $\gamma_0 \in [\pi, \alpha]$ such that $v(\gamma_0) = 0$. Then $g_{2m+1} = (v(\gamma_0))^2 = 0$, which leads to orthogonality of the design, where γ_0 is given by

(15)

$$2k_1\cos(\alpha/2) + 2\cos(\gamma_0/2) + 1 = 0,$$

that is,

$$\gamma_0 = 2\pi - 2 \arccos(k_1 \cos(\alpha/2) + 1/2).$$

4. Optimality criteria. When orthogonality cannot be achieved, one may instead choose some optimality criterion. For $M(\tau)$ and $d(\tau)$ given in (4) and (5), let Φ denote the class of all optimality criteria ϕ that are of the form

$$\phi(M(\tau)) = \psi(d(\tau)),$$

for some monotonic function $\psi: [0,1] \to [-\infty,\infty]$. That is, any criterion in Φ depends on the design τ only through $d(\tau)$.

If ϕ is an information function and ψ is antitonic, then maximizing ϕ is the same as minimizing $d(\tau)$. If ϕ behaves like a variance and ψ is isotonic, then minimizing ϕ again means minimizing $d(\tau)$. Therefore, we have the following definition.

DEFINITION 2. Designs that minimize $d(\tau)$ are called Φ -optimal.

Hence every orthogonal design is Φ -optimal. It is interesting to explore the relationships between Φ -optimality and other design criteria in the literature. So far the two most popular criteria are (1) minimizing det{Cov[$\hat{\theta}$]}, or equivalently, maximizing det $M(\tau)$, which is the *D*-criterion, and (2) minimizing the total or average variance of $\hat{\theta}$, that is, minimizing tr[$(M(\tau))^{-1}$] (*A*-criterion). These two criteria give the so-called optimal exact designs which are very important in practice. So far, many algorithms are available for constructing *D*-optimal exact designs [Cook and Nachtsheim (1980), Li and Wu (1997)]. However, the global optimality of the resulting designs is not guaranteed. It is also worth noting that the design issue here is for the case of bivariate observations, which causes the numerical algorithms for finding optimal designs to be more complicated. More generally, we can consider a class of ϕ_p -criteria [Pukelsheim (1993)]. When $p = -\infty, -1, 0, 1$, we obtain the *E*-, *A*-, *D*- and *T*-criteria, respectively. Let $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4$ be the four eigenvalues of the moment matrix $M(\tau)$. Then the ϕ_p -criteria ($p \in [-\infty, 1]$) maximize the following ϕ_p functions:

(16)
$$\phi_p(M(\tau)) = \begin{cases} \lambda_4, & \text{for } p = -\infty, \\ \left(\prod_{j \le 4} \lambda_j\right)^{1/4}, & \text{for } p = 0, \\ \left(\frac{1}{4} \sum_{j \le 4} \lambda_j^p\right)^{1/p}, & \text{for } p \ne 0, \pm \infty, \\ \lambda_1, & \text{for } p = \infty. \end{cases}$$

It is easy to show that $\lambda_1 = \lambda_2 = 1 + \sqrt{d(\tau)}$ and $\lambda_3 = \lambda_4 = 1 - \sqrt{d(\tau)}$. Hence

$$\begin{aligned} \phi_p(M(\tau)) &= \psi_p(d(\tau)) \\ (17) &= \begin{cases} 1 - \sqrt{d(\tau)}, & \text{for } p = -\infty, \\ \sqrt{1 - d(\tau)}, & \text{for } p = 0, \\ \left(\frac{\left(1 + \sqrt{d(\tau)}\right)^p}{2} + \frac{\left(1 - \sqrt{d(\tau)}\right)^p}{2}\right)^{1/p}, & \text{for } p \neq 0, \pm \infty, \\ 1 + \sqrt{d(\tau)}, & \text{for } p = \infty. \end{cases} \end{aligned}$$

