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EXACT OPTIMAL DESIGNS FOR WEIGHTED LEAST SQUARES ANALYSIS WITH CORRELATED ERRORS

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Abstract: In the common linear and quadratic regression model with an autoregressive error structure exact D-optimal designs for weighted least squares analysis are determined. It is demonstrated that for highly correlated observations the D-optimal design is close to the equally spaced design. Moreover, the equally spaced design is usually very efficient, even for moderate sizes of the correlation, while the D-optimal design obtained under the assumptions of independent observations yields a substantial loss in efficiency. We also consider the problem of designing experiments for weighted least squares estimation of the slope in a linear regression and compare the exact D-optimal designs for weighted and ordinary least squares analysis.

Key words and phrases: Autoregressive errors, linear regression; quadratic regression, exact D-optimal designs, estimation of the slope, generalized MANOVA.

1. Introduction

The main purpose of the present paper is the construction of exact optimal designs for weighted least squares estimation in the common linear and quadratic regression model with correlated observations. Our research was motivated by an example from toxicology where, in a factorial design, several ingredients at different doses were compared in their capacity to inhibit bacterial growth. For each setting of the factorial design, a bacteria growth was observed at three time points. The influence of the single ingredients on the regression curves was measured. We assume that observations from different settings are independent, but that observations at different time points of the same setting are correlated, with the same covariance matrix for each setting. Therefore the covariance structure can be estimated from the data and, if a parametric model for the bacterial growth has been fixed, each of these curves can be fitted by weighted least squares. Note that this analysis is in accordance with Potthoff and Roy's (1964) generalized MANOVA (GMANOVA). The problem of experimental design now consists in the specification of the experimental conditions for the estimation of each curve.

The problem of determining exact optimal designs has found considerable interest for models with uncorrelated observations (see e.g., Hohmann and Jung (1975), Gaffke and Krafft (1982), Imhof (1998, 2000) and Imhof, Krafft and Schaefer (2000)). These papers deal with D-, G-, A- and D_1-criteria for linear or quadratic regression. The determination of optimal designs for models with a correlated error structure is substantially more difficult and for this reason not so well developed. To the best knowledge of the authors the first paper dealing with the optimal design problem for a linear regression model with correlated observations is the work by Hoel (1958), who considered the weighted least squares estimate, but restricted attention to equally spaced designs. Bickel and Herzberg (1979) and Bickel, Herzberg and Schilling (1981) considered least squares estimation and determined asymptotic (for an increasing sample size) optimal designs for the constant regression, the straight line through the origin, and the estimation of the slope in the common linear regression model. Optimal designs were also studied by Abt, Liski, Mandal and Sinha (1997, 1998) for the linear and quadratic regression model with autocorrelated error structure, respectively. Following Hoel (1958) these authors determined the optimal designs among all equally spaced designs. Müller and Pazman (2003) determine an algorithm to approximate optimal designs for linear regression with correlated errors. There is also a vast literature on optimal designs with correlated errors when the variance-covariance structure does not depend on the chosen design. This generally is the case for ANOVA-models, see e.g., Martin (1996), but there are also some papers dealing with regression models, see e.g., Bischoff (1995).

In the present paper we relax some of these restrictions and consider the problem of determining exact optimal designs for regression models in the case where the correlation structure depends on the design and where the number n of available observations for the estimation of each growth curve is relatively small.

In Section 2 we introduce the model and present some preliminary notation. In Section 3 we concentrate on the linear regression model and derive properties of exact D-optimal designs that substantially simplify their numerical construction. In particular we show that one should always take an observation at the extreme points of the design space and that for highly correlated data the exact D-optimal designs converge to an equally spaced design. We also investigate similar problems for weighted least squares estimation of the slope in a linear regression. In Section 4 we present several numerical results for sample sizes $n = 3, 4, 5$ and 6. In Section 5 several exact D-optimal designs for weighted least squares estimation in a quadratic regression model with correlated observations are calculated.

We also investigate the efficiency of the design which is derived under the assumption of uncorrelated observations (see Hohmann and Jung (1975) and

Gaffke and Krafft (1982)) and the equally spaced design. While the latter design is very efficient and can be recommended, the design determined under the assumptions of uncorrelated observations yields to a substantial loss in efficiency, in particular if the correlation is small. Finally, in Section 6 some exact optimal designs for ordinary least squares estimation are presented and compared with the optimal designs for weighted least squares estimation. In particular, it is shown that for highly correlated data the D-optimal designs for weighted and ordinary least squares estimation differ substantially. On the other hand, the equally spaced design is usually very efficient for both estimation methods provided the correlation is not too small.

2. Preliminaries

Consider the common linear regression model

$$Y_{t_i} = \beta_1 f_1(t_i) + \cdots + \beta_p f_p(t_i) + \varepsilon_{t_i} \ , \quad i = 1, \ldots, n, \tag{2.1}$$

where $f_1, \ldots, f_p$ ($p \in \mathbb{N}$) are given regression functions. The independent variables t_i can be chosen by the experimenter from a compact interval, say $[0, 1]$. The parameters $\beta_1, \ldots, \beta_p$ are unknown and have to be estimated from the data. We assume that the errors $\varepsilon_{t_1}, \ldots, \varepsilon_{t_n}$ are centered and follow a stationary autoregressive process, where the correlation between two measurements depends on the distance in t, that is $E[\varepsilon_t] = 0$ and

$$\sigma_{ts} := \mathrm{Cov}(Y_t, Y_s) = \mathrm{Cov}(\varepsilon_t, \varepsilon_s) = \sigma^2 \lambda^{|t-s|}. \tag{2.2}$$

Here $t, s \in [0, 1]$ and λ is a known constant, such that $0 \leq \lambda < 1$. For the determination of an optimal design we can assume without loss of generality that $\sigma^2 = 1$. An exact design $\xi = \{t_1, \ldots, t_n\}$ is a vector of n positions, say $0 \leq t_1 \leq \ldots \leq t_n \leq 1$ describing the experimental conditions in the regression model (2.1). If n observations are taken according to the design ξ, model (2.1) can be written as $Y = X_\xi \beta + \varepsilon_\xi$, where $Y = [Y_{t_1}, \ldots, Y_{t_n}]^T$ denotes the vector of observations, $\beta = (\beta_1, \ldots, \beta_p)^T$, $X_\xi = (f_i(t_j))_{i,j=1}^{p,n}$ is the design matrix and the (random) vector $\varepsilon_\xi = (\varepsilon_{t_1}, \ldots, \varepsilon_{t_n})^T$ has expectation 0 and covariance matrix $\Sigma_\xi = (\sigma_{t_i,t_j})_{i,j=1}^n$.

