

OPTIMAL DESIGN FOR LINEAR MODELS WITH CORRELATED OBSERVATIONS¹

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In the common linear regression model the problem of determining optimal designs for least squares estimation is considered in the case where the observations are correlated. A necessary condition for the optimality of a given design is provided, which extends the classical equivalence theory for optimal designs in models with uncorrelated errors to the case of dependent data. If the regression functions are eigenfunctions of an integral operator defined by the covariance kernel, it is shown that the corresponding measure defines a universally optimal design. For several models universally optimal designs can be identified explicitly. In particular, it is proved that the uniform distribution is universally optimal for a class of trigonometric regression models with a broad class of covariance kernels and that the arcsine distribution is universally optimal for the polynomial regression model with correlation structure defined by the logarithmic potential. To the best knowledge of the authors these findings provide the first explicit results on optimal designs for regression models with correlated observations, which are not restricted to the location scale model.

1. Introduction. Consider the common linear regression model

$$(1.1) \quad y(x) = \theta_1 f_1(x) + \cdots + \theta_m f_m(x) + \varepsilon(x),$$

where $f_1(x), \dots, f_m(x)$ are linearly independent, continuous functions, $\varepsilon(x)$ denotes a random error process or field, $\theta_1, \dots, \theta_m$ are unknown parameters and x is the explanatory variable, which varies in a compact design space $\mathcal{X} \subset \mathbb{R}^d$. We assume that N observations, say y_1, \dots, y_N , can be taken at experimental conditions x_1, \dots, x_N to estimate the parameters in the linear regression model (1.1). If an appropriate estimate, say $\hat{\theta}$, of the parameter $\theta = (\theta_1, \dots, \theta_m)^T$ has been chosen, the quality of the statistical analysis can be further improved by choosing an appropriate design for the experiment. In particular, an optimal design minimizes a functional of the variance–covariance matrix of the estimate $\hat{\theta}$, where the functional should reflect certain aspects of the goal of the experiment. In contrast to the

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case of uncorrelated errors, where numerous results and a rather complete theory are available [see, e.g., the monograph of Pukelsheim (2006)], the construction of optimal designs for dependent observations is intrinsically more difficult. On the other hand, this problem is of particular practical interest as in most applications there exists correlation between different observations. Typical examples include models, where the explanatory variable x represents the time and all observations correspond to one subject. In such situations optimal experimental designs are very difficult to find even in simple cases. Some exact optimal design problems were considered in Boltze and Näther (1982), Näther [(1985a), Chapter 4], Näther (1985b), Pázman and Müller (2001) and Müller and Pázman (2003), who derived optimal designs for the location scale model

$$(1.2) \quad y(x) = \theta + \varepsilon(x).$$

Exact optimal designs for specific linear models have been investigated in Dette, Kunert and Pepelyshev (2008), Harman and Štulajter (2010), Kiseľák and Stehlík (2008). Because explicit solutions of optimal design problems for correlated observations are rarely available, several authors have proposed to determine optimal designs based on asymptotic arguments [see, e.g., Sacks and Ylvisaker (1966, 1968), Bickel and Herzberg (1979), Näther (1985a), Zhigljavsky, Dette and Pepelyshev (2010)]. Roughly speaking, there exist three approaches to embed the optimal design problem for regression models with correlated observations in an asymptotic optimal design problem. The first one is due to Sacks and Ylvisaker (1966, 1968), who assumed that the covariance structure of the error process $\varepsilon(x)$ is fixed and that the number of design points tends to infinity. Alternatively, Bickel and Herzberg (1979) and Bickel, Herzberg and Schilling (1981) considered a different model, where the correlation function depends on the sample size. Recently, Zhigljavsky, Dette and Pepelyshev (2010) extended the Bickel–Herzberg approach and allowed the variance (in addition to the correlation function) to vary as the number of observations changes. As a result, the corresponding optimality criteria contain a kernel with singularity at zero. The focus in all these papers is again mainly on the location scale model (1.2).

The difficulties in the development of the optimal design theory for correlated observations can be explained by a different structure of the covariance of the least squares estimator in model (1.1), which is of the form $M^{-1}BM^{-1}$ for certain matrices M and B depending on the design. As a consequence, the corresponding design problems are in general not convex [except for the location scale model (1.2) where $M = 1$].

The present paper is devoted to the problem of determining optimal designs for more general models with correlated observations than the simple location scale model (1.2). In Section 2 we present some preliminary discussion and introduce the necessary notation. In Section 3 we investigate general conditions for design optimality. One of the main results of the paper is Theorem 3.3, where we derive necessary and sufficient conditions for the universal optimality of designs.

By relating the optimal design problems to eigenvalue problems for integral operators we identify a broad class of multi-parameter regression models where the universally optimal designs can be determined explicitly. It is also shown that in this case the least squares estimate with the corresponding optimal design has the same covariance matrix as the weighted least squares estimates with its optimal design. In other words, under the conditions of Theorem 3.3 least squares estimation combined with an optimal design can never be improved by weighted least squares estimation. In Section 4 several applications are presented. In particular, we show that for a trigonometric system of regression functions involving only cosine terms with an arbitrary periodic covariance kernel, the uniform distribution is universally optimal. We also prove that the arcsine design is universally optimal for the polynomial regression model with the logarithmic covariance kernel and derive some universal optimality properties of the Beta distribution. To our best knowledge these results provide the first explicit solution of optimal design problems for regression models with correlated observations which differ from the location scale model.

In Section 5 we provide an algorithm for computing optimal designs for any regression model with specified covariance function and investigate the efficiency of the arcsine and uniform distribution in polynomial regression models with exponential correlation functions. Finally, Section 6 contains some conclusions and technical details are given in the Appendix.

2. Preliminaries.

2.1. *The asymptotic covariance matrix.* Consider the linear regression model (1.1), where $\varepsilon(x)$ is a stochastic process with

$$(2.1) \quad E\varepsilon(x) = 0, \quad E\varepsilon(x)\varepsilon(x') = K(x, x'); \quad x, x' \in \mathcal{X} \subset \mathbb{R}^d;$$

the function $K(x, x')$ is called covariance kernel. If N observations, say $y = (y_1, \dots, y_N)^T$, are available at experimental conditions x_1, \dots, x_N and the covariance kernel is known, the vector of parameters can be estimated by the weighted least squares method, that is, $\hat{\theta} = (\mathbf{X}^T \boldsymbol{\Sigma}^{-1} \mathbf{X})^{-1} \mathbf{X}^T \boldsymbol{\Sigma}^{-1} y$, where $\mathbf{X} = (f_i(x_j))_{j=1, \dots, N}^{i=1, \dots, m}$ and $\boldsymbol{\Sigma} = (K(x_i, x_j))_{i, j=1, \dots, N}$. The variance-covariance matrix of this estimate is given by

$$\text{Var}(\hat{\theta}) = (\mathbf{X}^T \boldsymbol{\Sigma}^{-1} \mathbf{X})^{-1}.$$

If the correlation structure of the process is not known, one usually uses the ordinary least squares estimate $\tilde{\theta} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T y$, which has the covariance matrix

$$(2.2) \quad \text{Var}(\tilde{\theta}) = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \boldsymbol{\Sigma} \mathbf{X} (\mathbf{X}^T \mathbf{X})^{-1}.$$

An exact experimental design $\xi_N = \{x_1, \dots, x_N\}$ is a collection of N points in \mathcal{X} , which defines the time points or experimental conditions where observations

are taken. Optimal designs for weighted or ordinary least squares estimation minimize a functional of the covariance matrix of the weighted or ordinary least squares estimate, respectively, and numerous optimality criteria have been proposed in the literature to discriminate between competing designs; see [Pukelsheim \(2006\)](#).

Note that the weighted least squares estimate can only be used if the correlation structure of the errors is known, and its misspecification can lead to a considerable loss of efficiency. At the same time, the ordinary least squares estimate does not employ the structure of the correlation. Obviously the ordinary least squares estimate can be less efficient than the weighted least squares estimate, but in many cases the loss of efficiency is small. For example, consider the location scale model (1.2) with a stationary error process, the Gaussian correlation function $\rho(t) = e^{-\lambda t^2}$ and the exact design $\xi = \{-1, -2/3, -1/3, 1/3, 2/3, 1\}$. Suppose that the guessed value of λ equals 1 while the true value is 2. Then the variance of the weighted least squares estimate is 0.528 computed as

$$(\mathbf{X}^T \Sigma_{\text{guess}}^{-1} \mathbf{X})^{-1} \mathbf{X}^T \Sigma_{\text{guess}}^{-1} \Sigma_{\text{true}} \Sigma_{\text{guess}}^{-1} \mathbf{X} (\mathbf{X}^T \Sigma_{\text{guess}}^{-1} \mathbf{X})^{-1},$$

while the variance of the ordinary least squares estimate is 0.433. If the guessed value of λ equals the true value, then the variance of the weighted least squares estimate is 0.382. A similar relation between the variances holds if the location scale model and the Gaussian correlation function are replaced by a polynomial model and a triangular or exponential correlation function, respectively. For a more detailed discussion concerning advantages of the ordinary least squares against the weighted least squares estimate, see [Bickel and Herzberg \(1979\)](#) and Section 5.1 in [Näther \(1985a\)](#).

Throughout this article we will concentrate on optimal designs for the ordinary least squares estimate. These designs also require the specification of the correlation structure but a potential loss by its misspecification in the stage of design construction is typically much smaller than the loss caused by the misspecification of the correlation structure in the weighted least squares estimate. Moreover, in this paper we will demonstrate that there are many situations, where the combination of the ordinary least squares estimate with the corresponding (universally) optimal design yields the same covariance matrix as the weighted least squares estimate on the basis of a (universally) optimal design for weighted least squares estimation; see the discussions in Sections 4 and 6.

Because even in simple models the exact optimal designs are difficult to find, most authors usually use asymptotic arguments to determine efficient designs for the estimation of the model parameters; see [Sacks and Ylvisaker \(1966, 1968\)](#), [Bickel and Herzberg \(1979\)](#) or [Zhigljavsky, Dette and Pepelyshev \(2010\)](#). [Sacks and Ylvisaker \(1966, 1968\)](#) and [Näther \[\(1985a\), Chapter 4\]](#), assumed that the design points $\{x_1, \dots, x_N\}$ are generated by the quantiles of a distribution function, that is,

$$(2.3) \quad x_i = a((i-1)/(N-1)), \quad i = 1, \dots, N,$$

where the function $a : [0, 1] \rightarrow \mathcal{X}$ is the inverse of a distribution function. If ξ_N denotes a design with N points and corresponding quantile function $a(\cdot)$, the covariance matrix of the least squares estimate $\tilde{\theta} = \tilde{\theta}_{\xi_N}$ given in (2.2) can be written as

$$(2.4) \quad \text{Var}(\tilde{\theta}) = D(\xi_N) = M^{-1}(\xi_N)B(\xi_N, \xi_N)M^{-1}(\xi_N),$$

where

$$(2.5) \quad M(\xi_N) = \int_{\mathcal{X}} f(u) f^T(u) \xi_N(du),$$

$$(2.6) \quad B(\xi_N, \xi_N) = \iint K(u, v) f(u) f^T(v) \xi_N(du) \xi_N(dv),$$

and $f(u) = (f_1(u), \dots, f_m(u))^T$ denotes the vector of regression functions. Following Kiefer (1974) we call any probability measure ξ on \mathcal{X} (more precisely on an appropriate Borel field) an approximate design or simply design. The definition of the matrices $M(\xi)$ and $B(\xi, \xi)$ can be extended to an arbitrary design ξ , provided that the corresponding integrals exist. The matrix

$$(2.7) \quad D(\xi) = M^{-1}(\xi)B(\xi, \xi)M^{-1}(\xi)$$

is called the covariance matrix for the design ξ and can be defined for any probability measure ξ supported on the design space \mathcal{X} such that the matrices $B(\xi, \xi)$ and $M^{-1}(\xi)$ are well defined. This set will be denoted by Ξ . An (approximate) optimal design minimizes a functional of the covariance matrix $D(\xi)$ over the set Ξ and a universally optimal design ξ^* (if it exists) minimizes the matrix ξ with respect to the Loewner ordering, that is,

$$D(\xi^*) \leq D(\xi) \quad \text{for all } \xi \in \Xi.$$

Note that on the basis of this asymptotic analysis the kernel $K(u, v)$ has to be well defined for all $u, v \in \mathcal{X}$. On the other hand, Zhigljavsky, Dette and Pepelyshev (2010) extended the approach in Bickel and Herzberg (1979) and proposed an alternative approximation for the covariance matrix in (2.2), where the variance of the observations also depends on the sample size. As a result they obtained an approximating matrix of the form (2.6), where the kernel $K(u, v)$ in the matrix $B(\xi, \xi)$ may have singularities at the diagonal.