Here the *T*-criterion (trace criterion) is useless since $\phi_1(M(\tau)) \equiv 1$. Since $\phi_p(M(\tau)) = \psi_p(d(\tau))$ decreases in $d(\tau)$ for any $p \in [-\infty, 1)$, all the ϕ_p -criteria with $p \in [-\infty, 1)$ are equivalent to Φ -optimality. Since

(18)
$$\operatorname{Cov}[\hat{\theta}] = \frac{\sigma^2}{n} (M(\tau))^{-1} = \frac{\sigma^2}{n(1-d(\tau))} \begin{pmatrix} I_2 & -A(\tau) \\ -A(\tau)' & I_2 \end{pmatrix},$$

we can see that Φ -optimality also leads to minimizing the common variance of the unbiased estimators $\hat{\theta}$. This property is stronger and more interpretable than the *E*-, *A*- and *D*-criteria. However, since θ_3 and θ_4 are not of direct interest, one question is whether Φ -optimality can lead to minimizing the mean-squared error of the biased estimator $\hat{\rho} = \sqrt{\hat{\theta}_3^2 + \hat{\theta}_4^2}$ of the radius ρ . This turns out to be true and its proof is given in the Appendix. In summary, we have the following lemma.

LEMMA 2. For Berman's model (2), Φ -optimality is equivalent to (a) ϕ_p -criteria with $p \in [-\infty, 1)$; (b) minimizing the common variance $\sigma^2/(n(1-d(\tau)))$ of the (unbiased) least squares estimators $\hat{\theta}$ of θ ; and (c) minimizing the mean-squared error of $\hat{\rho}$.

5. Φ -optimal exact designs. In Section 3, we obtained orthogonal designs for (i) n = 2m and $\pi \le \alpha \le 2\pi$, and (ii) n = 2m + 1 and $\beta_m \le \alpha \le 2\pi$. In this section, we will construct Φ -optimal exact designs for other cases. When n = 2m and $0 < \alpha < \pi$, Φ -optimality can be achieved by m endpoint pairs. When n = 2m + 1, we may try to set m endpoint pairs, but the "extra" support point needs special care by setting it as an endpoint, a midpoint or an arbitrary point, depending on the length of α . This gives the second main result as follows.

THEOREM 2. (a) If n = 2m and $0 < \alpha < \pi$, then the design with m endpoint pairs is Φ -optimal.

If n = 2m + 1, then the Φ -optimal exact designs are:

(b) *m* endpoint pairs and an endpoint, if $0 < \alpha < \pi$;

(c) m endpoint pairs and a midpoint, if $\pi < \alpha < \beta_m$, where β_m is given by (9);

(d) *m* endpoint pairs and any other point, if $\alpha = \pi$.

PROOF. Since Φ -optimality is equivalent to minimizing g_n defined in (7), we only need to show that the above designs have the smallest g_n values among any designs with the same sample size n on the same circular arc $[-\alpha/2, \alpha/2]$. It is easy to see that the g_n values of the above designs are (a) $(2m\cos(\alpha/2))^2$, (b) $1 + 4m(m+1)(\cos(\alpha/2))^2$, (c) $(1 + 2m\cos(\alpha/2))^2$, and (d) 1, respectively. Recall that $\mathcal{T} = [-\alpha/2, \alpha/2]$ and that all t_j 's fall in \mathcal{T} . (a) If $0 < \alpha < \pi$, then $\cos t_j \ge \cos(\alpha/2) > 0$ for $j = 1, \ldots, 2m$. Hence

(19)
$$g_{2m}(t_1, \dots, t_{2m}) \ge \left(\sum_{j=1}^{2m} \cos t_j\right)^2 \ge \left(\sum_{j=1}^{2m} \cos(\alpha/2)\right)^2 = \left(2m\cos(\alpha/2)\right)^2.$$

For the proofs of (b), (c) and (d), noting that g_{2m+1} is symmetric in t_1, \ldots, t_{2m+1} , we assume $t_1 \leq \cdots \leq t_{2m+1}$. As argued at the beginning of Section 3, rotation of t_1, \ldots, t_{2m+1} does not matter, so we can also assume $t_1 = -\delta/2$ and $t_{2m+1} = \delta/2$, where $0 \leq \delta \leq \alpha$.