In the case $t_i = t_{i+1}$ for some $1 \leq i \leq n-1$, the corresponding observations have correlation 1 and taking an additional observation under the experimental condition t_{i+1} does not increase the information of the experiment. Such a situation is typical for experiments at the same object. For example the growth of a plant is a function of time (thus the observations are correlated), but no additional information is obtained measuring the same object twice at the same time. For this reason we assume throughout this paper that $t_1 < \cdots < t_n$. In this case the matrix Σ_ξ is invertible and a straightforward calculation yields $\Sigma_\xi^{-1} = V_\xi^T V_\xi$, where the matrix V_ξ is defined by

$$V_\xi = \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 & 0 \\ -\frac{\lambda^{(t_2-t_1)}}{\sqrt{1-\lambda^{2(t_2-t_1)}}} & \frac{1}{\sqrt{1-\lambda^{2(t_2-t_1)}}} & 0 & \cdots & 0 & 0 \\ 0 & -\frac{\lambda^{(t_3-t_2)}}{\sqrt{1-\lambda^{2(t_3-t_2)}}} & \frac{1}{\sqrt{1-\lambda^{2(t_3-t_2)}}} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -\frac{\lambda^{(t_n-t_{n-1})}}{\sqrt{1-\lambda^{2(t_n-t_{n-1})}}} & \frac{1}{\sqrt{1-\lambda^{2(t_n-t_{n-1})}}} \end{bmatrix}.$$

This is a straightforward generalization of the situation considered in ANOVA-models, see e.g., Kunert (1985).

The weighted least squares estimate of β is given by $\hat\beta = (X_\xi^T V_\xi^T V_\xi X_\xi)^{-1} X_\xi^T V_\xi^T V_\xi Y$ with covariance matrix $\mathrm{Cov}(\hat\beta) = (X_\xi^T V_\xi^T V_\xi X_\xi)^{-1}$. An exact D-optimal design ξ^* minimizes the determinant $\det(\mathrm{Cov}(\hat\beta))$ with respect to the choice of the experimental design $\xi = \{t_1, \ldots, t_n\}$. This is equivalent to maximize $\det M_\xi$, where the matrix M_ξ is given by

$$M_\xi = X_\xi^T V_\xi^T V_\xi X_\xi. \tag{2.3}$$

In the following sections we will concentrate on the linear ($p = 2, f_1(t) = 1, f_2(t) = t$) and the quadratic regression model ($p = 3, f_1(t) = 1, f_2(t) = t, f_3(t) = t^2$).

3. The Linear Regression Model

We start with the simple linear regression model

$$Y_{t_i} = \mu + \beta t_i + \varepsilon_{t_i}\ , \quad i = 1, \ldots, n, \tag{3.1}$$

the quadratic model is investigated in Section 5. We first derive a more transparent representation of the determinant of the matrix M_ξ defined in (2.3). For this purpose we introduce the notation $d_1 = 0$, $d_i = t_i - t_{i-1}$, $2 \le i \le n$, $a_1 = 1$, $b_1 = 0$,

$$a_j = \frac{1}{\sqrt{1-\lambda^{2d_j}}}, \quad b_j = \frac{\lambda^{d_j}}{\sqrt{1-\lambda^{2d_j}}}, \quad j = 2, \ldots, n, \tag{3.2}$$

and find that

$$V_\xi X_\xi = \begin{bmatrix} 1 & t_1 \\ a_2 - b_2 & t_1(a_2 - b_2) + d_2 a_2 \\ a_3 - b_3 & t_1(a_3 - b_3) + d_2(a_3 - b_3) + d_3 a_3 \\ & \\ a_n - b_n & t_1(a_n - b_n) + (d_2 + \ldots + d_{n-1})(a_n - b_n) + d_n a_n \end{bmatrix}.$$

From the Cauchy-Binet formula (see Karlin and Studden (1966)) we obtain, for the determinant of the matrix (2.3),

$$\det M_\xi = \sum_{1\le i<j\le n} \det{}^2 \begin{pmatrix} a_i - b_i & (d_1+\cdots+d_{i-1})(a_i-b_i)+d_ia_i \\ a_j-b_j & (d_1+\cdots+d_{j-1})(a_j-b_j)+d_ja_j \end{pmatrix}. \quad (3.3)$$

It therefore follows that a design $\tilde{\xi}$ with points $\tilde{t}_1 = 0$, $\tilde{t}_2 = t_2 - t_1, \ldots, \tilde{t}_n = t_n - t_1$ yields the same value in the D-criterion as the design ξ with points $t_1, \ldots, t_n$, i.e. $\det M_\xi = \det M_{\tilde{\xi}}$. Note that all points $\tilde{t}_i$ are located in the interval $[0,1]$, and therefore the design $\tilde{\xi}$ is in fact of interest. We begin with a technical lemma, that will be helpful for the numerical determination of optimal designs in Section 4.

Lemma 3.1. *Let $\tilde{\xi} = \{1-t_n, \ldots, 1-t_1\}$ denote the design obtained from $\xi = \{t_1, \ldots, t_n\}$ by reflecting the points t_i at $t = 1/2$, then $\det M_{\tilde{\xi}} = \det M_\xi$, where the matrix M_ξ is defined in (2.3) with $p = 2, f_1(t) = 1$ and $f_2(t) = t$.*

Proof. Note that the determinants in the representaion (3.3) can be rewritten as

$$\det{}^2 \begin{pmatrix} a_i - b_i & a_it_i - b_it_{i-1} \\ a_j - b_j & a_jt_j - b_jt_{j-1} \end{pmatrix}.$$

Now a careful calculation of the expressions for a_i, b_i and d_i for the design $\tilde{\xi}$ yields the assertion of the Lemma.

Proposition 3.2. *Let ξ be an arbitrary design with points $0 \le t_1 < \cdots < t_n \le 1$, and take ξ^* to be the design that has the experimenter take observations at the points $t_1^* = 0$, $t_2^* = t_2 - t_1 = d_2$, $t_3^* = t_3 - t_1 = d_2 + d_3, \ldots, t_{n-1}^* = t_{n-1} - t_1 = d_2 + \cdots + d_{n-1}$, and $t_n^* = 1$. Then the design ξ^* performs at least as well under the D-criterion as the design ξ, i.e. $\det M_\xi \le \det M_{\xi^*}$.*

Proof. We have already seen that a design $\tilde{\xi}$ defined in the previous paragraph yields the same value of the D-criterion as ξ. The only difference between the designs ξ^* and $\tilde{\xi}$ is that the point $t_n^* \in [0,1]$ is as large as possible and therefore ξ^* has the largest possible value for d_n. We now show that the derivative of the function $\det(X_{\tilde{\xi}}^T V_{\tilde{\xi}}^T V_{\tilde{\xi}} X_{\tilde{\xi}})$ with respect to the variable d_n is positive, which proves the assertion of the proposition. For the design $\tilde{\xi}$, take

$$f_i(d_j) = \det \begin{pmatrix} a_i - b_i & (d_1+\cdots+d_{i-1})(a_i-b_i)+d_ia_i \\ a_j-b_j & (d_1+\cdots+d_{j-1})(a_j-b_j)+d_ja_j \end{pmatrix}$$

for $1 \le i < j \le n$. It follows from (3.3) that $\det M_{\tilde{\xi}} = \sum_{1\le i<j\le n} (f_i(d_j))^2$ and, therefore,

$$\frac{\partial}{\partial d_n} \det M_{\tilde{\xi}} = \sum_{1\le i<n} 2 f_i(d_n) f_i'(d_n),$$

where $f_i'(d_n)$ is the derivative of $f_i(d_n)$ with respect to the variable d_n. Consequently, it is sufficient to show that $f_i(d_n) > 0$ and $f_i'(d_n) > 0$ for all $1 \le i < n$ and for all $0 < d_n \le 1$.