Note that in general the function $D(\xi)$ is not convex (with respect to the Loewner ordering) on the space of all approximate designs. This implies that even if one determines optimal designs by minimizing a convex functional, say Φ , of the matrix $D(\xi)$, the corresponding functional $\xi \rightarrow \Phi(D(\xi))$ is generally not convex on the space of designs Ξ . Consider, for example, the case $m = 1$ where $D(\xi)$ is given by

$$(2.8) \quad D(\xi) = \left[\int f^2(u) \xi(du) \right]^{-2} \iint K(u, v) f(u) f(v) \xi(du) \xi(dv),$$

and it is obvious that this functional is not necessarily convex. On the other hand, for the location scale model (1.2) we have $m = 1$, $f(x) = 1$ for all x and this expression reduces to $D(\xi) = \iint K(u, v)\xi(du)\xi(dv)$. In the stationary case $K(u, v) = \sigma^2\rho(u - v)$, where $\rho(\cdot)$ is a correlation function, this functional is convex on the set of all probability measures on the domain \mathcal{X} ; see Lemma 1 in Zhigljavsky, Dette and Pepelyshev (2010) and Lemma 4.3 in N  ther (1985a). For this reason [namely the convexity of the functional $D(\xi)$] most of the literature discussing asymptotic optimal design problems for least squares estimation in the presence of correlated observations considers the location scale model, which corresponds to the estimation of the mean of a stationary process; see, for example, Boltze and N  ther (1982), N  ther (1985a, 1985b).

2.2. Covariance kernels. Consider the covariance kernels $K(u, v)$ that appeared in (2.1). An important case appears when the error process is stationary and the covariance kernel is of the form $K(u, v) = \sigma^2\rho(u - v)$, where $\rho(0) = 1$ and $\rho(\cdot)$ is called the correlation function.

Because in this paper we are interested in designs maximizing functionals of the matrix $D(\xi)$ independently of the type of approximation which has been used to derive it, we will also consider singular kernels in the following discussion. Moreover, we call $K(u, v)$ covariance kernel even if it has singularities at the diagonal.

The covariance kernels with singularities at the diagonal can be used as approximations to the standard covariance kernels. They naturally appear as limits of sequences of covariance kernels satisfying $K_N(u, v) = \sigma_N^2\rho_N(u - v)$, where $\rho_N(t) = \rho(a_N t)$, $\sigma_N^2 = a_N^\alpha \tau^2$, $\tau > 0$, $0 < \alpha \leq 1$, is a constant depending on the asymptotic behavior of the function $\rho(t)$ as $t \rightarrow \infty$, and $\{a_N\}_{N \in \mathbb{N}}$ denotes a sequence of positive numbers satisfying $a_N \rightarrow \infty$ as $N \rightarrow \infty$. Consider, for example, the correlation function $\rho(t) = 1/(1 + |t|)^\alpha$ which is nonsingular. Then the sequence of functions

$$\sigma_N^2\rho_N(t) = a_N^\alpha \tau^2 \frac{1}{(1 + |a_N t|)^\alpha} = \tau^2 \frac{1}{(1/a_N + |t|)^\alpha}$$

converges to $r_\alpha(t) = 1/|t|^\alpha$ as $N \rightarrow \infty$. For slightly different types of approximation, see Examples 4.2 and 4.3 below.

Let us summarize the assumptions regarding the covariance kernel. First, we assume that K is symmetric and continuous at all points $(u, v) \in \mathcal{X} \times \mathcal{X}$ except possibly at the diagonal points (u, u) . We also assume that $K(u, v) \neq 0$ for at least one pair (u, v) with $u \neq v$. Any covariance kernel $K(\cdot, \cdot)$ considered in this paper is assumed to be positive definite in the following sense: for any signed measure $\nu(du)$ on \mathcal{X} , we have

$$(2.9) \quad \iint K(u, v)\nu(du)\nu(dv) \geq 0.$$

If the kernel $K(u, v)$ has singularities at the diagonal then the assumptions we make are as follows. We assume that $K(u, v) = r(u - v)$, where $r(\cdot)$ is a function on $\mathbb{R} \setminus \{0\}$ with $0 \leq r(t) < \infty$ for all $t \neq 0$ and $r(0) = +\infty$. We also assume that there exists a monotonously increasing sequence $\{\sigma_N^2 \rho_N(t)\}_{N \in \mathbb{N}}$ of covariance functions such that $0 \leq \sigma_N^2 \rho_N(t) \leq r(t)$ for all t and all $N = 1, 2, \dots$ and $r(t) = \lim_{N \rightarrow \infty} \sigma_N^2 \rho_N(t)$. Theorem 5 in Zhigljavsky, Dette and Pepelyshev (2010) then guarantees that for this kernel we also have the property of positive definiteness (2.9).

2.3. The set of admissible design points. Consider the vector-function $f(x) = (f_1(x), \dots, f_m(x))^T$ used in the definition of the regression model (1.1). Define the sets $\mathcal{X}_0 = \{x \in \mathcal{X} : f(x) = 0\}$ and $\mathcal{X}_1 = \mathcal{X} \setminus \mathcal{X}_0 = \{x \in \mathcal{X} : f(x) \neq 0\}$ and assume that designs ξ_0 and ξ_1 are concentrated on \mathcal{X}_0 and \mathcal{X}_1 correspondingly. Consider the design $\xi_\alpha = \alpha \xi_0 + (1 - \alpha) \xi_1$ with $0 \leq \alpha < 1$; note that if the design ξ_α is concentrated on the set \mathcal{X}_0 only (corresponding to the case $\alpha = 1$), then the construction of estimates is not possible. We have

$$M(\xi_\alpha) = \int f(x) f^T(x) \xi_\alpha(dx) = (1 - \alpha) M(\xi_1), \quad M^{-1}(\xi_\alpha) = \frac{1}{1 - \alpha} M^{-1}(\xi_1)$$

and

$$B(\xi_\alpha, \xi_\alpha) = \iint K(x, u) f(x) f^T(u) \xi_\alpha(dx) \xi_\alpha(du) = (1 - \alpha)^2 B(\xi_1, \xi_1).$$

Therefore, for all $0 \leq \alpha < 1$ we have

$$D(\xi_\alpha) = M^{-1}(\xi_\alpha) B(\xi_\alpha, \xi_\alpha) M^{-1}(\xi_\alpha) = M^{-1}(\xi_1) B(\xi_1, \xi_1) M^{-1}(\xi_1) = D(\xi_1).$$

Consequently, observations taken at points from the set \mathcal{X}_0 do not change the estimate $\hat{\theta}$ and its covariance matrix. If we use the convention $0 \cdot \infty = 0$, it follows that $\iint K(x, u) f(x) f^T(u) \xi_0(dx) \xi_0(du) = 0$, and this statement is also true for the covariance kernels $K(x, u)$ with singularity at $x = u$.

Summarizing this discussion, we assume throughout this paper that $f(x) \neq 0$ for all $x \in \mathcal{X}$.

3. Characterizations of optimal designs.

3.1. General optimality criteria. Recall the definition of the information matrix in (2.5) and define

$$B(\xi, \nu) = \int_{\mathcal{X}} \int_{\mathcal{X}} K(u, v) f(u) f^T(v) \xi(du) \nu(dv),$$

where ξ and $\nu \in \Xi$ are two arbitrary designs, and $K(u, v)$ is a covariance kernel.

According to the discussion in the previous paragraph, the asymptotic covariance matrix of the least squares estimator $\hat{\theta}$ is proportional to the matrix $D(\xi)$

defined in (2.4). Let $\Phi(\cdot)$ be a monotone, real valued functional defined on the space of symmetric $m \times m$ matrices where the monotonicity of $\Phi(\cdot)$ means that $A \geq B$ implies $\Phi(A) \geq \Phi(B)$. Then the optimal design ξ^* minimizes the function

$$(3.1) \quad \Phi(D(\xi))$$

on the space Ξ of all designs. In addition to monotonicity, we shall also assume differentiability of the functional $\Phi(\cdot)$; that is, the existence of the matrix of derivatives

$$C = \frac{\partial \Phi(D)}{\partial D} = \left(\frac{\partial \Phi(D)}{\partial D_{ij}} \right)_{i,j=1,\dots,m},$$

where D is any symmetric nonnegative definite matrix of size $m \times m$. The following lemma is crucial in the proof of the optimality theorem below.

LEMMA 3.1. *Let ξ and ν be two designs and Φ be a differentiable functional. Set $\xi_\alpha = (1 - \alpha)\xi + \alpha\nu$ and assume that the matrices $M(\xi)$ and $B(\xi, \xi)$ are non-singular. Then the directional derivative of Φ at the design ξ in the direction of $\nu - \xi$ is given by*

$$\left. \frac{\partial \Phi(D(\xi_\alpha))}{\partial \alpha} \right|_{\alpha=0} = 2[\mathbf{b}(\nu, \xi) - \boldsymbol{\varphi}(\nu, \xi)],$$

where

$$\boldsymbol{\varphi}(\nu, \xi) = \text{tr}(M(\nu)D(\xi)C(\xi)M^{-1}(\xi)),$$

$$\mathbf{b}(\nu, \xi) = \text{tr}(M^{-1}(\xi)C(\xi)M^{-1}(\xi)B(\xi, \nu))$$

and

$$C(\xi) = \left. \frac{\partial \Phi(D)}{\partial D} \right|_{D=D(\xi)}.$$

PROOF. Straightforward calculation shows that

$$\left. \frac{\partial}{\partial \alpha} M^{-1}(\xi_\alpha) \right|_{\alpha=0} = M^{-1}(\xi) - M^{-1}(\xi)M(\nu)M^{-1}(\xi)$$

and

$$\left. \frac{\partial}{\partial \alpha} B(\xi_\alpha, \xi_\alpha) \right|_{\alpha=0} = B(\xi, \nu) + B(\nu, \xi) - 2B(\xi, \xi).$$

Using the formula for the derivative of a product and the two formulas above, we obtain

$$\left. \frac{\partial}{\partial \alpha} D(\xi_\alpha) \right|_{\alpha=0} = -2M^{-1}(\xi)M(\nu)D(\xi) + 2M^{-1}(\xi)B(\xi, \nu)M^{-1}(\xi).$$

Note that the matrices $M(\xi_\alpha)$ and $B(\xi_\alpha, \xi_\alpha)$ are nonsingular for small nonnegative α (i.e., for all $\alpha \in [0, \alpha_0)$ where α_0 is a small positive number) which follows from the nondegeneracy of $M(\xi)$ and $B(\xi, \xi)$ and the continuity of $M(\xi_\alpha)$ and $B(\xi_\alpha, \xi_\alpha)$ with respect to α .