(b) It suffices to show that, for any $m \ge 0$ and $-\alpha/2 \le t_1 \le \cdots \le t_{2m+1} \le \alpha/2$,

(20)
$$g_{2m+1}(t_1,\ldots,t_{2m+1}) \ge 1 + 4m(m+1)(\cos(\alpha/2))^2.$$

We use induction on m. When m = 0, (20) holds since $g_1(t_1) = 1$. Assume that (20) holds for 2m - 1 ($m \ge 1$). Then

(21)
$$g_{2m-1}(t_2,...,t_{2m}) \equiv A^2 + B^2 \ge 1 + 4m(m-1)(\cos(\alpha/2))^2,$$

where $A = \sum_{j=2}^{2m} \cos t_j$ and $B = \sum_{j=2}^{2m} \sin t_j$. Hence

$$g_{2m+1}(t_1, \dots, t_{2m+1}) = g_{2m+1}(-\delta/2, t_2, \dots, t_{2m}, \delta/2)$$

= $(2\cos(\delta/2) + A)^2 + B^2$
= $A^2 + B^2 + 4\cos(\delta/2)(\cos(\delta/2) + A)$
 $\ge A^2 + B^2 + 8m(\cos(\alpha/2))^2$
 $\ge 1 + 4m(m+1)(\cos(\alpha/2))^2$,

that is, (20) holds. The first inequality in (22) follows by the facts that $A \ge (2m - 1)\cos(\alpha/2) > 0$ and $\cos(\delta/2) \ge \cos(\alpha/2) > 0$, since $0 < \alpha < \pi$, and then $\cos t_j \ge \cos(\alpha/2) > 0$ for $j = 1, \ldots, 2m + 1$. The second inequality in (22) follows by the inductive hypothesis (21).

(c) As in (b), we use induction on $m \ge 0$ to show that

(23)
$$g_{2m+1}(t_1,\ldots,t_{2m+1}) \ge (1+2m\cos(\alpha/2))^2,$$

for $\pi \leq \alpha < \beta_m$. Using (9) and noting that $\pi \leq \alpha < \beta_m < 4\pi/3$, we have

(24)
$$0 = 1 + 2m \cos(\beta_m/2) \le 1 + 2m \cos(\alpha/2) \le 1.$$

If $\delta < \pi$, then $t_1, \ldots, t_{2m+1} \in [-\delta/2, \delta/2]$ implies that (20) holds. Then from (20) and (24) we have

$$g_{2m+1}(t_1, \dots, t_{2m+1}) \ge 1 + 4m(m+1)(\cos(\delta/2))^2$$
$$\ge 1 \ge (1 + 2m\cos(\alpha/2))^2,$$

that is, (23) holds. Thus we only need to consider $\pi \le \delta \le \alpha$. Let $K = \sqrt{A^2 + B^2}$. Then $A \le K$, where A and B are defined below (21). Induction on m is then applied. When m = 0, (23) holds. If we assume that it holds for $2m - 1 \ge 1$, then, from (24) and the inductive hypothesis, we have

(25)
$$K = \left(g_{2m-1}(t_2, \dots, t_{2m})\right)^{1/2} \ge 1 + 2(m-1)\cos(\alpha/2) \ge 0.$$

Since $\cos(\delta/2) \ge \cos(\alpha/2)$, then, from the above inequality and (24), we have

(26) $K + 2\cos(\delta/2) \ge 1 + 2m\cos(\alpha/2) \ge 0.$

Therefore, by (22),

$$g_{2m+1}(t_1, \dots, t_{2m+1}) = A^2 + B^2 + 4\cos(\delta/2)(\cos(\delta/2) + A)$$
(27)

$$\geq K^2 + 4\cos(\delta/2)(\cos(\delta/2) + K)$$

$$= (K + 2\cos(\delta/2))^2 \geq (1 + 2m\cos(\alpha/2))^2,$$

that is, (23) holds. The first inequality in (27) holds since $A \leq K$ and $\cos(\delta/2) \leq 0$ from $\pi \leq \delta \leq \alpha < \beta_m < 4\pi/3$. The second inequality in (27) is from (26).