For this purpose we note for $2 \le j \le n$ and $d_j > 0$ that $a_j = (a_j - b_j)/(1-\lambda^{d_j})$. Consequently, for $2 \le i < n$, we can rewrite

$$f_i(d_n) = (a_i - b_i)(a_n - b_n)[d_{i+1} + \cdots + d_{n-1} + g(d_n) + \ell(d_i)],$$

where the functions g and ℓ are defined as $g(x) = x/(1-\lambda^x)$ and $\ell(x) = x - (x/(1-\lambda^x))$, respectively. Note that $a_j - b_j \ge 0$ for all j, which yields $f_i(d_n) \ge (a_i - b_i)(a_n - b_n)[g(d_n) + \ell(d_i)]$. If $x \to 0$ we have $g(x) \to -1/\ln\lambda > 0$, and the derivative of g is

$$g'(x) = \frac{1}{(1-\lambda^x)^2}(1 - \lambda^x + x\lambda^x \ln\lambda).$$

Let $h(x)$ be the numerator of g'. Then $h(0) = 0$, while

$$h'(x) = -\lambda^x \ln(\lambda) + \lambda^x \ln(\lambda) + x\lambda^x(\ln\lambda)^2 = x\lambda^x(\ln\lambda)^2 > 0,$$

for all $x > 0$. Consequently, $h(x) > 0$ for all $x > 0$ and it follows that $g'(x) > 0$. Therefore we obtain $g(x) > \lim_{x\to 0} g(x) = -1/\ln\lambda$ for all $x > 0$. On the other hand,

$$\ell'(x) = 1 - \frac{1}{(1-\lambda^x)^2}(1 - \lambda^x + x\lambda^x \ln\lambda) = -\frac{\lambda^x}{(1-\lambda^x)^2}(1 - \lambda^x + x\ln\lambda).$$

Defining $q(x) = 1 - \lambda^x + x\ln\lambda$, we find that $q'(x) = -\lambda^x \ln\lambda + \ln\lambda < 0$, which yields $q(x) < q(0) = 0$, for all $x > 0$. Therefore it follows that $\ell'(x) > 0$, for all $x > 0$ and $\ell(x) > \lim_{x\to 0} \ell(x) = 1/\ln\lambda$ for all $x > 0$. In all, we have shown for all $d_i \ge 0$ and for all $d_n > 0$ that $g(d_n) + \ell(d_i) > -1/\ln\lambda + 1/\ln\lambda = 0$. This, however, implies that $f_i(d_n) > 0$, for all $2 \le i < n$ and all $d_n > 0$. Now consider $f_i'(d_n)$. We obtain for $2 \le i < n$ that

$$\begin{aligned} f_i'(d_n) = {} & (a_i - b_i)(a_n' - b_n')(d_{i+1} + \cdots + d_{n-1} + g(d_n) + \ell(d_i)) \\ & + (a_i - b_i)(a_n - b_n)g'(d_n), \end{aligned}$$

where $(a_n' - b_n')$ is the derivative of $(a_n - b_n)$ with respect to the variable d_n. We have already seen that $a_i - b_i > 0$, $a_n - b_n > 0$, $g'(d_n) > 0$ and that $d_{i+1} + \cdots + d_{n-1} + g(d_n) + \ell(d_i) > 0$. Since $a_n - b_n = \sqrt{(1-\lambda^{d_n})/(1+\lambda^{d_n})}$, we obtain $a_n' - b_n' = -\lambda^{d_n} \ln\lambda (1+\lambda^{d_n})^{-1}(1-\lambda^{2d_n})^{-1/2} > 0$, for all $d_n > 0$. Therefore, $f_i'(d_n) > 0$ for all $d_n > 0$ $(i = 2, \ldots, n-1)$.

It remains to consider the case $i = 1$, where $f_1(d_n) = (a_n - b_n)(d_1 + \cdots + d_{n-1} + g(d_n))$, which is clearly positive. Similarly, $f_1'(d_n) = (a_n' - b_n')(d_1 + \cdots + d_{n-1} + g(d_n)) + (a_n - b_n)g'(d_n)$ is also positive. Summarizing our arguments we have shown that $\frac{\partial}{\partial d_n} \det M_{\tilde{\xi}} > 0$, for all $d_n > 0$, which yields the assertion of the proposition.

Remark 3.3. If $d_k \to 0$ for some $k \geq 2$, then the corresponding $f_i(d_k) \to 0$ for all $1 \leq i < k$. This underlines the fact that a second observation under the same experimental condition does not provide any additional information in the experiment.

Remark 3.4. Note that in the case $\lambda \to 0$ we obtain the linear regression model with uncorrelated observations. In this case the corresponding information matrix $M_{\xi^*}(\lambda)$ in (2.3) of the exact D-optimal design does not necessarily converge to the information matrix of the D-optimal design for uncorrelated observations. For the limiting case of pairwise uncorrelated observations it is well-known that an exact n-point D-optimal design is $\xi^*_{\mathrm{uc}} = \{0, 0, \ldots, 0, 1, \ldots, 1\}$ where $k = \mathrm{int}(n/2)$ observations are taken at each boundary point of the interval $[0, 1]$ and the last one is taken either at the point 0 or at the point 1 (see Hohmann and Jung (1975)). For this design, however, we have that $\det M_{\xi^*_{\mathrm{uc}}} = 1/(1 - \lambda^2)$ irrespective of the sample size n.

Remark 3.5. A simple calculation shows that the optimal designs on the interval $[a, a + c]$ $(c > 0)$ with correlation structure $\sigma^2 \lambda^{|t-s|}$ can be obtained from the optimal designs on the interval $[0, 1]$ with correlation structure $\sigma^2 \lambda^{c|t-s|}$.

We now concentrate on the case $\lambda \to 1$ which corresponds to highly correlated observations. The following result shows, that in this case the exact D-optimal design converges to an equally spaced design on the interval $[0, 1]$.

Theorem 3.6. *If $\lambda \to 1$, then any exact n-point D-optimal design in the linear regression model with correlation structure* (2.2) *converges to the equally spaced design $\xi_n = \{0, 1/(n-1), 2/(n-1), \ldots, 1\}$.*

Proof. Recalling the definition of a_i, b_i in (3.2), a Taylor expansion at the point $\lambda = 1$ yields

$$
\begin{aligned}
(a_i - b_i)^2 &= (t_i - t_{i-1})\frac{1-\lambda}{2} + (t_i - t_{i-1})\frac{(1-\lambda)^2}{4} \\
&\quad - (t_i - t_{i-1})((t_i - t_{i-1})^2 - 4)\frac{(1-\lambda)^3}{24} + o((1-\lambda)^3), \\
(a_i t_i - b_i t_{i-1})^2 &= \frac{(t_i - t_{i-1})(1-\lambda)^{-1}}{2} + \frac{(t_i - t_{i-1})(2t_i + 2t_{i-1} - 1)}{4} \\
&\quad + (t_{i-1} - 4t_{i-1}^3 - t_i + 4t_i^3)\frac{(1-\lambda)}{24} \\
&\quad + (t_{i-1} - 4t_{i-1}^3 - t_i + 4t_i^3)\frac{(1-\lambda)^2}{48} + o((1-\lambda)^2),
\end{aligned}
$$

$$(a_i - b_i)(a_i t_i - b_i t_{i-1}) = \frac{(t_i - t_{i-1})}{2} + (t_i^2 - t_{i-1}^2)(1-\lambda)\Big(\frac{1}{4} + \frac{1-\lambda}{8}\Big) + o((1-\lambda)^2).$$

Proposition 3.2 allows us to restrict attention to designs with $t_1 = 0$ and $t_n = 1$. For such designs, $\sum_{i=2}^n t_i^k - t_{i-1}^k = 1$ for every k.