Using the above formula and the fact that $\text{tr}(H(A + A^T)) = 2 \text{tr}(HA)$ for any $m \times m$ matrix A and any $m \times m$ symmetric matrix H , we obtain

$$\left. \frac{\partial \Phi(D(\xi_\alpha))}{\partial \alpha} \right|_{\alpha=0} = \text{tr} \left(C(\xi) \frac{\partial}{\partial \alpha} D(\xi_\alpha) \right) \Big|_{\alpha=0} = 2[\mathbf{b}(\nu, \xi) - \boldsymbol{\varphi}(\nu, \xi)]. \quad \square$$

Note that the functions $\mathbf{b}(\nu, \xi)$ and $\boldsymbol{\varphi}(\nu, \xi)$ can be represented as

$$\mathbf{b}(\nu, \xi) = \int b(x, \xi) \nu(dx), \quad \boldsymbol{\varphi}(\nu, \xi) = \int \varphi(x, \xi) \nu(dx),$$

where

$$(3.2) \quad \varphi(x, \xi) = \boldsymbol{\varphi}(\xi_x, \xi) = f^T(x) D(\xi) C(\xi) M^{-1}(\xi) f(x),$$

$$(3.3) \quad b(x, \xi) = \mathbf{b}(\xi_x, \xi) = \text{tr}(C(\xi) M^{-1}(\xi) B(\xi, \xi_x) M^{-1}(\xi)),$$

and ξ_x is the probability measure concentrated at a point x .

LEMMA 3.2. *For any design ξ such that the matrices $M(\xi)$ and $B(\xi, \xi)$ are nonsingular we have*

$$(3.4) \quad \int \varphi(x, \xi) \xi(dx) = \int b(x, \xi) \xi(dx) = \text{tr} D(\xi) C(\xi),$$

where the functions $\varphi(x, \xi)$ and $b(x, \xi)$ are defined in (3.2) and (3.3), respectively.

PROOF. Straightforward calculation shows that

$$\int \varphi(x, \xi) \xi(dx) = \text{tr} \left(D(\xi) C(\xi) M^{-1}(\xi) \int f(x) f^T(x) \xi(dx) \right) = \text{tr}(D(\xi) C(\xi)).$$

We also have

$$\begin{aligned} \int B(\xi, \xi_x) \xi(dx) &= \int \left[\iint K(u, v) f(u) f^T(v) \xi(du) \xi_x(dv) \right] \xi(dx) \\ &= \int \left[\int K(u, x) f(u) f^T(x) \xi(du) \right] \xi(dx) = B(\xi, \xi), \end{aligned}$$

which implies

$$\begin{aligned} \int b(x, \xi) \xi(dx) &= \text{tr} \left(M^{-1}(\xi) C(\xi) M^{-1}(\xi) \int B(\xi, \xi_x) \xi(dx) \right) \\ &= \text{tr}(D(\xi) C(\xi)). \end{aligned} \quad \square$$

The first main result of this section provides a necessary condition for the optimality of a given design.

THEOREM 3.1. *Let ξ^* be any design minimizing the functional $\Phi(D(\xi))$. Then the inequality*

$$(3.5) \quad \varphi(x, \xi^*) \leq b(x, \xi^*)$$

holds for all $x \in \mathcal{X}$, where the functions $\varphi(x, \xi)$ and $b(x, \xi)$ are defined in (3.2) and (3.3), respectively. Moreover, there is equality in (3.5) for ξ^ -almost all x , that is, $\xi^*(\mathcal{A}) = 0$ where*

$$\mathcal{A} = \mathcal{A}(\xi^*) = \{x \in \mathcal{X} \mid \varphi(x, \xi^*) < b(x, \xi^*)\}$$

is the set of $x \in \mathcal{X}$ such that the inequality (3.5) is strict.

PROOF. Consider any design ξ^* minimizing the functional $\Phi(D(\xi))$. The necessary condition for an element to be a minimizer of a differentiable functional states that the directional derivative from this element in any direction is nonnegative. In the case of the design ξ^* and the functional $\Phi(D(\xi))$ this yields for any design ν

$$\left. \frac{\partial \Phi(D(\xi_\alpha))}{\partial \alpha} \right|_{\alpha=0} \geq 0,$$

where $\xi_\alpha = (1 - \alpha)\xi^* + \alpha\nu$. Inequality (3.5) follows now from Lemma 1. The assumption that inequality (3.5) is strict for all $x \in \mathcal{A}$ with $\xi^*(\mathcal{A}) > 0$ is in contradiction with identity (3.4). \square

REMARK 3.1. In the classical theory of optimal design, convex optimality criteria are almost always considered. However, in at least one paper, namely [Torsney \(1986\)](#), an optimality theorem for a rather general nonconvex optimality criteria was established and used (in the case of noncorrelated observations).

3.2. An alternative representation of the necessary condition of optimality. For a given design $\xi \in \Xi$, introduce the vector-valued function

$$(3.6) \quad g(x) = \int K(x, u) f(u) \xi(du) - \Lambda f(x), \quad x \in \mathcal{X},$$

where $\Lambda = B(\xi, \xi)M^{-1}(\xi)$. This function satisfies the equality

$$(3.7) \quad \int g(x) f^T(x) \xi(dx) = 0.$$

Additionally, as the vector of regression functions $f(\cdot)$ is continuous on \mathcal{X} , the function $g(\cdot)$ is continuous too.

Note that $f_1, \dots, f_m \in L_2(\mathcal{X}, \xi)$ where

$$L_2(\mathcal{X}, \xi) = \left\{ h : \mathcal{X} \rightarrow \mathbb{R} \mid \int h^2(x) \xi(dx) < \infty \right\}.$$

Formula (3.6) implies that $g(x)$ is the residual obtained after component-wise projection of the vector-valued function $\int K(x, u) f(u) \xi(du)$ onto the subspace $\text{span}\{f_1, \dots, f_m\} \subset L_2(\mathcal{X}, \xi)$.

Using (3.6), (3.7) and the symmetry of the matrix $B(\xi, \xi)$ we obtain

$$\begin{aligned} B(\xi, \xi) &= \iint K(x, u) f(u) \xi(du) f^T(x) \xi(dx) \\ &= \int \Lambda f(x) f^T(x) \xi(dx) + \int g(x) f^T(x) \xi(dx) \\ &= \Lambda M(\xi) = M(\xi) \Lambda^T, \end{aligned}$$

which gives for the matrix D in (2.7),

$$D(\xi) = M^{-1}(\xi) B(\xi, \xi) M^{-1}(\xi) = M^{-1}(\xi) \Lambda = \Lambda^T M^{-1}(\xi).$$

For the function (3.2), we obtain

$$\begin{aligned} \varphi(x, \xi) &= f^T(x) D(\xi) C(\xi) M^{-1}(\xi) f(x) \\ &= f^T(x) \Lambda^T M^{-1}(\xi) C(\xi) M^{-1}(\xi) f(x) \\ &= f^T(x) M^{-1}(\xi) C(\xi) M^{-1}(\xi) \Lambda f(x). \end{aligned}$$

We also have

$$B(\xi, \xi_x) = \int K(x, u) f(u) \xi(du) f^T(x) = \Lambda f(x) f^T(x) + g(x) f^T(x),$$

which gives for function (3.3)

$$\begin{aligned} b(x, \xi) &= \text{tr}(C(\xi) M^{-1}(\xi) B(\xi, \xi_x) M^{-1}(\xi)) \\ &= \varphi(x, \xi) + r(x, \xi), \end{aligned}$$

where the function r is defined by

$$r(x, \xi) = f^T(x) M^{-1}(\xi) C(\xi) M^{-1}(\xi) g(x).$$

The following result is now an obvious corollary of Theorem 3.1.

COROLLARY 3.1. *If a design ξ is optimal, then $r(x, \xi) \geq 0$ for all $x \in \mathcal{X}$ and $r(x, \xi) = 0$ for all x in the support of the measure ξ .*

3.3. D -optimality. For the D -optimality there exists an analogue of the celebrated “equivalence theorem” of Kiefer and Wolfowitz (1960), which characterizes optimal designs minimizing the D -optimality criterion $\Phi(D(\xi)) = \ln \det(D(\xi))$.

THEOREM 3.2. *Let ξ^* be any D -optimal design. Then for all $x \in \mathcal{X}$ we have*

$$(3.8) \quad d(x, \xi^*) \leq b(x, \xi^*),$$

where the functions d and b are defined by $d(x, \xi) = f^T(x)M^{-1}(\xi)f(x)$ and

$$(3.9) \quad \begin{aligned} b(x, \xi) &= \text{tr}(B^{-1}(\xi, \xi)B(\xi, \xi_x)) \\ &= f^T(x)B^{-1}(\xi, \xi) \int K(u, x)f(u)\xi(du), \end{aligned}$$

respectively. Moreover, there is equality in (3.8) for ξ^* -almost all x .

PROOF. In the case of the D -optimality criterion $\Phi(D(\xi)) = \ln \det(D(\xi))$, we have $C(\xi) = D^{-1}(\xi)$, which gives

$$\varphi(x, \xi) = f^T(x)D(\xi)D^{-1}(\xi)M^{-1}(\xi)f(x) = d(x, \xi).$$

Similarly, we simplify an expression for $b(x, \xi)$. Reference to Theorem 3.1 completes the proof. \square

Note that the function $r(x, \xi)$ for the D -criterion is given by

$$r(x, \xi) = f^T(x)B^{-1}(\xi, \xi)g(x)$$

and, consequently, the necessary condition of the D -optimality can be written as $f^T(x)B^{-1}(\xi, \xi)g(x) \geq 0$ for all $x \in \mathcal{X}$.

The following statement illustrates a remarkable similarity between D -optimal design problems in the cases of correlated and noncorrelated observations. The proof easily follows from Lemma 3.2 and Theorem 3.2.

COROLLARY 3.2. *For any design ξ such that the matrices $M(\xi)$ and $B(\xi, \xi)$ are nonsingular we have*

$$\int d(x, \xi)\xi(dx) = \int b(x, \xi)\xi(dx) = m,$$

where $b(x, \xi)$ is defined in (3.9) and m is the number of parameters in the regression model (1.1).

EXAMPLE 3.1. Consider the quadratic regression model $y(x) = \theta_1 + \theta_2x + \theta_3x^2 + \varepsilon(x)$ with design space $\mathcal{X} = [-1, 1]$. In Figure 1 we plot functions $b(x, \xi)$ and $d(x, \xi)$ for the covariance kernels $K(u, v) = e^{-|u-v|}$, $K(u, v) = \max\{0, 1 - |u - v|\}$ and $K(u, v) = -\log(u - v)^2$, where the design is the arcsine distribution with density

$$(3.10) \quad p(x) = 1/(\pi\sqrt{1 - x^2}), \quad x \in (-1, 1).$$

Throughout this paper this design will be called ‘‘arcsine design’’ and denoted by ξ_a . By the definition, the function $d(x, \xi)$ is the same for different covariance kernels, but the function $b(x, \xi)$ depends on the choice of the kernel. From the left

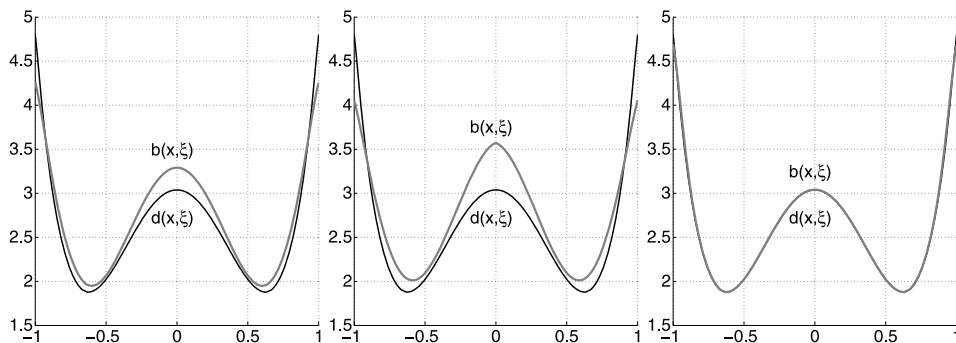


FIG. 1. The functions $b(x, \xi)$ and $d(x, \xi)$ for the regression model (1.1) with $f(x) = (1, x, x^2)^T$ and the covariance kernels $K(u, v) = e^{-|u-v|}$ (left), $K(u, v) = \max(0, 1 - |u - v|)$ (middle) and $K(u, v) = -\log(u - v)^2$ (right) and the arcsine design ξ_a .

and middle panel we see that the arcsine design does not satisfy the necessary condition of Theorem 3.1 for the kernels $K(u, v) = e^{-|u-v|}$ and $\max\{0, 1 - |u - v|\}$ and is therefore not D -optimal for the quadratic regression model. On the other hand, for the logarithmic kernel $K(u, v) = -\log(u - v)^2$ the necessary condition is satisfied, and the arcsine design ξ_a is a candidate for the D -optimal design. We will show in Theorem 4.5 that the design ξ_a is universally optimal and as a consequence optimal with respect to a broad class of criteria including the D -optimality criterion.