(d) Since (23) holds for $\alpha = \pi$, then $g_{2m+1}(t_1, \ldots, t_{2m+1}) \ge 1$ and (d) follows. \Box

It is interesting to look at the special cases of Theorems 1 and 2 with n = 2 and n = 3.

COROLLARY 1. (a) If n = 2 and $0 < \alpha < \pi$, then an endpoint pair form an Φ -optimal exact design.

(b) If n = 2 and $\pi \le \alpha \le 2\pi$, then any diametrical pair form an orthogonal design.

COROLLARY 2. For n = 3, Φ -optimal exact designs are:

(a) an endpoint pair and an endpoint, if $0 < \alpha < \pi$;

(b) an endpoint pair and any other point, if $\alpha = \pi$;

(c) an endpoint pair and a midpoint, if $\pi < \alpha < 4\pi/3$;

(d) if n = 3 and $4\pi/3 \le \alpha \le 2\pi$, then three equidistant points on a complete circle form an orthogonal design.

An illustration of Theorems 1 and 2 is given in Figure 1 which provides Φ -optimal exact designs for sample sizes n = 10 and n = 11 with different α values.

Theorems 1 and 2 provide Φ -optimal exact designs on a circle or a circular arc for any sample size and sampling range. In particular, Theorem 1 gives orthogonal designs for all the situations in which orthogonality can be achieved. As a by-product of these results, we obtain Φ -optimal approximate designs which minimize

$$d(\tau) \equiv \left(\int \cos(t) d\tau\right)^2 + \left(\int \sin(t) d\tau\right)^2$$

with respect to a probability measure (an approximate design) τ on \mathcal{T} . Since orthogonal designs attain the minimum value 0 of $d(\tau)$, they are also Φ -optimal approximate designs. Other Φ -optimal approximate designs are easily obtained by the following argument.

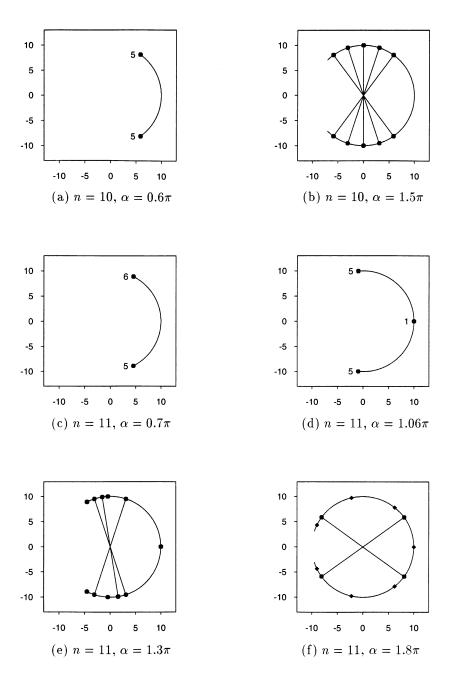


FIG. 1. Examples of Φ -optimal exact designs. The diametrical pairs in (b), (e) and (f) are connected by line segments. The diamond points in (f) form an equidistant sampling on a complete circle.

In the approximate theory, the design problem is invariant with respect to reflection across the midpoint of the arc, that is, $t \to -t$ when $\mathscr{T} = [-\alpha/2, \alpha/2]$. The symmetrized design $\bar{\tau} = \frac{1}{2}(\tau + \tau^R)$ has a vanishing sineterm, $s(\bar{\tau}) = 0$. Hence $d(\bar{\tau}) = (c(\bar{\tau}))^2$, and minimizing $d(\bar{\tau})$ is the same as minimizing $|c(\bar{\tau})|$. Thus Φ -optimal approximate designs are obtained by placing half of the observations at each of the two support points $\pm \min\{\alpha/2, \pi/2\}$.