From the representation $M_\xi = (V_\xi X_\xi)^T (V_\xi X_\xi)$ we therefore obtain $\det M_\xi = AB - C^2$ where the quantities A, B and C are calculated as follows:

$$\begin{aligned} A &= \sum_{i=1}^n (a_i - b_i)^2 = 1 + \sum_{i=2}^n (a_i - b_i)^2 \\ &= 1 + \sum_{i=2}^n (t_i - t_{i-1})\big(\frac{1-\lambda}{2} + \frac{(1-\lambda)^2}{4} + \frac{(1-\lambda)^3}{6}\big) \\ &\quad - \sum_{i=2}^n (t_i - t_{i-1})^3 \frac{(1-\lambda)^3}{24} + o((1-\lambda)^3) \\ &= 1 + \frac{1-\lambda}{2} + \frac{(1-\lambda)^2}{4} + (1-\lambda)^3 \Big(\frac{1}{6} - \sum_{i=2}^n \frac{(t_i - t_{i-1})^3}{24}\Big) + o((1-\lambda)^3), \end{aligned} \tag{3.4}$$

where we have used the fact that $a_1 - b_1 = 1$. By a similar calculation we obtain

$$B = \sum_i (a_i t_i - b_i t_{i-1})^2 = \frac{(1-\lambda)^{-1}}{2} + \frac{1}{4} + \frac{(1-\lambda)}{8} + \frac{(1-\lambda)^2}{16} + o((1-\lambda)^2), \tag{3.5}$$

$$C = \sum_i (a_i - b_i)(a_i t_i - b_i t_{i-1}) = \frac{1}{2} + \frac{1-\lambda}{4} + \frac{(1-\lambda)^2}{8} + o((1-\lambda)^2), \tag{3.6}$$

respectively. Therefore the determinant of the matrix M_ξ can be expanded as

$$\det M_\xi = \frac{(1-\lambda)^{-1}}{2} + \frac{1}{4} + \frac{1-\lambda}{8} + \frac{(1-\lambda)^2}{12} - \sum_{i=2}^n (t_i - t_{i-1})^3 \frac{(1-\lambda)^2}{48} + o((1-\lambda)^2),$$

and it follows that the D-optimal design converges (as $\lambda \to 1$) to the design that minimizes the expression $\sum_{i=2}^n (t_i - t_{i-1})^3 = \sum_{i=2}^n d_i^3$, with $d_i = t_i - t_{i-1}$, as above. Since $\sum_{i=2}^n d_i = 1$ for the designs considered, it is obvious that the minimum is attained if and only if all $d_i = 1/(n-1)$. This completes the proof of the Theorem.

Theorem 3.6 indicates that uniform designs are very efficient for highly correlated data. In the following section we demonstrate that even for rather small values of the parameter λ the equally spaced design $\xi_n = \{0, 1/(n-1), 2/(n-1), \ldots, 1\}$ yields large D-efficiencies.

Before we present these numerical results we briefly discuss the optimal design problem for estimating the slope in the linear regression model with correlated observations. If the main interest of the experiment is the estimation of the slope an optimal design should maximize

$$D_1(\xi) = (e_2^T M_\xi^{-1} e_2)^{-1} = \det M_\xi \cdot \Big(\sum_{j=1}^{n} (a_j - b_j)^2\Big)^{-1}, \tag{3.7}$$

where $e_2 = (0,1)^T, a_1 = 1, b_1 = 0$. Throughout this paper optimal designs maximizing the function in (3.7) are called exact D_1-optimal designs.

Theorem 3.7.
(a) *Let $\xi = \{t_1, \ldots, t_n\}$ denote a design and $\tilde{\xi} = \{1-t_n, \ldots, 1-t_1\}$ its reflection at the point $t = 1/2$, then $D_1(\xi) = D_1(\tilde{\xi})$.*
(b) *If $\xi = \{t_1, \ldots, t_n\}$ is an exact D_1-optimal design for the linear regression model* (3.1) *with correlation structure* (2.2)*, then $t_1 = 0, t_n = 1$.*
(c) *If $\lambda \to 1$ any exact n-point D_1-optimal design for the linear regression model* (3.1) *with correlation structure* (2.2) *converges to the design $\bar{\xi} = \{0, t_2, t_3, \ldots, t_{n-1}, 1\}$, where the points $t_2 < \cdots < t_{n-1}$ minimize the function*

$$\frac{S_{1,2}}{6} - \frac{S_{1,1}}{8} - \frac{S_{2,1}}{18} - \frac{S_{1,3}}{18} \tag{3.8}$$

with $(t_1 = 0,\ t_n = 1)$

$$S_{p,q} = \sum_{i=2}^{n} t_i^p t_{i-1}^p (t_i^q - t_{i-1}^q). \tag{3.9}$$

Proof. Because part (a) and (b) can be proved in a similar manner as Lemma 3.1 and Proposition 3.2 we restrict ourselves to a proof of part (c). For this we need a more refined expansion of $\det M_\xi = AB - C^2$. More precisely we have for the expression A, B, and C in (3.4), (3.5) and (3.6), respectively,

$$\begin{aligned}
A &= 1 + \frac{(1-\lambda)}{2} + \frac{(1-\lambda)^2}{4} + (1+S_{1,1})\frac{(1-\lambda)^3}{8} + (1+3S_{1,1})\frac{(1-\lambda)^4}{16} \\
&\quad + o((1-\lambda)^4), \\
B(1-\lambda)^2 &= \frac{(1-\lambda)}{2} + \frac{(1-\lambda)^2}{4} + \frac{(1-\lambda)^3}{8} + \frac{(1-\lambda)^4}{16} \\
&\quad + \Big(\frac{1}{32} + \frac{S_{2,1}+S_{1,3}}{72}\Big)(1-\lambda)^5 + o((1-\lambda)^5), \\
C(1-\lambda) &= \frac{(1-\lambda)}{2} + \frac{(1-\lambda)^2}{4} + \frac{(1-\lambda)^3}{8} + (3+2S_{1,2})\frac{(1-\lambda)^4}{48} + o((1-\lambda)^4).
\end{aligned}$$

Straightforward calculations now yield

$$\det M_\xi = \frac{(1-\lambda)^{-1}}{2} + \frac{1}{4} + \frac{(1-\lambda)}{8} + (1+S_{1,1})\frac{(1-\lambda)^2}{16}$$

$$+\Big(\frac{1}{32}+\frac{S_{1,1}}{8}-\frac{S_{1,1}}{24}+\frac{S_{2,1}+S_{1,3}}{72}\Big)(1-\lambda)^3+o((1-\lambda)^3),$$
$$\{D_1(\xi)\}^{-1}=\frac{A}{\det M_\xi}=2(1-\lambda)+\left(\frac{S_{1,2}}{6}-\frac{S_{1,1}}{8}-\frac{S_{2,1}}{18}-\frac{S_{1,3}}{18}\right)(1-\lambda)^2+o((1-\lambda)^2).$$

Therefore the exact D_1-optimal design in the linear regression model with correlation structure (2.2) converges to the the designs $\xi=\{0,t_2,t_3,\ldots,t_{n-1},1\}$ where the points $t_2,\ldots,t_{n-1}$ minimize the function in (3.8).