3.4. c -optimality. For the c -optimality criterion $\Phi(D(\xi)) = c^T D(\xi)c$, we have $C(\xi) = cc^T$. Consequently,

$$\varphi(x, \xi) = f^T(x)M^{-1}(\xi)cc^T M^{-1}(\xi)\Lambda f(x) = c^T M^{-1}(\xi)\Lambda f(x)f^T(x)M^{-1}(\xi)c$$

and

$$r(x, \xi) = b(x, \xi) - \varphi(x, \xi) = f^T(x)M^{-1}(\xi)cc^T M^{-1}(\xi)g(x).$$

Therefore, the necessary condition for c -optimality simplifies to

$$(3.11) \quad f^T(x)M^{-1}(\xi)cc^T M^{-1}(\xi)g(x) \geq 0 \quad \text{for all } x \in \mathcal{X}.$$

EXAMPLE 3.2. Consider again the quadratic regression model $y(x) = \theta_1 + \theta_2 x + \theta_3 x^2 + \varepsilon(x)$ with design space $\mathcal{X} = [-1, 1]$. Assume the triangular correlation function $\rho(x) = \max\{0, 1 - |x|\}$.

Let $\xi = \{-1, 0, 1; 1/3, 1/3, 1/3\}$ be the design assigning weights $1/3$ to the points $-1, 0$ and 1 . For this design, we have the matrices $M(\xi)$ and $D(\xi)$

$$M(\xi) = \begin{pmatrix} 1 & 0 & 2/3 \\ 0 & 2/3 & 0 \\ 2/3 & 0 & 2/3 \end{pmatrix}, \quad D(\xi) = \begin{pmatrix} 1 & 0 & -1 \\ 0 & 1/2 & 0 \\ -1 & 0 & 3/2 \end{pmatrix},$$

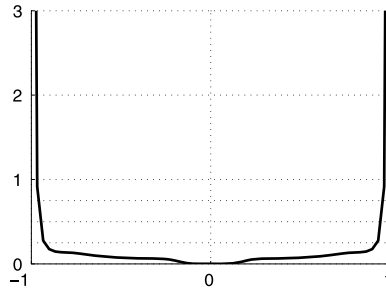


FIG. 2. The c -optimal design for the quadratic model and the triangular correlation function, where $c = (1, 0, 0)^T$.

and the matrix Λ and the vector g are given by

$$\Lambda = \text{diag}(1/3, 1/3, 1/3), \quad g(x) = (1/3, x/3, |x|/3)^T.$$

If $c = (0, 1, 0)^T$, then $r(x, \xi) = 0$ for all $x \in [-1, 1]$ and thus the design ξ satisfies the necessary condition for c -optimality in (3.11). If $c = (1, 0, 1)^T$, then $r(x, \xi) = \frac{3}{4}|x|^3(1 - |x|) \geq 0$ for all $x \in [-1, 1]$ and the design ξ also satisfies (3.11). The corresponding functions b and φ are displayed in the left and middle panels of Figure 3. Numerical analysis shows that for both vectors this design is in fact c -optimal. However, it is not optimal for any c -optimality criteria. For example, if $c = (1, 0, 0)^T$, then $r(x, \xi) = -3x(1 - |x|)(1 - x^2) \leq 0$ for all $x \in [-1, 1]$, showing that the design is not c -optimal; see the middle panel of Figure 3. For this case, the density function of the c -optimal design is displayed in Figure 2. The corresponding functions b and φ are shown in the right panel of Figure 3.

3.5. *Universal optimality.* In this section we consider the matrix $D(\xi)$ defined in (2.7) as the matrix optimality criterion which we are going to minimize on the

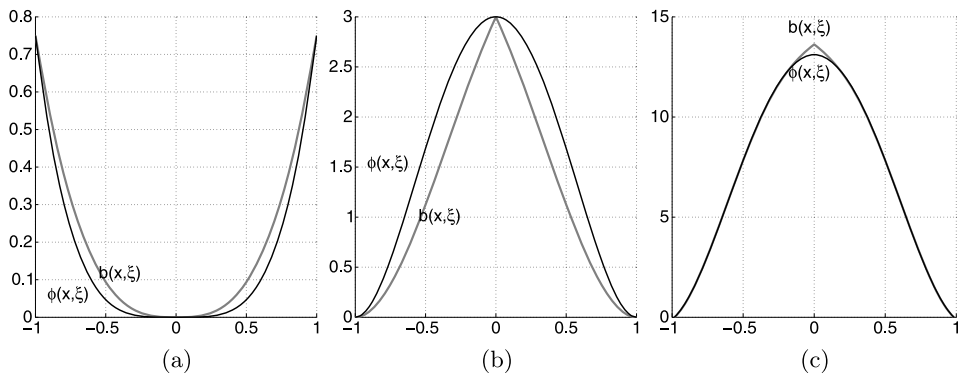


FIG. 3. The functions $b(x, \xi)$ and $\phi(x, \xi)$ for the c -optimality criterion. (a): $c = (1, 0, 1)^T$, design $\xi = \{-1, 0, 1; 1/3, 1/3, 1/3\}$; (b): $c = (1, 0, 0)^T$, design $\xi = \{-1, 0, 1; 1/3, 1/3, 1/3\}$; (c): $c = (1, 0, 0)^T$, design is displayed in Figure 2.

set Ξ of all designs, such that the matrices $B(\xi, \xi)$ and $M^{-1}(\xi)$ [and therefore the matrix $D(\xi)$] are well defined. Recall that a design ξ^* is universally optimal if $D(\xi^*) \leq D(\xi)$ in the sense of the Loewner ordering for any design $\xi \in \Xi$. Note that a design ξ^* is universally optimal if and only if ξ^* is c -optimal for any vector $c \in \mathbb{R}^m \setminus \{0\}$; that is, $c^T D(\xi^*)c \leq c^T D(\xi)c$ for any $\xi \in \Xi$ and any $c \in \mathbb{R}^m$.

THEOREM 3.3. *Consider the regression model (1.1) with a covariance kernel K , a design $\xi \in \Xi$ and the corresponding the vector-function $g(\cdot)$ defined in (3.6).*

- (a) *If $g(x) = 0$ for all $x \in \mathcal{X}$, then the design ξ is universally optimal;*
- (b) *If the design ξ is universally optimal, then the function $g(\cdot)$ can be represented in the form $g(x) = \gamma(x)f(x)$, where $\gamma(x)$ is a nonnegative function defined on \mathcal{X} such that $\gamma(x) = 0$ for all x in the support of the design ξ .*

In the proof of Theorem 3.3 we shall need the following two auxiliary results which will be proved in the [Appendix](#).

LEMMA 3.3. *Let $c \in \mathbb{R}^m$, and \mathcal{M} be the set of all signed vector measures supported on \mathcal{X} . Then the functional $\Phi_c: \mathcal{M} \rightarrow \mathbb{R}_+$ defined by*

$$(3.12) \quad \Phi_c(\mu) = c^T \iint K(x, u)\mu(dx)\mu^T(du)c$$

is convex.

LEMMA 3.4. *Let $m > 1$ and $a, b \in \mathbb{R}^m$ be two linearly independent vectors. Then there exists a vector $c \in \mathbb{R}^m$ such that $S_c = c^T ab^T c < 0$.*

PROOF OF THEOREM 3.3. Consider the regression model $y(x) = f^T(x)\theta + \varepsilon(x)$, where the full trajectory $\{y(x)|x \in \mathcal{X}\}$ can be observed. Let $\hat{\theta}(\mu) = \int y(x)\mu(dx)$ be a general linear unbiased estimate of the parameter θ , where $\mu = (\mu_1, \dots, \mu_m)^T$ is a vector of signed measures. For example, the least squares estimate for a design ξ in this model is obtained as $\hat{\theta}(\mu_\xi)$, where $\mu_\xi(dx) = M^{-1}(\xi)f(x)\xi(dx)$. The condition of unbiasedness of the estimate $\hat{\theta}(\mu)$ means that

$$\theta = E[\hat{\theta}(\mu)] = E\left[\int \mu(dx)y(x)\right] = \int \mu(dx)f^T(x)\theta$$

for all $\theta \in \mathbb{R}^m$, which is equivalent to the condition

$$(3.13) \quad \int \mu(dx)f^T(x) = \int f(x)\mu^T(dx) = I_m,$$

where I_m denotes the $m \times m$ identity matrix. In the following discussion we define \mathcal{M}_0 as a subset of \mathcal{M} containing the signed measures which satisfy condition (3.13). Note that both sets, \mathcal{M} and \mathcal{M}_0 , are convex.

For a given vector $c \in \mathbb{R}^m$, the variance of the estimate $c^T \hat{\theta}(\mu)$ is given by

$$\begin{aligned} \text{Var}(c^T \hat{\theta}(\mu)) &= c^T \iint \mathbb{E}[\varepsilon(x)\varepsilon(u)]\mu(\mathrm{d}x)\mu^T(\mathrm{d}u)c \\ &= c^T \iint K(x, u)\mu(\mathrm{d}x)\mu^T(\mathrm{d}u)c = \Phi_c(\mu), \end{aligned}$$

and a minimizer of this expression with respect to $\mu \in \mathcal{M}_0$ determines the best linear unbiased estimate for $c^T \theta$ and the corresponding c -optimal design simultaneously.