REMARKS. (i) It is known that equidistant sampling is optimal for the trigonometric model on the complete circle $[-\pi, \pi)$; see, for example, Section 9.16 in Pukelsheim (1993). The technique used in this paper might be helpful for finding optimal trigonometric designs for proper circular arcs $\mathcal{T} \neq [-\pi, \pi)$.

(ii) The fact that optimality is achieved by two-point designs seems to imply limitations of Φ -optimality. Fortunately, designs consisting of diametrical pairs—of which there are many, provided $\alpha > \pi$ —leave a wide choice among optimal designs.

(iii) If the model is slightly wrong, optimal designs that are far from equidistant will be in trouble because they make no provision for checking model inadequacy. From the practical point of view, study of efficiency of equidistant and related designs is important, as we will discuss in the next section.

6. Efficiency comparisons. As a result of its simplicity and intuitive appeal, equidistant sampling is widely used in practice for sampling circular measurement data. It is important to consider its efficiency. Since the common variance of the parameter estimators $\hat{\theta}$ is $\sigma^2/(n(1 - d(\tau)))$, it is natural to define $1 - d(\tau)$ to be the *efficiency* of a sampling scheme for any fixed sample size *n*. Recall from the proof of Lemma 1(a) that equidistant sampling on a complete circle is achieved when $\alpha = ((n - 1)/n)2\pi$. Then, for any $((n - 1)/n)2\pi \le \alpha \le 2\pi$, we can also have equidistant sampling on a complete circle. Therefore, the efficiency of equidistant sampling is

$$\operatorname{Eff}_{\mathbf{E}}(n,\alpha) = \begin{cases} 1 - \frac{1}{n^2} \frac{1 - \cos\left(\frac{n}{n-1}\alpha\right)}{1 - \cos\left(\frac{\alpha}{n-1}\right)}, & \text{if } 0 < \alpha < \frac{n-1}{n} 2\pi, \\ 1, & \text{if } \frac{n-1}{n} 2\pi \le \alpha \le 2\pi; \end{cases}$$

that of Φ -optimal approximate designs is

$$\operatorname{Eff}_{\mathbf{\Phi}\mathbf{A}}(\alpha) = \begin{cases} \sin^2(\alpha/2), & \text{if } 0 < \alpha < \pi, \\ 1, & \text{if } \pi \le \alpha \le 2\pi; \end{cases}$$

and that of Φ -optimal exact designs is

$$\begin{split} \mathrm{Eff}_{\Phi\mathbf{E}}(n,\alpha) & \text{if } n = 2m, \\ & \left\{ \begin{aligned} \mathrm{Eff}_{\Phi\mathbf{A}}(\alpha), & \text{if } n = 2m, \\ \sin^2(\alpha/2) \left(1 - \frac{1}{(2m+1)^2} \right), & \text{if } n = 2m+1 \text{ and } 0 < \alpha \leq \pi, \\ & 1 - \frac{\left(2m\cos(\alpha/2) + 1 \right)^2}{\left(2m+1 \right)^2}, & \text{if } n = 2m+1 \text{ and } \pi < \alpha < \beta_m, \\ & 1, & \text{if } n = 2m+1 \text{ and } \beta_m \leq \alpha \leq 2\pi \end{aligned} \right. \end{split}$$

where β_m is given by (9).

Since Φ -optimal approximate designs attain maximum efficiency among designs on the same experimental domain $\mathcal{T} = [-\alpha/2, \alpha/2]$, another type of efficiency of a design can be defined by the ratio of its efficiency to that of Φ -optimal approximate designs with the same α . This type of efficiency is called *standardized efficiency*. Then, for equidistant sampling, its standardized efficiency is