4. Numerical Results

In this section we present several numerical results for the exact D-optimal designs maximizing the determinant in (2.3) in the linear regression model. We will also investigate the efficiency of the exact D-optimal design ξ^*_{uc} for the linear regression model with uncorrelated observations and the equally spaced design ξ_n considered in Theorem 3.6.

Example 4.1. *The case* $n=3$. It follows from Proposition 3.2 that it is sufficient to search among designs with $t_1=0$, $t_2=d$, say, and $t_3=1$. For such a design, the D-criterion simplifies to

$$\det(X_\xi^T V_\xi^T V_\xi X_\xi)=\frac{2\left((1-(1-d)\lambda^d)(1-d\lambda^{1-d})-d(1-d)\right)}{(1-\lambda^{2d})(1-\lambda^{2(1-d)})}=\psi(d), \quad (4.1)$$

say. Therefore the exact D-optimal design can be determined maximizing the function ψ with respect to $d\in(0,1)$. From Lemma 3.1, it is obvious that this function is symmetric around the point $d=1/2$.

We have evaluated this criterion numerically for several values of the parameter λ. It turns out that for all sufficiently large λ the function ψ has a unique maximum at $d=1/2$. In other words, if the parameter λ is not too small, then the design $\xi=\{0,1/2,1\}$ is D-optimal for the linear regression model (3.1). If λ approaches 0 the situation changes and gets more complicated. For instance, if $\lambda=0.0001$ the function ψ has a local minimum at the point $d=1/2$ and there are two maxima at $d=0.2459$ and $d=0.7541$. Hence, there are two non-equally spaced exact D-optimal designs, given by $\{0,0.2459,1\}$ and $\{0,0.7541,1\}$.

To continue these investigations we consider

$$\psi''(\frac{1}{2})=-4\Big((1-\lambda)^2\Big[\lambda+\frac{1}{2}\sqrt{\lambda}\,(\ln(\lambda))^2-2\sqrt{\lambda}\ln(\lambda)-1\Big]$$
$$-(-4\sqrt{\lambda}+\lambda+3)\lambda\,(\ln(\lambda))^2\Big),$$

which is negative whenever $\lambda>0.0007798=\lambda^*$, say. It is positive whenever $\lambda<\lambda^*$, which leads us to the conjecture that the optimum design is equally spaced at the points 0, 1/2, 1 for all $\lambda \geq \lambda^*$. In the case $\lambda < \lambda^*$, the optimal design is not equally spaced and places the inner point nearer to the boundary of the design space. Based on an exhaustive numerical search we confirmed this conjecture and derived the following numerical result.

Numerical Result 4.2. *For the linear regression with correlated observations, an exact* 3*-point* D*-optimal design is given by* $\xi_3 = \{0, 1/2, 1\}$ *if and only if* $\lambda \geq \lambda^*$*, and by the design* $\xi^* = \{0, d(\lambda), 1\}$ *or* $\{0, 1-d(\lambda), 1\}$ *if and only if* $\lambda < \lambda^*$*. Here* $d(\lambda) \in [0, 1/2)$ *is the unique solution of the equation* $\psi'(d) = 0$*, where the function* ψ *is defined in* (4.1).

In Table 4.1 we display the non-trivial point $d(\lambda)$ of the exact D-optimal designs for weighted least squares estimation in the linear regression model (3.1) with correlation structure (2.2) and $n = 3$ observations. The point $d(\lambda)$ will go to 0 when λ approaches 0. This can be seen as follows: for any given $d > 0$, if $\lambda \to 0$ then $\psi(d) \to 2(1-d(1-d))$. Hence, if we compare $0 < d_1 < d_2 < 1/2$ then there is a $\lambda_0 > 0$ such that $\psi(d_1) > \psi(d_2)$ for all $\lambda < \lambda_0$. Therefore, the optimal design $\{0, d(\lambda), 1\}$ gets near to the design $\xi_{\text{uc}^*} = \{0, 0, 1\}$, which is D-optimal for uncorrelated observations. The table also shows the D-efficiency,

$$\text{eff}(\xi^*_{\text{uc}}) = \frac{\sqrt{\det(X^T_{\xi^*_{\text{uc}}} V^T_{\xi^*_{\text{uc}}} V_{\xi^*_{\text{uc}}} X_{\xi^*_{\text{uc}}})}}{\sqrt{\det(X^T_{\xi^*} V^T_{\xi^*} V_{\xi^*} X_{\xi^*})}},$$

of the design ξ^*_{uc} and the analogously defined efficiency of the equally spaced design ξ_3. Note that, somewhat surprisingly, the efficiency of ξ^*_{uc} gets less for smaller λ, while the equally spaced design is extremely efficient for the estimation of the parameters in the linear regression model with correlated observations.

Example 4.3. *The case* $n = 4, 5, 6$. In the case $n = 4$ it follows from Theorem 4.1 that the exact D-optimal design for the linear regression model (3.1) with correlation structure (2.2) is of the form $\xi^* = \{0, t_2, t_3, 1\}$. However, our extensive numerical study shows that the exact 4-point D-optimal design has an even

Table 4.1. The non-trivial point $d(\lambda)$ of the exact D-optimal designs for weighted least squares estimation in the linear regression model (3.1) with correlation structure (2.2) and $n = 3$ observations for various values of the parameter λ. The exact D-optimal design is given by $\xi^* = \{0, d(\lambda), 1\}$. The table also shows the D-efficiency of the design $\xi^*_{\text{uc}} = \{0, 0, 1\}$, D-optimal for uncorrelated observations, and the efficiency of the equally spaced design $\xi_3 = \{0, 0.5, 1\}$.

λ	0.9	0.5	0.1	0.01	0.001	10^{-4}	10^{-5}	10^{-6}	10^{-7}	10^{-8}	10^{-9}	10^{-10}
$d(\lambda)$	0.5	0.5	0.5	0.5	0.5	0.305	0.246	0.211	0.187	0.169	0.155	0.143
eff(ξ_3)	1.0	1.0	1.0	1.0	1.0	0.995	0.983	0.972	0.962	0.954	0.947	0.941
eff(ξ^*_{uc})	0.999	0.996	0.944	0.867	0.831	0.817	0.804	0.794	0.786	0.779	0.773	0.768

simpler form, given by $\{0, d, 1-d, 1\}$ where $d = d(\lambda) \in (0, 0.5)$. In the first part of Table 4.2 we present the D-optimal designs for the linear regression model (3.1) with correlation structure (2.2) and $n = 4$ observations for various values of λ. We also display the D-efficiencies of the designs $\xi^*_{\mathrm{uc}} = \{0, 0, 1, 1\}$ and the equally spaced design $\xi_4 = \{0, 1/3, 2/3, 1\}$. It is interesting to note that the equally spaced design is again very efficient for all values of the parameter λ. The design ξ^*_{uc} which is D-optimal for uncorrelated observations is very efficient for highly correlated data and gets less efficient if $\lambda \to 0$.