Note that the sets \mathcal{M} and \mathcal{M}_0 are convex and in view of Lemma 3.3 the functional $\Phi_c(\mu)$ defined in (3.12) is convex on \mathcal{M} . Similar arguments as given in Section 3.1 show that the directional derivative of Φ_c at μ^* in the direction of $\nu - \mu^*$ is given by

$$\begin{aligned} &\left. \frac{\partial}{\partial \alpha} \Phi_c(\mu_\alpha) \right|_{\alpha=0} \\ &= \left. \frac{\partial}{\partial \alpha} \Phi_c((1-\alpha)\mu^* + \alpha\nu) \right|_{\alpha=0} \\ &= 2c^T \left[\iint K(x, u)\mu^*(\mathrm{d}x)v^T(\mathrm{d}u) - \iint K(x, u)\mu^*(\mathrm{d}x)\mu^{*T}(\mathrm{d}u) \right] c. \end{aligned}$$

Because Φ_c is convex, the optimality of μ^* in the set \mathcal{M}_0 is equivalent to the condition $\left. \frac{\partial}{\partial \alpha} \Phi_c(\mu_\alpha) \right|_{\alpha=0} \geq 0$ for all $\nu \in \mathcal{M}_0$. Therefore, the signed measure $\mu^* \in \mathcal{M}_0$ minimizes the functional $\Phi_c(\mu)$ if and only if the inequality

$$(3.14) \quad \Phi_c(\mu^*, \nu) \geq \Phi_c(\mu^*)$$

holds for all $\nu \in \mathcal{M}_0$, where

$$\Phi_c(\mu^*, \nu) := c^T \iint K(x, u)\mu^*(\mathrm{d}x)v^T(\mathrm{d}u)c.$$

Let us prove part (a) of Theorem 3.3. Consider a design $\xi \in \Xi$ such that $g(x) = 0$ for all $x \in \mathcal{X}$ and define the vector-valued measure $\mu_0(\mathrm{d}x) = M^{-1}(\xi) \times f(x)\xi(\mathrm{d}x)$. It follows for all $\nu \in \mathcal{M}_0$,

$$\begin{aligned} \Phi_c(\mu_0, \nu) &= c^T \iint K(x, u)M^{-1}(\xi)f(x)\xi(\mathrm{d}x)v^T(\mathrm{d}u)c \\ &= c^T M^{-1}(\xi)\Lambda \int f(u)v^T(\mathrm{d}u)c = c^T M^{-1}(\xi^*)\Lambda c, \end{aligned}$$

where we used (3.13) for the measure ν in the last identity. On the other hand, $\mu_0 \in \mathcal{M}$ also satisfies (3.13), and we obtain once more using identity (3.6) with

$g(x) \equiv 0$,

$$\begin{aligned}\Phi_c(\mu_0) &= c^T \iint K(x, u) \mu_0(dx) \mu_0^T(du) c \\ &= c^T \int \left[\int K(x, u) M^{-1}(\xi) f(x) \xi(dx) \right] \mu_0^T(du) c \\ &= c^T M^{-1}(\xi) \Lambda \int f(u) \mu_0^T(du) c = c^T M^{-1}(\xi) \Lambda c.\end{aligned}$$

This yields that for $\mu^* = \mu_0$ we have equality in (3.14) for all $v \in \mathcal{M}_0$, which shows that the vector-valued measure $\mu_0(dx) = M^{-1}(\xi) f(x) \xi(dx)$ minimizes the function Φ_c for any $c \neq 0$ over the set \mathcal{M}_0 of signed vector-valued measures satisfying (3.13).

Now we return to the minimization of the function $D(\eta)$ in the class of all designs $\eta \in \Xi$. For any $\eta \in \Xi$, define the corresponding vector-valued measure $\mu_\eta(dx) = M^{-1}(\eta) f(x) \eta(dx)$ and note that $\mu_\eta \in \mathcal{M}_0$. We obtain

$$\begin{aligned}c^T D(\eta) c &= c^T M^{-1}(\eta) B(\eta, \eta) M^{-1}(\eta) c = \Phi_c(\mu_\eta) \\ &\geq \min_{\mu \in \mathcal{M}_0} \Phi_c(\mu) = \Phi_c(\mu_0) = c^T D(\xi) c.\end{aligned}$$

Since the design ξ does not depend on the particular vector c , it follows that ξ is universally optimal.

Let us now prove (b) of Theorem 3.3. Assume that the design ξ is universally optimal and let $g(x)$ be the function associated with this design and computed by (3.6).

Consider first the case $m = 1$. In this case, the assumption that ξ is universally optimal design coincides with the assumption of simple optimality. Also, since $f(x) \neq 0$ for all $x \in \mathcal{X}$, we can define $\gamma(x) = g(x)/f(x)$ for all $x \in \mathcal{X}$. In this notation, the statement (b) of Theorem 3.3 coincides with the statement of Corollary 3.1.

Assume now $m > 1$. Since the design ξ is universally optimal it is c -optimal for any vector c and therefore the necessary condition for c -optimality should be satisfied; this condition is

$$r_c(x, \xi) = c^T M^{-1}(\xi) g(x) f^T(x) M^{-1}(\xi) c \geq 0$$

for all $x \in \mathcal{X}$ and $r_c(x, \xi) = 0$ for all x in the support of the measure ξ . If $g(x) = \gamma(x) f(x)$, where $\gamma(x) \geq 0$, then

$$r_c(x, \xi) = \gamma(x) [c^T M^{-1}(\xi) f(x) f^T(x) M^{-1}(\xi) c] \geq 0$$

for any vector c and all x so that the necessary condition for c -optimality is satisfied. On the other hand, if $g(x) = \gamma(x) f(x)$, but $\gamma(x_0) < 0$ for some $x_0 \in \mathcal{X}$ then [in view of the fact that the matrix $M^{-1}(\xi) f(x_0) f^T(x_0) M^{-1}(\xi)$ is nondegenerate]

there exists c such that $r_c(x_0, \xi) < 0$ and the necessary condition for c -optimality of the design ξ is not satisfied.

Furthermore, if the representation $g(x) = \gamma(x)f(x)$ does not hold, then there exists a point $x_0 \in \mathcal{X}$ such that $g(x_0) \neq 0$ and $g(x_0)$ is not proportional to $f(x_0)$ [recall also that $f(x) \neq 0$ for all $x \in \mathcal{X}$]. Then

$$r_c(x_0, \xi) = c^T M^{-1}(\xi)g(x_0)f^T(x_0)M^{-1}(\xi)c = c^T ab^T c$$

with $a = M^{-1}(\xi)g(x_0)$ and $b = M^{-1}(\xi)f(x_0)$. Using Lemma 3.4, we deduce that there exists a vector c such that $r_c(x_0, \xi) < 0$. Therefore the design ξ is not c -optimal and as a consequence also not universally optimal. \square

In the one-parameter case ($m = 1$) it is easy to construct examples where the function $g(x)$ corresponding to the optimal design is nonzero. For example, consider the regression model $y(t) = \theta t + \varepsilon(t)$, $t \in [-1, 1]$, with the so-called spherical correlation function

$$\rho(u) = 1 - \frac{3}{2}|u|/R + \frac{1}{2}(|u|/R)^3$$

with $R = 2$. Then the design assigning weights 0.5 to the points -1 and 1 is optimal. For this design, the function $g(x)$ defined in (3.6) is equal to $g(x) = x(1 - x^2)/16$, while the function $\gamma(x)$ is $\gamma(x) = (1 - x^2)/16$, $x \in [-1, 1]$.

4. Optimal designs for specific kernels and models.

4.1. *Optimality and Mercer's theorem.* In this section we consider the case when the regression functions are proportional to eigenfunctions from Mercer's theorem. To be precise, let \mathcal{X} denote a compact subset of a metric space, and let ν denote a measure on the corresponding Borel field with positive density. Consider the integral operator

$$(4.1) \quad T_K(f)(\cdot) = \int_{\mathcal{X}} K(\cdot, u)f(u)\nu(du)$$

on $L_2(\nu)$. Under certain assumptions on the kernel [e.g., if $K(u, v)$ is symmetric, continuous and positive definite] T_K defines a symmetric, compact self-adjoint operator. In this case Mercer's theorem [see, e.g., Kanwal (1997)] shows that there exist a countable number of eigenfunctions $\varphi_1, \varphi_2, \dots$ with positive eigenvalues $\lambda_1, \lambda_2, \dots$ of the operator K , that is,

$$(4.2) \quad T_K(\varphi_\ell) = \lambda_\ell \varphi_\ell, \quad \ell = 1, 2, \dots$$

The next statement follows directly from Theorem 3.3.

THEOREM 4.1. *Let \mathcal{X} be a compact subset of a metric space, and assume that the covariance kernel $K(x, u)$ defines an integral operator T_K of the form (4.1), where the eigenfunctions satisfy (4.2). Consider the regression model (1.1) with $f(x) = L(\varphi_{i_1}(x), \dots, \varphi_{i_m}(x))^T$ and the covariance kernel $K(x, u)$, where $L \in \mathbb{R}^{m \times m}$ is a nonsingular matrix. Then the design ν is universally optimal.*

We note that the Mercer expansion is known analytically for certain covariance kernels. For example, if ν is the uniform distribution on the interval $\mathcal{X} = [-1, 1]$, and the covariance kernel is of exponential type, that is, $K(x, u) = e^{-\lambda|x-u|}$, then the eigenfunctions are given by

$$\varphi_k(x) = \sin(\omega_k x + k\pi/2), \quad k \in \mathbb{N},$$

where $\omega_1, \omega_2, \dots$ are positive roots of the equation $\tan(2\omega) = -2\lambda\omega/(\lambda^2 - \omega^2)$. Similarly, consider as a second example, the covariance kernel $K(x, u) = \min\{x, u\}$ and $\mathcal{X} = [0, 1]$. In this case, the eigenfunctions of the corresponding integral operator are given by

$$\varphi_k(x) = \sin((k + 1/2)\pi x), \quad k \in \mathbb{N}.$$

In the following subsection we provide a further example of the application of Mercer's theorem, which is of importance for series estimation in nonparametric regression.

4.2. Uniform design for periodic covariance functions. Consider the regression functions

$$(4.3) \quad f_j(x) = \begin{cases} 1, & \text{if } j = 1, \\ \sqrt{2} \cos(2\pi(j-1)x), & \text{if } j \geq 2, \end{cases}$$

and the design space $\mathcal{X} = [0, 1]$. Linear models of the form (1.1) with regression functions (4.3) are widely applied in series estimation of a nonparametric regression function [see, e.g., Efromovich (1999, 2008) or Tsybakov (2009)]. Assume that the correlation function $\rho(x)$ is periodic with period 1, that is, $\rho(x) = \rho(x + 1)$, and let a covariance kernel be defined by $K(u, v) = \sigma^2 \rho(u - v)$ with $\sigma^2 = 1$. An example of the covariance kernel $\rho(x)$ satisfying this property is provided by a convex combination of the functions $\{\cos(2\pi x), \cos^2(2\pi x), \dots\}$.

THEOREM 4.2. *Consider regression model (1.1) with regression functions $f_{i_1}(x), \dots, f_{i_m}(x)$ ($1 \leq i_1 < \dots < i_m$) defined in (4.3) and a correlation function $\rho(t)$ that is periodic with period 1. Then the uniform design is universally optimal.*

PROOF. We will show that the identity

$$(4.4) \quad \int_0^1 K(u, v) f_j(u) du = \int_0^1 \rho(u - v) f_j(u) du = \lambda_j f_j(v)$$

holds for all $v \in [0, 1]$, where $\lambda_j = \int \rho(u) f_j(u) du$ ($j \geq 1$). The assertion then follows from Theorem 4.1.

To prove (4.4), we define $A_j(v) = \int_0^1 \rho(u - v) f_j(u) du$ which should be shown to be $\lambda_j f_j(v)$. For $j = 1$ we have $A_1(v) = \lambda_1$ because $\int_0^1 \rho(u - v) du =$

$\int_0^1 \rho(u) du = \lambda_1$ by the periodicity of the function $\rho(x)$. For $j = 2, 3, \dots$ we note that

$$\begin{aligned} A_j(v) &= \int_0^1 \rho(u-v) f_j(u) du = \int_{-v}^{1-v} f_j(u+v) \rho(u) du \\ &= \int_0^{1-v} f_j(u+v) \rho(u) du + \int_{-v}^0 f_j(u+v) \rho(u) du. \end{aligned}$$

Because of the periodicity we have

$$\int_{-v}^0 f_j(u+v) \rho(u) du = \int_{1-v}^1 f_j(u+v) \rho(u) du,$$

which gives $A_j(v) = \int_0^1 f_j(u+v) \rho(u) du$. A simple calculation now shows

$$(4.5) \quad A_j''(v) = -b_j^2 A_j(v),$$

where $b_j^2 = (2\pi(j-1))^2$ and

$$A_j(0) = \sqrt{2} \int_0^1 \cos(2\pi(j-1)u) \rho(u) du = \sqrt{2} \lambda_j,$$

$$A_j'(0) = -b_j \sqrt{2} \int_0^1 \sin(2\pi(j-1)u) \rho(u) du = 0.$$

Therefore (from the theory of differential equations) the unique solution of (4.5) is of the form $A_j(v) = c_1 \cos(b_j v) + c_2 \sin(b_j v)$, where c_1 and c_2 are determined by initial conditions, that is, $A_j(0) = c_1 = \sqrt{2} \lambda_j$, $A_j'(0) = b_j c_2 = 0$. This yields $A_j(v) = \lambda_j \sqrt{2} \cos(2\pi(j-1)v) = \lambda_j f_j(v)$ and proves identity (4.4). \square

4.3. *Optimal designs for the triangular covariance function.* Let us now consider the triangular correlation function defined by

$$(4.6) \quad \rho(x) = \max\{0, 1 - \lambda|x|\}.$$

On the one hand this function arises as a correlation function of the process of increments of a Brownian motion which is in turn related to a Brownian bridge after a suitable conditioning is made; see [Mehr and McFadden \(1965\)](#). On the other hand it is motivated by the fact that for “small” values of the parameter λ , it provides a good approximation of the exponential correlation kernel $\rho_\lambda(x) = \exp(-\lambda|x|)$, which is widely used for modeling correlations in regression models; see [Ucinski and Atkinson \(2004\)](#) or [Dette, Pepelyshev and Holland-Letz \(2010\)](#), among others. For the exponential correlation kernel optimal designs are difficult to find, even in the linear regression model; see [Dette, Kunert and Pepelyshev \(2008\)](#). However, as the next theorem shows, it is possible to explicitly derive optimal designs for the linear model with a triangular correlation function. It will be demonstrated in [Example 4.1](#) below that for “small” and “moderate” values of the parameter λ , these designs provide also an efficient solution of the design problem for the exponential correlation kernel.