 $\text{Stdeff}_{\mathbf{E}}(n, \alpha)$

$$= \left\{ \begin{aligned} \left(1 - \frac{1}{n^2} \frac{1 - \cos\left(\frac{n}{n-1}\alpha\right)}{1 - \cos\left(\frac{\alpha}{n-1}\right)} \right) \middle/ \sin^2(\alpha/2), & \text{if } 0 < \alpha < \pi, \\ 1 - \frac{1}{n^2} \frac{1 - \cos\left(\frac{n}{n-1}\alpha\right)}{1 - \cos\left(\frac{\alpha}{n-1}\right)}, & \text{if } \pi < \alpha < \frac{n-1}{n} 2\pi, \\ 1, & \text{if } \frac{n-1}{n} 2\pi \le \alpha \le 2\pi \end{aligned} \right.$$

If n=2, then ${\rm Stdeff}_{\rm E}(2,\,\alpha)=1.$ For a $\Phi\mbox{-optimal exact design, its standard-ized efficiency is$

$$\begin{split} & \text{Stdeff}_{\Phi \mathbf{E}}(n, \alpha) \\ & = \begin{cases} 1, & \text{if } n = 2m, \\ 1 - \frac{1}{(2m+1)^2}, & \text{if } n = 2m+1 \text{ and } 0 < \alpha \leq \pi, \\ 1 - \frac{(2m\cos(\alpha/2) + 1)^2}{(2m+1)^2}, & \text{if } n = 2m+1 \text{ and } \pi < \alpha < \beta_m, \\ 1, & \text{if } n = 2m+1 \text{ and } \beta_m \leq \alpha \leq 2\pi. \end{cases} \end{split}$$

Numerical results show that for equidistant sampling and Φ -optimal exact designs the above-defined efficiency and standardized efficiency do not vary

much with sample size n when $n \ge 10$. Thus we can focus on their limits as $n \to \infty$, and define those limits to be the efficiency and standardized efficiency of these designs. This gives the efficiency of equidistant sampling to be

$$\operatorname{Eff}_{\mathbf{E}}(\alpha) = 1 - \left(\frac{\sin(\alpha/2)}{\alpha/2}\right)^2, \quad 0 < \alpha \le 2\pi,$$

and its standardized efficiency

$$\begin{aligned} \text{Stdeff}_{\mathbf{E}}(\alpha) &= \text{Eff}_{\mathbf{E}}(\alpha)/\text{Eff}_{\Phi \mathbf{A}}(\alpha) \\ &= \begin{cases} \frac{1}{\sin^2(\alpha/2)} - \left(\frac{2}{\alpha}\right)^2, & \text{if } 0 < \alpha < \pi, \\ \\ 1 - \left(\frac{2}{\alpha}\right)^2 \sin^2(\alpha/2), & \text{if } \pi \le \alpha \le 2\pi. \end{cases} \end{aligned}$$

The efficiency of Φ -optimal exact designs is $\text{Eff}_{\Phi E}(\alpha) = \text{Eff}_{\Phi A}(\alpha)$ and their standardized efficiency is 1.

It is interesting to note the monotonicity of $\text{Eff}_{\mathbf{E}}(\alpha)$, $\text{Stdeff}_{\mathbf{E}}(\alpha)$ and $\text{Eff}_{\mathbf{\Phi}\mathbf{E}}(\alpha) = \text{Eff}_{\mathbf{\Phi}\mathbf{A}}(\alpha)$ in $\alpha \in (0, 2\pi]$. More precisely, we have the following proposition.

PROPOSITION. (a) For equidistant sampling, $\text{Eff}_{\mathbf{E}}(\alpha)$ and $\text{Stdeff}_{\mathbf{E}}(\alpha)$ are both strictly increasing on $(0, 2\pi]$, and $\lim_{\alpha \to 0^+} \text{Stdeff}_{\mathbf{E}}(\alpha) = 1/3$.

(b) For Φ -optimal designs, $\text{Eff}_{\Phi \mathbf{E}}(\alpha) = \text{Eff}_{\Phi \mathbf{A}}(\alpha)$ strictly increases on $(0, \pi)$ and attains 1 if $\alpha \in [\pi, 2\pi]$.