The situation in the cases $n = 5$ and $n = 6$ is very similar. Exact optimal designs for $n = 5$ and $n = 6$ observations are displayed in the second and third part of Table 4.2, respectively. Our numerical results show that for five observations the exact D-optimal design is of the form $\{0, d_1, d_2, 1-d_1, 1\}$ (or its reflection at the point $t = 1/2$), where $d_1 = d_1(\lambda) \in (0, 0.5)$ and $d_2 = d_2(\lambda) \in (0, 0.5]$. Similarly, exact D-optimal designs for the linear regression model (3.1) with correlation structure (2.2) and $n = 6$ observations are of the form $\{0, d_1, d_2, 1-d_2, 1-d_1, 1\}$, where $d_1 = d_1(\lambda) \in (0, 0.5)$ and $d_2 = d_2(\lambda) \in (0, 0.5)$. We have also performed calculations for a larger sample size but the results are not presented here for the sake of brevity. However the structure of the exact D-

Table 4.2. The non-trivial support points of the exact D-optimal designs for weighted least squares estimation in the linear regression model (3.1) with correlation structure (2.2) and $n = 4$ (first row), $n = 5$ (second row) and $n = 6$ (third row) observations. The exact D-optimal design is of the form (4.2) or (4.3) if n is even or odd, respectively. The table also shows the D-efficiency of the design ξ^*_{uc}, D-optimal for uncorrelated observations, and the efficiency of the equally spaced design ξ_n.

$n=4$												
λ	0.9	0.5	0.1	0.01	0.001	10^{-4}	10^{-5}	10^{-6}	10^{-7}	10^{-8}	10^{-9}	10^{-10}
$d(\lambda)$	0.332	0.328	0.317	0.303	0.281	0.249	0.217	0.192	0.174	0.159	0.146	0.136
eff(ξ_4)	1.0	1.0	1.0	0.998	0.993	0.982	0.966	0.947	0.930	0.914	0.900	0.888
eff(ξ^*_{uc})	1.0	0.996	0.928	0.806	0.731	0.689	0.662	0.642	0.626	0.614	0.604	0.596
$n=5$												
λ	0.9	0.5	0.1	0.01	0.001	10^{-4}	10^{-5}	10^{-6}	10^{-7}	10^{-8}	10^{-9}	10^{-10}
$d_1(\lambda)$	0.249	0.243	0.233	0.224	0.215	0.204	0.191	0.181	0.167	0.153	0.142	0.133
$d_2(\lambda)$	0.5	0.5	0.5	0.5	0.5	0.5	0.5	0.424	0.345	0.304	0.276	0.255
eff(ξ_5)	1.0	1.0	1.0	1.0	0.996	0.991	0.984	0.975	0.962	0.947	0.931	0.917
eff(ξ^*_{uc})	1.0	1.0	0.922	0.780	0.685	0.628	0.594	0.573	0.556	0.542	0.530	0.521
$n=6$												
λ	0.9	0.5	0.1	0.01	0.001	10^{-4}	10^{-5}	10^{-6}	10^{-7}	10^{-8}	10^{-9}	10^{-10}
$d_1(\lambda)$	0.199	0.194	0.184	0.177	0.171	0.164	0.156	0.146	0.134	0.124	0.115	0.107
$d_2(\lambda)$	0.399	0.397	0.391	0.385	0.380	0.372	0.361	0.340	0.311	0.283	0.261	0.242
eff(ξ_6)	1.0	1.0	1.0	0.999	0.997	0.993	0.988	0.981	0.970	0.957	0.942	0.927
eff(ξ^*_{uc})	1.0	0.995	0.919	0.767	0.659	0.591	0.548	0.519	0.499	0.483	0.469	0.458

optimal designs can be described as follows: If $n = 2k$ our numerical calculations indicate that an exact $2k$-point D-optimal design is of the form

$$\{0, d_1, \ldots, d_{k-1}, 1 - d_{k-1}, \ldots, 1 - d_1, 1\}, \tag{4.2}$$

where $d_i = d_i(\lambda) \in (0, 0.5)$ while in the case $n = 2k + 1$ an exact $2k + 1$-point D-optimal design is of the form

$$\{0, d_1, \ldots, d_{k-1}, d_k, 1 - d_{k-1}, \ldots, 1 - d_1, 1\} \tag{4.3}$$

(or its reflection at the point $t = 1/2$), where $d_i = d_i(\lambda) \in (0, 0.5)$.

Example 4.4. *Estimation of the slope.* In this example we briefly present some exact optimal designs for weighted least squares estimation of the slope in the linear regression model. Some exact optimal designs for weighted least squares estimation of the slope in the linear regression model. In Table 4.3 we show the

Table 4.3. The non-trivial points of the exact optimal designs for weighted least squares estimation of the slope in the linear regression model (3.1) with correlation structure (2.2) and $n = 3$ (first row), $n = 4$ (second row), $n = 5$ (third row) and $n = 6$ (fourth row) observations. The exact D_1-optimal design is of the form (4.2) or (4.3) if n is even or odd, respectively. The table also shows the D_1-efficiency of the design ξ^*_{uc}, D_1-optimal for uncorrelated observations, and the efficiency of the equally spaced design ξ_n.

$n = 3$												
λ	0.9	0.5	0.1	0.01	0.001	10^{-4}	10^{-5}	10^{-6}	10^{-7}	10^{-8}	10^{-9}	10^{-10}
$d(\lambda)$	0.146	0.147	0.151	0.151	0.145	0.136	0.126	0.118	0.110	0.103	0.097	0.092
$\mathrm{eff}_1(\xi_3)$	1.0	1.0	0.996	0.975	0.947	0.923	0.904	0.888	0.876	0.866	0.857	0.850
$\mathrm{eff}_1(\xi^*_{\mathrm{uc}})$	1.0	1.0	0.996	0.975	0.947	0.923	0.904	0.888	0.876	0.866	0.857	0.850
$n = 4$												
λ	0.9	0.5	0.1	0.01	0.001	10^{-4}	10^{-5}	10^{-6}	10^{-7}	10^{-8}	10^{-9}	10^{-10}
$d(\lambda)$	0.180	0.180	0.178	0.172	0.163	0.153	0.142	0.133	0.124	0.116	0.109	0.103
$\mathrm{eff}_1(\xi_4)$	1.0	1.0	0.996	0.973	0.935	0.895	0.858	0.826	0.799	0.777	0.759	0.743
$\mathrm{eff}_1(\xi^*_{\mathrm{uc}})$	1.0	1.0	0.990	0.941	0.877	0.823	0.780	0.747	0.721	0.700	0.683	0.669
$n = 5$												
λ	0.9	0.5	0.1	0.01	0.001	10^{-4}	10^{-5}	10^{-6}	10^{-7}	10^{-8}	10^{-9}	10^{-10}
$d_1(\lambda)$	0.186	0.186	0.184	0.177	0.168	0.158	0.147	0.138	0.129	0.121	0.114	0.107
$d_2(\lambda)$	0.239	0.239	0.238	0.235	0.229	0.221	0.211	0.200	0.190	0.180	0.171	0.163
$\mathrm{eff}_1(\xi_5)$	1.0	1.0	0.998	0.986	0.962	0.931	0.898	0.866	0.837	0.812	0.789	0.769
$\mathrm{eff}_1(\xi^*_{\mathrm{uc}})$	1.0	1.0	0.989	0.935	0.863	0.800	0.749	0.710	0.679	0.654	0.634	0.617
$n = 6$												
λ	0.9	0.5	0.1	0.01	0.001	10^{-4}	10^{-5}	10^{-6}	10^{-7}	10^{-8}	10^{-9}	10^{-10}
$d_1(\lambda)$	0.112	0.112	0.111	0.109	0.106	0.102	0.098	0.093	0.089	0.085	0.081	0.077
$d_2(\lambda)$	0.252	0.251	0.250	0.246	0.239	0.231	0.221	0.210	0.200	0.190	0.181	0.172
$\mathrm{eff}_1(\xi_6)$	1.0	1.0	0.999	0.989	0.970	0.943	0.913	0.882	0.852	0.823	0.798	0.775
$\mathrm{eff}_1(\xi^*_{\mathrm{uc}})$	1.0	1.0	0.988	0.928	0.847	0.774	0.715	0.669	0.632	0.603	0.579	0.559

