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# Optimal designs for quadratic regression with random block effects: The case of block size two

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Optimal approximate designs for quadratic regression with random block effects in the case of block size two are considered. We obtain, with respect to the Schur ordering, an essentially complete class consisting of designs with a simple structure. The locally $D$- and $A$-optimal designs given in Cheng (1995a) and Atkins and Cheng (1999) belong to this class. We explicitly identify locally $E$-optimal designs and show that for each $p$, $-\infty \leq p \leq 1$, there is a unique $\phi_p$-design in this class. Bayesian $\phi_p$-optimal designs are also considered.


## 1. Introduction

Optimal designs for linear and nonlinear regression models with uncorrelated errors have been investigated extensively, but the case of correlated errors has not received much attention in the literature. In experiments where the observations are taken in blocks such as the experiment on eyes in Cheng (1995a), the experiment on feet in Draper and Guttman (1997), and the valve wear experiment and the food additives experiment in Goos and Donev (2006), it is more appropriate to treat the block effects as random, and the observations in the same block are no longer uncorrelated.

Cheng (1995a) and Atkins and Cheng (1999) studied $D$- and $A$-optimal designs for quadratic regression with random block effects in the case of constant block size under the assumption that the intra-block correlation is known. They obtained conditions under which the $D$- and $A$-optimal designs do not depend on the intra-block correlation. Moreover, by applying the equivalence theorem (Kiefer, 1974), they characterized $D$-optimal approximate designs for any block size and $A$-optimal designs with blocks of size two. Goos and Vandebroek (2001) provided a point exchange algorithm for generating $D$-optimal exact designs for models with random block effects. Recently, Dette et al. (2013) and Campos-Barreiro and Lopez-Fidalgo (2014) considered optimal designs under correlated errors in a different context.

In this paper we follow the framework of Atkins and Cheng (1999) and focus on designs with blocks of size two. We extend their results in two directions. The $D$- and $A$-criteria, along with the $E$-criterion, are the three most popular members of the family of $\phi_p$-criteria for $p \in [-\infty, 1]$. We develop a theory to determine the entire class of $\phi_p$-optimal designs; in particular, the $E$-optimal designs are explicitly identified. Secondly, the strategy of identifying optimal designs in Atkins and Cheng (1999) was to guess their structures and then use the equivalence theorem to determine the optimal designs and confirm their optimality. A better approach without guesswork is to first identify a small enough class of designs that is guaranteed to contain optimal designs and from which optimal designs can be more easily obtained. Such an approach

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based on the so-called essentially complete classes and minimal complete classes was used, e.g., in Cheng (1987, 1995b) to identify $\phi_p$-optimal designs in certain settings. In this paper, we obtain a class $\mathcal{C}$ of designs such that for an arbitrary design $\xi_1 \notin \mathcal{C}$, there exists a design $\xi_2 \in \mathcal{C}$ such that $\xi_1$ is not better than $\xi_2$ under every $\phi_p$-criterion. It follows that $\mathcal{C}$ contains a $\phi_p$-optimal design for every $p$. Furthermore, the designs in $\mathcal{C}$ have a very simple structure, from which the $\phi_p$-optimal designs can be determined. These results are presented in Section 3 after some preliminary materials and notations are reviewed in Section 2.

In general, the optimal designs depend on the intra-block correlation. Therefore they depend on an unknown parameter when the intra-block correlation is unknown; in this case they are said to be locally optimal. Under normality, since the estimators of the mean and the covariance matrix are independent, the $\phi_p$-optimal designs for known intra-block correlations can be shown to coincide with the locally $\phi_p$-optimal designs when the intra-block correlation is unknown.

When the experimenters can assume that the unknown parameters follow a prior distribution, a Bayesian approach can be employed. The class $\mathcal{C}$ mentioned above has the stronger property that for an arbitrary design $\xi_1 \notin \mathcal{C}$, there exists a design $\xi_2 \in \mathcal{C}$ such that $\xi_1$ is not better than $\xi_2$, not only for all $\phi_p$-criteria, but also for all intra-block correlations. In Section 4, this is used to show that for an arbitrary prior, a Bayesian $\phi_p$-optimal design can be found in $\mathcal{C}$. Moreover, it is observed that the Bayesian $D$, $A$, and $E$-optimal designs have the same structures as the corresponding locally optimal designs. We conclude the paper by presenting in Section 5 some designs that are highly efficient regardless of the unknown intra-block correlation.

All the proofs are presented in the Appendix.

## 2. Preliminaries

In this section, we introduce some notations, the information matrix of a design, and the $\phi_p$-optimality criteria.