PROOF. (a) The fact that $\sin(x)/x$ strictly decreases on $(0, \pi]$ leads to the monotonicity of $\text{Eff}_{\mathbf{E}}(\alpha)$ on $(0, 2\pi]$, and that of $\text{Stdeff}_{\mathbf{E}}(\alpha)$ on $[\pi, 2\pi]$. Since $\sin x/x > 1 - x^2/6$ and $\cos x < 1 - x^2/2 + x^4/24$, for any $x \in (0, \pi/2)$, the derivative of $\text{Stdeff}_{\mathbf{E}}(\alpha)$ is positive on $(0, \pi)$. Hence $\text{Stdeff}_{\mathbf{E}}(\alpha)$ also strictly increases on $(0, \pi)$. Part (b) is obvious. \Box

It can also be shown that, for any fixed n, $\operatorname{Eff}_{\mathbf{E}}(n, \alpha)$, $\operatorname{Eff}_{\Phi\mathbf{E}}(n, \alpha)$, Stdeff_E (n, α) and Stdeff_{$\Phi\mathbf{E}$} (n, α) are all increasing on $(0, 2\pi]$ (but not always strictly increasing). Here the monotonicity of Stdeff_{$\Phi\mathbf{E}$} (α) is of particular interest since it indicates that the efficiency of equidistant sampling approaches that of Φ -optimal designs as the experimental domain \mathcal{T} increases to a complete circle. Table 2 gives some selected values of efficiency and standardized efficiency for equidistant sampling and some values of efficiency for Φ -optimal designs. Standardized efficiency suggests a criterion for selection among available designs, and efficiency provides a method of choosing the sample size. For example, if the sampling range is only 1/8 of a complete circle, then, since $\operatorname{Eff}_{\mathbf{E}}(\pi/4) = 0.05$, to achieve the same accuracy of the estimators as that for a complete circle when equidistant sampling is used, the sample size should be almost 1/0.05 = 20 times that for a complete circle. This provides an important guide in practice.

TABLE 2 Efficiency comparisons of equidistant sampling versus Φ-optimal designs

α	2π	$\frac{7}{4}\pi$	$\frac{3}{2}\pi$	$rac{5}{4}\pi$	π	$\frac{7}{8}\pi$	$rac{3}{4}\pi$	$\frac{5}{8}\pi$	$\frac{1}{2}\pi$	$\frac{3}{8}\pi$	$\frac{1}{4}\pi$	$\frac{1}{8}\pi$
$Eff_{\Phi E}$	1.00	1.00	1.00	1.00	1.00	0.96	0.85	0.69	0.50	0.31	0.15	0.038
Eff_{E}	1.00	0.98	0.91	0.78	0.59	0.49	0.39	0.28	0.19	0.11	0.05	0.013
$\operatorname{Stdeff}_{\mathbf{E}}$	1.00	0.98	0.91	0.78	0.59	0.51	0.45	0.41	0.38	0.36	0.34	0.336

APPENDIX

PROOF OF LEMMA 2(c). Since $(\hat{\theta}_3, \hat{\theta}_4)'$ is normally distributed with mean $(\theta_3, \theta_4)'$ and covariance matrix $\sigma^2/(n(1 - d(\tau)))I_2$, then

$$\frac{n(1-d(\tau))\hat{\rho}^2}{\sigma^2} = \frac{n(1-d(\tau))}{\sigma^2} \Big(\hat{\theta}_3^2 + \hat{\theta}_4^2\Big) \equiv U \sim \chi_2^2(\omega^2),$$

where $\omega^2 = n(1 - d(\tau))\rho^2/\sigma^2$, and $\chi_2^2(\omega^2)$ denotes the noncentral χ^2 -distribution with 2 degrees of freedom and noncentrality parameter ω^2 . Then the mean-squared error of $\hat{\rho}$ is

$$\begin{split} \mathrm{E}(\hat{\rho}-\rho)^2 &= \frac{\rho^2}{\omega^2} \mathrm{E}(U) + \rho^2 - \frac{2\rho^2}{\omega} \mathrm{E}(U^{1/2}) \\ &= 2\rho^2 \Big\langle 1 + \frac{1}{\omega^2} - \frac{1}{\omega} u(\omega) \Big\rangle, \end{split}$$