exact optimal designs for sample sizes $n = 3, 4, 5, 6$. We also present the D_1-efficiency $\text{eff}_1(\xi) = D_1(\xi)/D_1(\xi_1^*)$ of the equally spaced design and the exact D_1-optimal design obtained under the assumption of uncorrelated observations. The form of the D_1 optimal design is given in (4.2) and (4.3) corresponding to the cases of an even and odd number of observations, respectively. Note that the optimal designs for estimating the slope are more concentrated at the boundary of the experimental region. For example, if $n = 4, \lambda = 0.01$, the exact D-optimal design for weighted least squares estimation is given by $\xi^* = \{0, 0.303, 0.697, 1\}$, while the exact D_1-optimal design is $\{0, 0.172, 0.828, 1\}$. As a consequence the design ξ^*_{uc} for the linear regression model with uncorrelated observations (which is the same for the D- and D_1-optimality criterion) yields larger efficiencies for estimating the slope, while the equally spaced design is less efficient for this purpose.

5. Exact Optimal Designs for Quadratic Regression

In this section we briefly discuss the problem of determining exact D-optimal designs for weighted least squares estimation in the quadratic regression model

$$Y_{t_i} = \beta_1 + \beta_2 t_i^2 + \beta_3 t_i^2 + \varepsilon_{t_i} \quad i = 1, \dots, n\,, \tag{5.1}$$

with an autoregressive error of the form (2.2). In all cases the exact optimal designs have to be determined numerically. However, it can be shown by similar arguments as presented in Section 3 that Proposition 3.2 also holds in the quadratic regression model. Moreover, the symmetry property in Lemma 3.1 is also valid in the quadratic case and it is possible to derive an analogue of Theorem 3.6 for highly correlated data.

Theorem 5.1.

(a) *Let* $\xi^- = \{1-t_n, \dots, 1-t_1\}$ *denote the design obtained from* $\xi = \{t_1, \dots, t_n\}$ *by reflecting the points* t_i *at the center* $t = 1/2$, *then* $\det M_\xi = \det M_{\xi^-}$, *where the matrix* M_ξ *is defined in* (2.3) *with* $p = 3$, $f_1(t) = 1$, $f_2(t) = t$, $f_3(t) = t^2$.

(b) *An exact* D*-optimal design* $\xi_n^* = \{t_1, \dots, t_n\}$ *for weighted least squares estimation in the quadratic regression model* (5.1) *with correlation structure* (2.2) *satisfies* $t_1 = 0$ *and* $t_n = 1$.

(c) *If* $\lambda \to 1$, *then any exact* n*-point* D*-optimal design for weighted least squares estimation in the quadratic regression model* (5.1) *with correlation structure* (2.2) *converges to the equally spaced design* $\xi_n = \{0, 1/(n-1), 2/(n-1), \dots, 1\}$.

Proof. We only prove part (c) of the Theorem. The remaining statements follow by similar arguments as presented in Section 3. If $\lambda \to 1$ the elements of the matrix

$$M_\xi = \begin{pmatrix} A & C & D \\ C & B & E \\ D & E & F \end{pmatrix}$$

satisfy

$$\begin{aligned}
A &= 1+\frac{1-\lambda}{2}+\frac{(1-\lambda)^2}{4}+(1+S_{1,1})\frac{(1-\lambda)^3}{8}+(1+3S_{1,1})\frac{(1-\lambda)^4}{16}+o((1-\lambda)^4),\\
B(1-\lambda)^2 &= \frac{(1-\lambda)}{2}+\frac{(1-\lambda)^2}{4}+\frac{(1-\lambda)^3}{8}+\frac{(1-\lambda)^4}{16}+o((1-\lambda)^4),\\
C(1-\lambda) &= \frac{(1-\lambda)}{2}+\frac{(1-\lambda)^2}{4}+\frac{(1-\lambda)^3}{8}+(3+2S_{1,2})\frac{(1-\lambda)^4}{48}+o((1-\lambda)^4),\\
D(1-\lambda) &= \frac{(1-\lambda)}{2}+(1-S_{1,1})\frac{(1-\lambda)^2}{4}+(1-S_{1,1})\frac{(1-\lambda)^3}{8}+o((1-\lambda)^3),\\
E(1-\lambda)^2 &= \frac{(1-\lambda)}{2}+\frac{(1-\lambda)^2}{4}+(3-2S_{1,2})\frac{(1-\lambda)^3}{24}+o((1-\lambda)^3),\\
F(1-\lambda)^2 &= (1+S_{1,1})\frac{(1-\lambda)}{2}+(1-S_{1,1})\frac{(1-\lambda)^2}{4}+o((1-\lambda)^2),
\end{aligned}$$

where $S_{1,1}$ and $S_{1,2}$ are defined in (3.9). A straightforward calculation of the determinant of the matrix M_ξ now yields the expansion $\det M_\xi = S_{1,1}(1-\lambda)^{-2}/16 + o((1-\lambda)^{-2})$, and the assertion follows by the same arguments as presented in the proof of Theorem 3.6.

Numerical calculations show that the exact optimal designs are of the form (4.2) in the case $n = 2k$ and (4.3) in the case $n = 2k + 1$. In Table 5.1 we display the exact D-optimal designs for weighted least squares estimation in the quadratic regression model with $n = 4$, $n = 5$ and $n = 6$ correlated observations for various values of the parameter λ. In the case $n = 3$ the equally spaced design $\xi_3 = \{0, 1/2, 1\}$ is D-optimal. We also show the D-efficiency of the equally spaced design ξ_n and the efficiency of the exact D-optimal design under the assumption of uncorrelated observations (see Gaffke and Krafft (1982)). We observe that the equally spaced design is extremely efficient for weighted least squares analysis in the quadratic regression model with autoregressive errors of the form (2.2). For example, if $n = 5$ observations can be taken, the D-efficiency of the design ξ_5 is at least 99.0% if the parameter λ varies in the interval $[10^{-10}, 1)$. It is also interesting to see that the exact D-optimal does not change substantially with the parameter λ. For example if $\lambda = 0.5$ and $\lambda = 10^{-7}$ the exact optimal designs differ only by one point, which is 0.252 in the first and 0.294 in the second case, respectively.