THEOREM 4.3. Consider model (1.1) with $f(x) = (1, x)^T$, $\mathcal{X} = [-1, 1]$ and the triangular correlation function (4.6).

(a) If $\lambda \in (0, 1/2]$, then the design $\xi^* = \{-1, 1; 1/2, 1/2\}$ is universally optimal.

(b) If $\lambda \in \mathbb{N}$, then the design supported at $2\lambda + 1$ points $x_k = -1 + k/\lambda$, $k = 0, 1, \dots, 2\lambda$, with equal weights is universally optimal.

PROOF. To prove part (a) we will show that $\int \rho(x - u) f_i(u) \xi^*(du) = \lambda_i f_i(x)$ for $i = 1, 2$ and some λ_1 and λ_2 . By direct calculations we obtain for $f_1(x) = 1$,

$$\int_{-1}^1 \rho(x - u) \xi^*(du) = \frac{-\lambda|x + 1|}{2} + \frac{1 - \lambda|x - 1|}{2} = 1 - \lambda$$

and, consequently, $\lambda_1 = 1 - \lambda$. Similarly, we have for $f_2(x) = x$,

$$\int_{-1}^1 u \rho(x - u) \xi^*(du) = -\frac{1 - \lambda|x + 1|}{2} + \frac{1 - \lambda|x - 1|}{2} = \lambda x$$

and, therefore, $\lambda_2 = \lambda$. Thus, the assumptions of Theorem 3.3 are fulfilled.

Part (b). Straightforward but tedious calculations show that $M(\xi^*) = \text{diag}(1, \gamma)$, where $\gamma = \sum_{k=0}^{2\lambda+1} x_k^2 / (2\lambda + 1) = (\lambda + 1) / (2\lambda)$. Also we have

$$\int \rho(x - u) f_i(u) \xi^*(du) = \lambda_i f_i(x)$$

for $i = 1, 2$ where $\lambda_1 = \lambda_2 = 1 / (2\lambda + 1)$. Thus, the assumptions of Theorem 3.3 are fulfilled. \square

The designs provided in Theorem 4.3 are also optimal for the location scale model; see Zhigljavsky, Dette and Pepelyshev (2010). However, unlike the results of previous subsections the result of Theorem 4.3 cannot be extended to polynomial models of higher order.

We conclude this section with an example illustrating the efficiency of the designs for the triangular kernel in models with correlation structure defined by the exponential kernel.

EXAMPLE 4.1. Consider the location scale model [$f(x) = 1$] and the linear regression model [$f(x) = (1, x)^T$], $\mathcal{X} = [-1, 1]$, and the correlation function $\rho(x) = \exp\{-\lambda|x|\}$. In Table 1 we display the D -efficiencies of the universally optimal design calculated under the assumption of the triangular kernel (4.6) for various values of the parameter $\lambda \in [0.1, 0.9]$. For this design we observe in all cases a D -efficiency of at least 90%. In most cases it is higher than 95%.

TABLE 1
D-Efficiencies of the universally optimal design
 $\xi = \{-1, 1; 0.5, 0.5\}$ calculated under the assumption of a
 triangular correlation function in the constant and linear
 regression model with the exponential
 correlation function $\rho(x) = e^{-\lambda|x|}$

λ	0.1	0.3	0.5	0.7	0.9
Constant	0.999	0.997	0.978	0.946	0.905
Linear	0.999	0.999	0.991	0.974	0.950

4.4. *Polynomial regression models and singular kernels.* In this section we consider the polynomial regression model, that is, $f(x) = (1, x, \dots, x^{m-1})^T$, with logarithmic covariance kernel

$$(4.7) \quad K(u, v) = \gamma - \beta \ln(u - v)^2, \quad \beta > 0, \gamma \geq 0,$$

and the kernel

$$(4.8) \quad K(u, v) = \gamma + \beta/|u - v|^\alpha, \quad 0 \leq \alpha < 1, \gamma \geq 0, \beta > 0,$$

for which the universally optimal designs can be found explicitly.

Covariance functions $K(u, v)$ with a singularity at $u = v$ appear naturally as approximations to many standard covariance functions $\tilde{K}(u, v) = \sigma^2 \tilde{\rho}(u - v)$ with $\tilde{\rho}(0) = 1$ if σ^2 is large. A general scheme for this type of approximation is investigated in Zhigljavsky, Dette and Pepelyshev (2010), Section 4. More precisely, these authors discussed the case where the covariance kernel can be represented as $\sigma_\delta^2 \tilde{\rho}_\delta(t) = r * h_\delta(t)$ with a singular kernel $r(t)$ and a smoothing kernel $h_\delta(\cdot)$ (here δ is a smoothing parameter and $*$ denotes the convolution operator). The basic idea is illustrated in the following example.

EXAMPLE 4.2. Consider the covariance kernel $\tilde{K}(u, v) = \rho_\delta(u - v)$, where

$$(4.9) \quad \rho_\delta(t) = 2 - \frac{1}{\delta} \log\left(\frac{|t + \delta|^{t+\delta}}{|t - \delta|^{t-\delta}}\right).$$

For several values of δ , the function ρ_δ is displayed in Figure 4. A straightforward calculation shows that $\rho_\delta(t) = r * h_\delta(t)$, where $r(t) = -\ln(t)^2$ and h_δ is the density of the uniform distribution on the interval on $[-\delta, \delta]$. As illustrated by Figure 4, the function $\rho_\delta(\cdot)$ is well approximated by the singular kernel $r(\cdot)$ if δ is small.

In Figure 5 we display the D -optimal designs (constructed numerically) for the quadratic model with a stationary error process with covariance kernel $\tilde{K}(u, u + t) = \rho_\delta(t)$, where ρ_δ is defined in (4.9) and $\delta = 0.02, 0.05, 0.1$. As one can see,

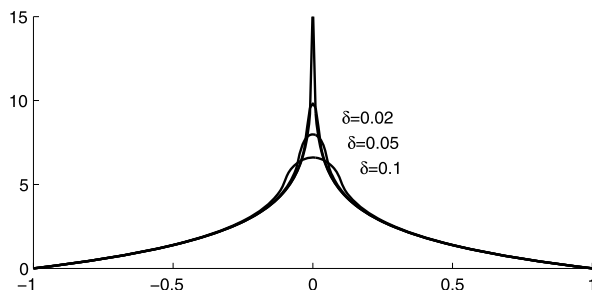


FIG. 4. The logarithmic covariance kernel $r(t) = -\ln(t)^2$ and the covariance kernel (4.9), where $\delta = 0.02, 0.05, 0.1$.

for small δ these designs are very close to the arcsine design, which is the D -optimal design for the quadratic model and the logarithmic kernel, as proved in Theorem 4.5 of the following section.

In Table 2 we show the efficiency of the arcsine distribution [obtained by maximizing $\det(D(\xi))$ with the logarithmic kernel] in the quadratic regression model with the kernel (4.9). We observe a very high efficiency with respect to the D -optimality criterion. Even in the case $\delta = 0.1$ the efficiency is 93.6% and it converges quickly to 100% as δ approaches 0.

EXAMPLE 4.3. The arcsine density can also be used as an alternative approximation to the exponential correlation function or correlation functions of a similar type, that is, $\rho_{\lambda, \nu}(t) = \exp(-\lambda|t|^\nu)$. For the case $\lambda = \nu = 1$ the function $\frac{7}{15}(1 - \frac{3}{17} \ln t^2)$ can be considered as a reasonable approximation to $\exp(-|t|)$ on the interval $[-1, 1]$; see the left part of Figure 6. Similarly, if $\lambda = 1, \nu = 1/4$, it is illustrated in the right part of Figure 6 that the function $\frac{3}{8} - \frac{1}{25} \ln t^2$ provides

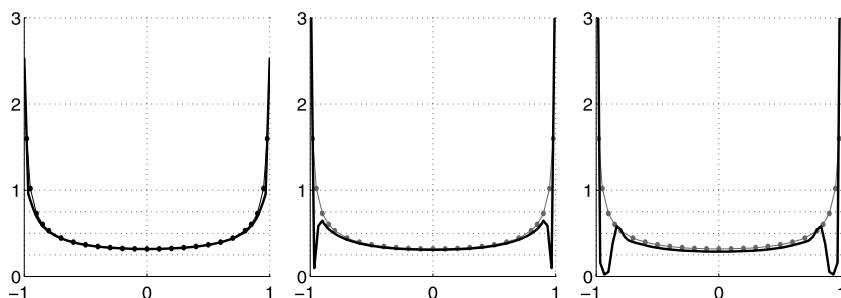


FIG. 5. Density functions corresponding to the D -optimal designs for the quadratic model with covariance kernel (4.9), where $\delta = 0.02$ (left), $\delta = 0.05$ (middle) and $\delta = 0.1$ (right). The y -axis corresponds to values of the density functions. The corresponding designs are obtained by (2.3), where a^{-1} is the distribution function corresponding to the displayed densities. The grey line corresponds to the arcsine density $p(x) = 1/\pi \sqrt{1-x^2}$.

TABLE 2
Efficiency of the arcsine design ξ_a for the quadratic model and the kernel (4.9)

δ	0.02	0.04	0.06	0.08	0.1
$\text{Eff}(\xi_a)$	0.998	0.978	0.966	0.949	0.936

a very accurate approximation of the exponential correlation function. As a consequence, the arcsine design (optimal for the logarithmic kernel) will also have a high efficiency with respect to these kernels, and this argument is illustrated in Table 3 of Section 5.2 where we calculate the D -efficiencies of the arcsine design in polynomial regression models with correlation function $\exp(-|t|)$. For the correlation function $\exp(-\lambda|t|^{1/4})$ a similar D -efficiency of the arcsine design can be observed. For example, if $\lambda = 0.5, 2.5$ the D -efficiencies of the arcsine design in the linear regression model are 100% and 96.9%, respectively, while they are 99.9% and 97.1% in the quadratic model. Other choices of λ and ν yield similar results, which are not displayed for the sake of brevity.

4.4.1. *Optimality of the arcsine design.* We will need the following lemma, which states a result in the theory of Fredholm–Volterra integral equations; see Mason and Handscomb (2003), Chapter 9, page 211.