where $u(\omega) = E(U^{1/2})$. Now, minimizing $E(\hat{\rho} - \rho)^2$ is equivalent to minimizing $f(\omega) = (1 - \omega u(\omega))/\omega^2$ with respect to $0 < \omega \le \sqrt{n} \rho/\sigma$. Since ω decreases as $d(\tau)$ increases, then Φ -optimality is equivalent to maximizing ω . Hence we need to show only that $f'(\omega) = (-2 - \omega^2 u'(\omega) + \omega u(\omega))/\omega^3 < 0$, or,

(28)
$$\omega^2 u'(\omega) - \omega u(\omega) + 2 > 0 \quad \text{for any } \omega > 0.$$

Using the density of U represented by a mixture of χ^2 -distributions with Poisson weights [Lehmann (1991), page 427], we can compute $u(\omega)$ and obtain that

$$u(\omega) = \mathrm{E}(U^{1/2}) = \exp\left(-\frac{\omega^2}{2}\right)\sqrt{\frac{\pi}{2}}\sum_{k=0}^{\infty}\frac{(2k+1)!!}{\left[(2k)!!\right]^2}\omega^{2k},$$

where $(2k)!! = 2 \cdot 4 \cdot 6 \cdots (2k)$ and $(2k + 1)!! = 1 \cdot 3 \cdot 5 \cdots (2k + 1)$, for $k = 1, 2, \dots$ Let (-1)!! = 1 and 0!! = 1. Then (28) becomes

(29)
$$\left(\sum_{k=0}^{\infty} \frac{(2k-1)!!}{\left[(2k)!!\right]^2} \omega^{2k+1}\right)^2 < \frac{8}{\pi} \exp(\omega^2).$$

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To show (29), first we use induction on k and verify that

(30)
$$\left(\frac{(2k-1)!!}{(2k)!!}\right)^2 \le \frac{1}{k+1} \text{ for } k \ge 1.$$

Then, using (30) and the Cauchy-Schwarz inequality, we have

$$\begin{split} \left(\sum_{k=0}^{\infty} \frac{(2k-1)!!}{\left[(2k)!!\right]^2} \omega^{2k+1}\right)^2 \\ &\leq \left(\sum_{k=0}^{\infty} \left(\frac{\omega^k}{\sqrt{(2k)!!}}\right) \left(\frac{\omega^{k+1}}{\sqrt{(2k)!!}} \frac{\sqrt{2}}{\sqrt{2(k+1)}}\right)\right)^2 \\ &\leq 2\sum_{k=0}^{\infty} \frac{\omega^{2k}}{(2k)!!} \sum_{k=0}^{\infty} \frac{\omega^{2k+2}}{(2k+2)!!} \\ &\leq 2\exp(\omega^2) < \frac{8}{\pi} \exp(\omega^2), \end{split}$$

that is, (29) holds, which concludes the proof. \Box

REMARK. Since $\hat{\rho}$ is a biased estimator of ρ , it would be interesting to know whether its bias is negligible. Let X and Y be N(0, 1) distributed. Then, for $\omega > 0$, $u(\omega) = E(\sqrt{(X - \omega)^2 + Y^2}) > E(|X - \omega|) \ge |E(X - \omega)| = \omega$. Hence,

$$\rho < \rho \frac{u(\omega)}{\omega} = \mathrm{E}(\hat{\rho}) < \sqrt{\mathrm{E}(\hat{\rho}^2)} = \rho \sqrt{1 + 2/\omega^2} < \rho (1 + 1/\omega^2).$$

The bias of $\hat{\rho}$ is therefore positive but less than $\rho/\omega^2 = \sigma^2/(n(1-d(\tau))\rho)$, which is of order 1/n. Since σ/ρ is usually small (less than 5%), the relative bias $E(\hat{\rho})/\rho - 1$ is very small (less than 0.05%) if $n \ge 10$ and $d(\tau) \le 0.5$.

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