As in Atkins and Cheng (1999), consider the following quadratic regression model on $[-1, 1]$ with blocks of size two. Each block $\{x_1, x_2\}$ can be considered as a point $\boldsymbol{x} = (x_1, x_2) \in [-1, 1]^2$. Let $\boldsymbol{y}(\boldsymbol{x}) = (y(x_1), y(x_2))^{\mathrm{T}}$ be the response at $\boldsymbol{x}$. We assume that $\boldsymbol{y}(\boldsymbol{x})$ has a normal distribution with

$$\mathrm{E}(\boldsymbol{y}(\boldsymbol{x})) = \begin{pmatrix} \mathrm{E}(y(x_1)) \\ \mathrm{E}(y(x_2)) \end{pmatrix} = \begin{pmatrix} \beta_0 + \beta_1 x_1 + \beta_2 x_1^2 \\ \beta_0 + \beta_1 x_2 + \beta_2 x_2^2 \end{pmatrix} = \boldsymbol{F}(\boldsymbol{x})^{\mathrm{T}}\boldsymbol{\beta},$$
$$\mathrm{Cov}(\boldsymbol{y}(\boldsymbol{x})) = \begin{pmatrix} 1 & r \\ r & 1 \end{pmatrix} \sigma^2,$$

where $\boldsymbol{F}(\boldsymbol{x}) = (\boldsymbol{f}(x_1), \boldsymbol{f}(x_2)), \boldsymbol{f}(x) = (1, x, x^2)^{\mathrm{T}}$, $\boldsymbol{\beta} = (\beta_0, \beta_1, \beta_2)^{\mathrm{T}}$ is the parameter vector of the regression model, and $\boldsymbol{\gamma} = (\sigma^2, r)^{\mathrm{T}}$. We assume that $\sigma^2 > 0$ and the observations in different blocks are independent; furthermore, we assume that the intra-block correlation $r$ is nonnegative since the dual responses are subject to the same random block effect.

The approach of approximate designs was adopted in Cheng (1995a) and Atkins and Cheng (1999). An approximate design here is a probability measure on $[-1, 1]^2$ and is denoted by $\xi = \{(\boldsymbol{x}_i, w_i)\}_{i=1}^k$ or

$$\xi = \begin{Bmatrix} \boldsymbol{x}_1 & \boldsymbol{x}_2 & \cdots & \boldsymbol{x}_k \\ w_1 & w_2 & \cdots & w_k \end{Bmatrix},$$

where $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_k \in [-1, 1]^2$ are distinct blocks (which together constitute the support of the design), and $(w_1, w_2, \ldots, w_k)$ is in the $(k-1)$-dimensional simplex, $\mathcal{S}^{k-1} = \{(w_1, w_2, \ldots, w_k) : w_i \geq 0, \sum_{i=1}^k w_i = 1\}$. The probabilities $w_1, w_2, \ldots, w_k$ are interpreted as the proportions of observations at the blocks $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_k$. Note that since $\boldsymbol{x} = (x_1, x_2)$ and $\boldsymbol{x}' = (x_2, x_1)$ represent the same block $\{x_1, x_2\}$, in implementing the design, $\xi(\boldsymbol{x}) + \xi(\boldsymbol{x}')$ is taken as the proportion of observations at the block $\{x_1, x_2\}$. Furthermore, let the single-block design at block $\boldsymbol{x}$ be $A_{\boldsymbol{x}} = \{(\boldsymbol{x}, 1)\}$; then the $\xi$ above can be expressed as $\sum_{i=1}^k w_i A_{\boldsymbol{x}_i}$.

Under an approximate design $\xi$, the covariance matrix of the maximum likelihood estimator of $\boldsymbol{\theta} = (\boldsymbol{\beta}^{\mathrm{T}}, \boldsymbol{\gamma}^{\mathrm{T}})^{\mathrm{T}}$ is proportional to the inverse of the information matrix of $\xi$,

$$M_0(\xi) = \begin{pmatrix} M_1(\xi) & \mathbf{0}_{3\times 2} \\ \mathbf{0}_{2\times 3} & M_2 \end{pmatrix}$$

where

$$M_1(\xi) = \frac{1}{\sigma^2(1-r^2)} M(\xi), \tag{1}$$
$$M_2 = \begin{pmatrix} \dfrac{1}{\sigma^4} & \dfrac{-r}{(1-r^2)\sigma^2} \\ \dfrac{-r}{(1-r^2)\sigma^2} & \dfrac{1+r^2}{(1-r^2)^2} \end{pmatrix},$$