LEMMA 4.1. *The Chebyshev polynomials of the first kind $T_n(x) = \cos(n \times \arccos x)$ are the eigenfunctions of the integral operator with the kernel $H(x, v) =$*

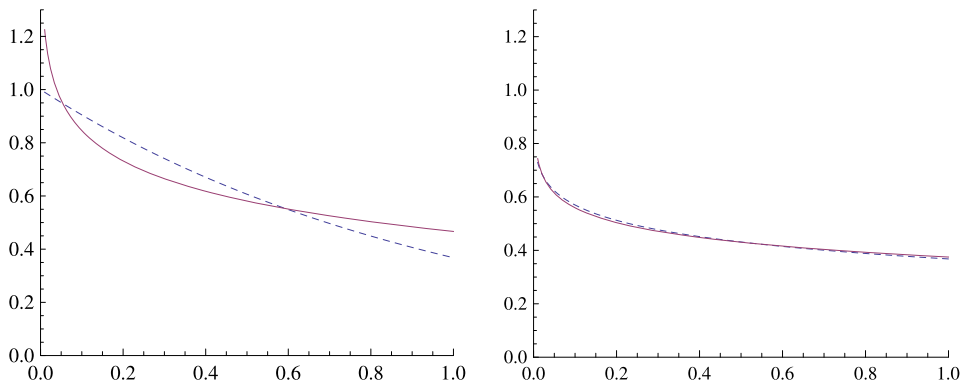


FIG. 6. *Left panel: the function $\frac{7}{15}(1 - \frac{3}{17} \ln t^2)$ (solid line) as an approximation of the exponential correlation function $\exp(-|t|)$. Right panel: the function $\frac{3}{8} - \frac{1}{25} \ln t^2$ (solid line) as an approximation of the exponential correlation function $\exp(-|t|^{1/4})$ (dashed line).*

$-\ln(x - v)^2/\sqrt{1 - v^2}$. More precisely, for all $n = 0, 1, \dots$ we have for all $n \in \mathbb{N}$

$$\lambda_n T_n(x) = - \int_{-1}^1 T_n(v) \ln(x - v)^2 \frac{dv}{\pi \sqrt{1 - v^2}}, \quad x \in [-1, 1],$$

where $\lambda_0 = 2 \ln 2$ and $\lambda_n = 2/n$ for $n \geq 1$.

With the next result we address the problem of uniqueness of the optimal design. In particular, we give a new characterization of the arcsine distribution. A proof can be found in the [Appendix](#).

THEOREM 4.4. *Let n be a nonnegative integer and ζ be a random variable supported on the interval $[-1, 1]$. Then the distribution of ζ has the arcsine density (3.10) if and only if the equality*

$$\mathbb{E}T_n(\zeta)(-\ln(\zeta - x)^2) = c_n T_n(x)$$

holds for almost all $x \in [-1, 1]$, where $c_n = 2/n$ if $n \in \mathbb{N}$ and $c_0 = 2 \ln 2$ if $n = 0$.

The following result is an immediate consequence of Theorems 3.3 and 4.4.

THEOREM 4.5. *Consider the polynomial regression model (1.1) with $f(x) = (1, x, x^2, \dots, x^{m-1})^T$, $x \in [-1, 1]$, and the covariance kernel (4.7). Then the arcsine design ξ_a with density (3.10) is the universally optimal design.*

PROOF. We assume without loss of generality that $\beta = 1$ and consider the function $\rho(x) = -\ln x^2 + \gamma$ with positive γ . From Lemma 4.1 we obtain

$$\begin{aligned} \int_{-1}^1 (-\ln(u - x)^2 + \gamma) T_n(u) p(u) du &= - \int_{-1}^1 \ln(u - x)^2 T_n(u) p(u) du \\ &= \lambda_n T_n(x) + \gamma \delta_{n0}, \end{aligned}$$

where δ_{xy} denotes Kronecker's symbol and we have used the fact that $\int_{-1}^1 T_n(u)/\sqrt{1 - u^2} du = 0$ whenever $n \geq 1$. This proves (3.6) for the arcsine distribution and the vector $t(x) = (T_0(x), \dots, T_{m-1}(x))^T$ where the function $g(x)$ is equal to 0 for all x . Now $f(x) = (1, x, \dots, x^{m-1})^T = Lt(x)$ for some nonsingular $m \times m$ matrix. Therefore (3.6) holds also for the vector $f(x)$ with $g(x) \equiv 0$ (and a different matrix Λ). The statement of the theorem now follows from Theorems 3.3 and 4.4. \square

4.4.2. Generalized arcsine designs. For $\alpha \in (0, 1)$ consider the Gegenbauer polynomials $C_m^{(\alpha)}(x)$ which are orthogonal with respect to the weight function

$$(4.10) \quad p_\alpha(x) = \frac{(\Gamma(\alpha + 1/2))^2}{2^\alpha \Gamma(2\alpha + 1)} (1 - x^2)^{(\alpha-1)/2}, \quad x \in [-1, 1].$$

For the choice $\alpha = 0$ the Gegenbauer polynomials $C_m^{(\alpha)}(x)$ are proportional to the Chebyshev polynomials of the first kind $T_m(x)$. Throughout this paper we will call the corresponding beta-distributions *generalized arcsine designs* emphasizing the fact that the distribution is symmetric and the parameter α varies in the interval $(0, 1)$. The following result [from the theory of Fredholm–Volterra integral equations of the first kind with special kernel, see Fahmy, Abdou and Darwish (1999)] establishes an analogue of Lemma 4.1 for the kernel

$$(4.11) \quad H(u, v) = \frac{1}{|u - v|^\alpha (1 - v^2)^{(1-\alpha)/2}}.$$

LEMMA 4.2. *The Gegenbauer polynomials $C_n^{(\alpha/2)}(x)$ are the eigenfunctions of the integral operator with the kernel defined in (4.11). More precisely, for all $n = 0, 1, \dots$ we have*

$$\lambda_n C_n^{(\alpha/2)}(x) = - \int_{-1}^1 \frac{1}{|x - v|^\alpha} C_n^{(\alpha/2)}(v) \frac{dv}{(1 - v^2)^{(1-\alpha)/2}}$$

for all $x \in [-1, 1]$, where $\lambda_n = \frac{\pi \Gamma(n+\alpha)}{\cos(\alpha\pi/2) \Gamma(\alpha)n!}$.

The following result generalizes Theorem 8 of Zhigljavsky, Dette and Pepelyshev (2010) from the case of a location scale model to polynomial regression models.

THEOREM 4.6. *Consider the polynomial regression model (1.1) with $f(x) = (1, x, x^2, \dots, x^{m-1})^T$, $x \in [-1, 1]$, and covariance kernel (4.8). Then the design with generalized arcsine density defined in (4.10) is universally optimal.*

PROOF. It is easy to see that the optimal design does not depend on β and we thus assume that $\beta = 1$ in (4.8).

To prove the statement for the kernel $\rho(x) = 1/|x|^\alpha + \gamma$ with positive γ we recall the definition of p_α in (4.10) and obtain from Lemma 4.2

$$\begin{aligned} \int \left(\frac{1}{|u - x|^\alpha} + \gamma \right) C_n^{(\alpha/2)}(u) p_{\alpha/2}(u) du &= \int \frac{1}{|u - x|^\alpha} C_n^{(\alpha/2)}(u) p_{\alpha/2}(u) du \\ &\propto C_n^{(\alpha/2)}(x) \end{aligned}$$

for any $n \in \mathbb{N}$ since $\int C_n^{(\alpha/2)}(u) p_{\alpha/2}(u) du = 0$. Consider the design ξ with density $p_{\alpha/2}$. For this design, the function $g(x)$ defined in (3.6) is identically zero; this follows from the formula above. It now follows by the same arguments as given at the end of the proof of Theorem 4.5 that the design with density $p_{\alpha/2}$ is universally optimal. \square

5. Numerical construction of optimal designs.

5.1. *An algorithm for computing optimal designs.* Numerical computation of optimal designs for a common linear regression model (1.1) with given correlation function can be performed by an extension of the multiplicative algorithm proposed by Dette, Pepelyshev and Zhigljavsky (2008) for the case of noncorrelated observations. Note that the proposed algorithm constructs a discrete design which can be considered as an approximation to a design which satisfies the necessary conditions of optimality of Theorem 3.1. By choosing a fine discretization $\{x_1, \dots, x_n\}$ of the design space \mathcal{X} and running the algorithm long enough, the accuracy of approximation can be made arbitrarily small (in the case when convergence is achieved).

Denote by $\xi^{(r)} = \{x_1, \dots, x_n; w_1^{(r)}, \dots, w_n^{(r)}\}$ the design at the iteration r , where $w_1^{(0)}, \dots, w_n^{(0)}$ are nonzero weights, for example, uniform. We propose the following updating rule for the weights:

$$(5.1) \quad w_i^{(r+1)} = \frac{w_i^{(r)}(\psi(x_i, \xi^{(r)}) - \beta_r)}{\sum_{j=1}^n w_j^{(r)}(\psi(x_j, \xi^{(r)}) - \beta_r)}, \quad i = 1, \dots, n,$$

where β_r is a tuning parameter [the only condition on β_r is the positivity of all the weights in (5.1)], $\psi(x, \xi) = \varphi(x, \xi)/b(x, \xi)$ and the functions $\varphi(x, \xi)$ and $b(x, \xi)$ are defined in (3.2) and (3.3), respectively. Condition (3.5) takes the form $\psi(x, \xi^*) \leq 1$ for all $x \in \mathcal{X}$. Rule (5.1) means that at the next iteration the weight of a point $x = x_j$ increases if condition (3.5) does not hold at this point.

A measure ξ_* is a fixed point of the iteration (5.1) if and only if $\psi(x, \xi_*) = 1$ for all $x \in \text{supp}(\xi_*)$ and $\psi(x, \xi_*) \leq 1$ for all $x \in \mathcal{X} \setminus \text{supp}(\xi_*)$. That is, a design ξ_* is a fixed point of the iteration (5.1) if and only if it satisfies the optimality condition of Theorem 3.1. We were not able to theoretically prove the convergence of iterations (5.1) to the design satisfying the optimality condition of Theorem 3.1, but we observed this convergence in all numerical studies. In particular, for the cases where we could derive the optimal designs explicitly, we observed convergence of the algorithm to the optimal design.

Algorithm (5.1) can be easily extended to cover the case of singular covariance kernels. Alternatively, a singular kernel can be approximated by a nonsingular one using the technique described in Zhigljavsky, Dette and Pepelyshev (2010), Section 4.

5.2. *Efficiencies of the uniform and arcsine densities.* In the present section we numerically study the efficiency (with respect to the D -optimality criterion) of the uniform and arcsine designs for the polynomial model (1.1) with $f(x) = (1, x, \dots, x^{m-1})^T$ and the exponential correlation function $\rho(t) = e^{-\lambda|t|}$, $t \in [-1, 1]$. We determine the efficiency of a design ξ as

$$\text{Eff}(\xi) = \left(\frac{\det D(\xi^*)}{\det D(\xi)} \right)^{1/m},$$

TABLE 3
Efficiencies of the uniform design ξ_u and the arcsine design ξ_a for the polynomial regression model of degree $m - 1$ and the exponential correlation function $\rho(x) = e^{-\lambda|x|}$

	λ	0.5	1.5	2.5	3.5	4.5	5.5
$m = 1$	Eff(ξ_u)	0.913	0.888	0.903	0.919	0.933	0.944
	Eff(ξ_a)	0.966	0.979	0.987	0.980	0.968	0.954
$m = 2$	Eff(ξ_u)	0.857	0.832	0.847	0.867	0.886	0.901
	Eff(ξ_a)	0.942	0.954	0.970	0.975	0.973	0.966
$m = 3$	Eff(ξ_u)	0.832	0.816	0.826	0.842	0.860	0.876
	Eff(ξ_a)	0.934	0.938	0.954	0.968	0.976	0.981
$m = 4$	Eff(ξ_u)	0.826	0.818	0.823	0.835	0.849	0.864
	Eff(ξ_a)	0.934	0.936	0.945	0.957	0.967	0.975

where ξ^* is the design computed by the algorithm described in the previous section (applied to the D -optimality criterion). The results are depicted in Table 3. We observe that the efficiency of the arcsine design is always higher than the efficiency of the uniform design. Moreover, the absolute difference between the efficiencies of the two designs increases as m increases. On the other hand, in most cases the efficiency of the uniform design and the arcsine design decreases as m increases.

6. Conclusions. In this paper we have addressed the problem of constructing optimal designs for least squares estimation in regression models with correlated observations. The main challenge in problems of this type is that—in contrast to “classical” optimal design theory for uncorrelated data—the corresponding optimality criteria are not convex (except for the location scale model). By relating the design problem to an integral operator problem, universally optimal design can be identified explicitly for a broad class of regression models and correlation structures. Particular attention is paid to a trigonometric regression model involving only cosines terms, where it is proved that the uniform distribution is universally optimal for any periodic kernel of the form $K(u, v) = \rho(u - v)$. For the classical polynomial regression model with a covariance kernel given by the logarithmic potential it is proved that the arcsine distribution is universally optimal. Moreover, optimal designs are derived for several other regression models.

So far optimal designs for regression models with correlated observations have only be derived explicitly for the location scale model, and to our best knowledge the results presented in this paper provide the first explicit solutions to this type of problem for a general class of models with more than one parameter.

We have concentrated on the construction of optimal designs for least squares estimation (LSE) because the best linear unbiased estimator (BLUE) requires the

knowledge of the correlation matrix. While the BLUE is often sensitive with respect to misspecification of the correlation structure, the corresponding optimal designs for the LSE show a remarkable robustness. Moreover, the difference between BLUE and LSE is often surprisingly small, and in many cases BLUE and LSE with certain correlation functions are asymptotically equivalent; see Rao (1967), Kruskal (1968).

Indeed, consider the location scale model $y(x) = \theta + \varepsilon(x)$ with $K(u, v) = \rho(u - v)$, where the knowledge of a full trajectory of a process $y(x)$ is available. Define the (linear unbiased) estimate $\hat{\theta}(G) = \int y(x) dG(x)$, where $G(x)$ is a distribution function of a signed probability measure. A celebrated result of Grenander (1950) states that the “estimator” $\hat{\theta}(G^*)$ is BLUE if and only if $\int \rho(u - x) dG^*(u)$ is constant for all $x \in \mathcal{X}$. This result was extended by Näther [(1985a), Section 4.3], to the case of random fields with constant mean. Consequently, if $G^*(x)$ is a distribution function of a nonsigned (rather than signed) probability measure, then LSE coincides with BLUE and an asymptotic optimal design for LSE is also an asymptotic optimal design for BLUE. Hájek (1956) proved that G^* is a distribution function of a nonsigned probability measure if the correlation function ρ is convex on the interval $(0, \infty)$. Zhigljavsky, Dette and Pepelyshev (2010) showed that G^* is a proper distribution function for a certain families of correlation functions including nonconvex ones.

In Theorem 3.3 we have characterized the cases where there exist universally optimal designs for ordinary least squares estimation. Specifically, a design ξ^* is universally optimal for least squares estimation if and only if condition (3.6) with $g(x) \equiv 0$ is satisfied. Moreover, the proof of Theorem 3.3 shows that in this case the signed vector-valued measure

$$\mu(dx) = M^{-1}(\xi^*)f(x)\xi^*(dx)$$

and the LSE minimizes (with respect to the Loewner ordering) the matrix

$$\iint K(x, u)\mu(dx)\mu^T(du)$$

in the space \mathcal{M} of all vector-valued signed measures. Because this matrix is the covariance of the linear estimate $\int y(x)\mu(dx)$ (where μ is a vector of signed measures) it follows that under the assumptions of Theorem 3.3, the LSE combined with the universally optimal design ξ^* give exactly the same asymptotic covariance matrix as the BLUE and the optimal design for the BLUE.

APPENDIX: SOME TECHNICAL DETAILS

PROOF OF LEMMA 3.3. For any $c \in \mathbb{R}^m$ and $\mu \in \mathcal{M}$ we set $\nu(\cdot) = c^T \mu(\cdot)$, where $\nu(dx)$ is a signed measure on \mathcal{X} . Then the functional

$$\Phi_c(\mu) = c^T \iint K(x, u)\mu(dx)\mu^T(du)c$$

can also be written as

$$\Phi_c(\mu) = \Psi(v) = \iint K(x, u)v(dx)v(du).$$

For any $\alpha \in [0, 1]$ and any two signed measures v_0 and v_1 on \mathcal{X} we have

$$\begin{aligned} &\Psi(\alpha v_0 + (1 - \alpha)v_1) \\ &= \iint K(u, v)[\alpha v_0(du) + (1 - \alpha)v_1(du)][\alpha v_0(dv) + (1 - \alpha)v_1(dv)] \\ &= \alpha^2 \iint K(u, v)v_0(du)v_0(dv) + (1 - \alpha)^2 \iint K(u, v)v_1(du)v_1(dv) \\ &\quad + 2\alpha(1 - \alpha) \iint K(u, v)v_0(du)v_1(dv) \\ &= \alpha^2\Psi(v_0) + (1 - \alpha)^2\Psi(v_1) + 2\alpha(1 - \alpha) \iint K(u, v)v_0(du)v_1(dv) \\ &= \alpha\Psi(v_0) + (1 - \alpha)\Psi(v_1) - \alpha(1 - \alpha)A, \end{aligned}$$

where

$$\begin{aligned} A &= \iint K(u, v)[v_0(du)v_0(dv) + v_1(du)v_1(dv) - 2v_0(du)v_1(dv)] \\ &= \iint K(u, v)\zeta(du)\zeta(dv) \end{aligned}$$

and $\zeta(du) = v_0(du) - v_1(du)$. In view of (2.9), we have $A \geq 0$ and therefore the functional $\Psi(\cdot)$ is convex. \square

PROOF OF LEMMA 3.4. As vectors a and b are linearly independent, we have $a^T a > 0$, $b^T b > 0$ and $(a')^T b' < 1$, where $a' = a/\sqrt{a^T a}$ and $b' = b/\sqrt{b^T b}$. For any vector $c \in \mathbb{R}^m$, we can represent S_c as

$$S_c = c^T a b^T c = \sqrt{a^T a \cdot b^T b} \cdot c^T a' \cdot c^T b'.$$

With the choice $c = a' - b'$ it follows

$$c^T a' = 1 - (a')^T b' > 0 \quad \text{and} \quad c^T b' = (a')^T b' - 1 < 0$$

implying $S_c < 0$. \square

PROOF OF THEOREM 4.4. Note that the part “if” of the statement follows from Lemma 4.1, and we should prove the part “only if.” Nevertheless, we provide a proof of the part “if” since it will be the base for proving the part “only if.”

Since the statement for $n = 0$ is proved in Schmidt and Zhigljavsky (2009), we consider the case $n \in \mathbb{N}$ in the rest of proof. Using the transformation $\varphi = \arccos u$ and $\psi = \arccos x$, we obtain $T_n(\cos \varphi) = \cos(n\varphi)$ and

$$\int_{-1}^1 \frac{\ln(u - x)^2}{\pi \sqrt{1 - u^2}} T_n(u) du = \int_0^\pi \frac{\ln(\cos \varphi - x)^2}{\pi \sin \varphi} \cos(n\varphi) \sin \varphi d\varphi.$$

Consequently, in order to prove Theorem 4.4 we have to show that the function

$$\int_0^\pi \ln(\cos \varphi - \cos \psi)^2 \cos(n\varphi) \mu(d\varphi)$$

is proportional to $\cos(n\psi)$ if and only if μ has a uniform density on the interval $[0, \pi]$. Extending μ to the interval $[0, 2\pi]$ as a symmetric (with respect to the center π) measure, $\mu(A) = \mu(2\pi - A)$, and defining the measure $\tilde{\mu}$ as $\tilde{\mu}(A) = \mu(2A)/2$ for all Borel sets $A \in [0, \pi]$, we obtain

$$\begin{aligned} & \int_0^\pi \ln(\cos \varphi - \cos \psi)^2 \cos(n\varphi) \mu(d\varphi) \\ &= \frac{1}{2} \int_0^{2\pi} \cos(n\varphi) \ln(\cos \varphi - \cos \psi)^2 \mu(d\varphi) \\ &= \frac{1}{2} \int_0^{2\pi} \cos(n\varphi) \ln\left(2 \sin \frac{\varphi - \psi}{2} \sin \frac{\varphi + \psi}{2}\right)^2 \mu(d\varphi) \\ &= \frac{1}{2} \int_0^{2\pi} \cos(n\varphi) \ln 2^2 \mu(d\varphi) \\ &\quad + \frac{1}{2} \int_0^{2\pi} \cos(n\varphi) \ln\left(\sin \frac{\varphi - \psi}{2}\right)^2 \mu(d\varphi) \\ &\quad + \frac{1}{2} \int_0^{2\pi} \cos(n\varphi) \ln\left(\sin \frac{\varphi + \psi}{2}\right)^2 \mu(d\varphi) \\ &= 0 + \int_0^\pi \cos(2n\varphi) \ln \sin^2(\varphi - \psi/2) \tilde{\mu}(d\varphi) \\ &\quad + \int_0^\pi \cos(2n\varphi) \ln \sin^2(\varphi + \psi/2) \tilde{\mu}(d\varphi) \\ &= 2 \int_0^\pi \cos(2n\varphi - n\psi + n\psi) \ln \sin^2(\varphi - \psi/2) \tilde{\mu}(d\varphi) \\ &= 2 \cos(n\psi) \int_0^\pi \cos(2n\varphi - n\psi) \ln \sin^2(\varphi - \psi/2) \tilde{\mu}(d\varphi) \\ &\quad + 2 \sin(n\psi) \int_0^\pi \sin(2n\varphi - n\psi) \ln \sin^2(\varphi - \psi/2) \tilde{\mu}(d\varphi). \end{aligned}$$

The “if” part follows from the facts that the functions $\cos(2nz) \ln \sin^2(z)$ and $\sin(2nz) \ln \sin^2(z)$ are π -periodic and

$$\begin{aligned} \int_0^\pi \sin(2n\varphi - n\psi) \ln \sin^2(\varphi - \psi/2) \frac{d\varphi}{\pi} &= \int_0^\pi \sin(2n\varphi) \ln \sin^2(\varphi) \frac{d\varphi}{\pi} = 0, \\ \int_0^\pi \cos(2n\varphi - n\psi) \ln \sin^2(\varphi - \psi/2) \frac{d\varphi}{\pi} &= \int_0^\pi \cos(2n\varphi) \ln \sin^2(\varphi) \frac{d\varphi}{\pi} = -1/n. \end{aligned}$$

To prove the “only if” part we need to show that the convolution of $\cos(2nz) \times \ln \sin^2(z)$ and $\tilde{\mu}(z)$, that is,

$$\int_0^\pi \cos(2n(\varphi - t)) \ln \sin^2(\varphi - t) \tilde{\mu}(d\varphi)$$

is constant for almost all $t \in [0, \pi]$ if and only if $\tilde{\mu}$ is uniform; and the same holds for the convolution of $\sin(2nz) \ln \sin^2(z)$ and $\tilde{\mu}(z)$. This, however, follows from Schmidt and Zhigljavsky [(2009), Lemma 3] since $\cos(2nz) \ln \sin^2(z) \in L^2([0, \pi])$, and all complex Fourier coefficients of these functions are nonzero. Indeed,

$$\int_0^\pi \cos(2nt) \ln \sin^2(t) \sin(2kt) dt = 0 \quad \forall k \in \mathbb{Z},$$

$$\int_0^\pi \cos(2nt) \ln \sin^2(t) \cos(2kt) dt = (\gamma_{|n+k|} + \gamma_{|n-k|})/2 \quad \forall k \in \mathbb{Z},$$

where $\gamma_0 = -2\pi \log 2$ and $\gamma_k = -\pi/k$ for $k \in \mathbb{N}$; see formula 4.384.3 in Gradshteyn and Ryzhik (1965). \square

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