Table 5.1. The non-trivial points of the exact D-optimal designs for weighted least squares estimation in the quadratic regression model (5.1), correlation structure (2.2) and $n = 4$ (first row), $n = 5$ (second row) and $n = 6$ (third row) observations. The exact D-optimal design is given by (4.2) or (4.3) if n is even or odd, respectively. The table also shows the D-efficiency of the designs $\xi^*_{\text{uc}} = \{0, 1/2, 1/2, 1\}$ (n=4), $\xi^*_{\text{uc}} = \{0, 1/2, 1/2, 1/2, 1\}$ ($n = 5$), $\xi^*_{\text{uc}} = \{0, 0, 1/2, 1/2, 1, 1\}$ ($n = 6$), D-optimal for uncorrelated observations, and the efficiency of the equally spaced design ξ_n.

$n = 4$												
λ	0.9	0.5	0.1	0.01	0.001	10^{-4}	10^{-5}	10^{-6}	10^{-7}	10^{-8}	10^{-9}	10^{-10}
$d(\lambda)$	0.333	0.335	0.345	0.355	0.362	0.369	0.378	0.386	0.394	0.400	0.407	0.412
eff(ξ_4)	1.0	1.0	1.0	0.998	0.995	0.992	0.988	0.984	0.981	0.978	0.975	0.973
eff(ξ^*_{uc})	0.945	0.944	0.929	0.892	0.860	0.840	0.828	0.820	0.815	0.811	0.809	0.807
$n = 5$												
λ	0.9	0.5	0.1	0.01	0.001	10^{-4}	10^{-5}	10^{-6}	10^{-7}	10^{-8}	10^{-9}	10^{-10}
$d_1(\lambda)$	0.250	0.252	0.265	0.273	0.274	0.276	0.279	0.286	0.294	0.304	0.315	0.325
$d_2(\lambda)$	0.500	0.500	0.500	0.500	0.500	0.500	0.500	0.500	0.500	0.500	0.500	0.500
eff(ξ_5)	1.0	1.0	1.0	0.999	0.998	0.998	0.997	0.996	0.995	0.993	0.992	0.990
eff(ξ^*_{uc})	0.928	0.926	0.907	0.854	0.803	0.767	0.744	0.730	0.722	0.716	0.712	0.710
$n = 6$												
λ	0.9	0.5	0.1	0.01	0.001	10^{-4}	10^{-5}	10^{-6}	10^{-7}	10^{-8}	10^{-9}	10^{-10}
$d_1(\lambda)$	0.200	0.202	0.215	0.220	0.214	0.208	0.201	0.194	0.182	0.164	0.142	0.124
$d_2(\lambda)$	0.400	0.401	0.407	0.410	0.409	0.409	0.408	0.409	0.410	0.412	0.415	0.419
eff(ξ_6)	1.0	1.0	1.0	0.999	0.999	0.999	0.999	0.999	0.998	0.996	0.992	0.987
eff(ξ^*_{uc})	0.921	0.919	0.897	0.835	0.772	0.724	0.690	0.668	0.653	0.642	0.634	0.627

Finally, we briefly compare the exact optimal designs for linear and quadratic regression. First we note that the optimal designs for the linear regression model are usually more concentrated at the boundary, in particular if λ is not too large. For example in the case $n = 6$ with $\lambda = 0.001$, the nontrivial points in the interval $[0, 0.5]$ are 0.171, 0.380 and 0.214, 0.409 corresponding to the linear and quadratic case. Secondly, both exact optimal designs approach the equally spaced design if $\lambda \to 1$. Therefore, it is intuitively clear that for highly correlated data the optimal design for the quadratic model is also very efficient in the linear model, and vice versa. For example, if $n = 6$ and $\lambda = 0.01$, the efficiency of the D-optimal design for the quadratic model in the linear regression is 99.7% and the efficiency of the D-optimal design for the linear model in the quadratic regression is 99.5%.

6. Ordinary Least Squares Estimation

In this section we briefly discuss exact D-optimal design problems for ordinary least squares estimation in the linear and quadratic model with correlation structure (2.2). Note that the covariance matrix of the ordinary least squares estimator is given by

$$\tilde{M}_{\xi}^{-1} = (X_{\xi}^T X_{\xi})^{-1}(X_{\xi}^T (V_{\xi}^T V_{\xi})^{-1} X_{\xi})(X_{\xi}^T X_{\xi})^{-1}, \tag{6.1}$$

where the matrices X_ξ and V_ξ are defined in Section 2. An exact D-optimal design for ordinary least squares estimation in a model with correlation structure (2.2) maximizes $\det \tilde{M}_\xi$.

Theorem 6.1. *Consider the linear or quadratic regression model.*

(a) *Let* $\tilde{\xi} = \{1-t_n, \dots, 1-t_1\}$ *denote the design obtained from* $\xi = \{t_1, \dots, t_n\}$ *by the reflection at the point* $t = 1/2$, *then* $\det \tilde{M}_{\tilde{\xi}} = \det \tilde{M}_\xi$, *where the matrix* $\tilde{M}_\xi$ *is defined in* (6.1).

(b) *Any exact* D*-optimal* $\xi = \{t_1, \dots, t_n\}$ *design for ordinary least squares estimation maximizing* $\det \tilde{M}_\xi$ *satisfies* $t_1 = 0, t_n = 1$.

In Table 6.1 we display the exact $D-$optimal designs for ordinary least squares estimation in a linear regression model with correlation structure (2.2). The corresponding results for the quadratic regression model are shown in Table 6.2, where for three observations the equally spaced design $\xi_3 = \{0, 1/2, 1\}$ is D-optimal independently of λ. In the case of a linear regression model these designs exhibit an interesting behaviour. There exist a threshold, say λ^* such that the exact D-optimal design for uncorrelated observations is also D-optimal for the correlation structure (2.2) whenever $\lambda > \lambda^*$. If $\lambda < \lambda^*$ the structure of the designs changes and the optimal designs can be found in Table 6.1. Such a threshold does not exist for the quadratic regression model. In both cases the equally spaced design is again very efficient, while the loss of efficiency of the exact D-optimal design for uncorrelated observations may be substantial if the correlation is small.

It is also of interest to compare these designs with the optimal designs for weighted least squares analysis derived in Section 4 and 5. In the linear regression the D-optimal designs for ordinary and weighted least squares estimation do not differ substantially if the correlation is small. For example, if $\lambda = 0.01$ and $n = 5$, the optimal design for weighted least squares estimation is $\{0, 0.224, 0.5, 0.776, 1\}$, while the optimal design for ordinary least squares estimation is $\{0, 0.216, 0.5, 0.784, 1\}$. However, if the correlation is larger, the difference is more substantial, because the optimal design for ordinary least squares estimation advises the experimenter to take repeated observations at the boundary of the experimental region. In the quadratic model the situation is similar, but the differences for strongly correlated data are smaller. For example, if $n = 6$ and $\lambda = 0.9$, the D-optimal design for weighted least squares estimation is $\{0, 0.2, 0.4, 0.6, 0.8, 1\}$, while the D-optimal design for ordinary least squares

Table 6.1. The non-trivial point of the exact D-optimal designs for ordinary least squares estimation in the linear regression model (3.1) with correlation structure (2.2) and $n = 3$ (first row), $n = 4$ (second row), $n = 5$ (third row) and and $n = 6$ (fourth row) observations. The exact D-optimal design is given by (4.2) or (4.3) if n is even or odd, respectively. The table also shows the D-efficiency of the exact D-optimal design ξ^*_{uc} for uncorrelated observations and the efficiency of the equally spaced design.

$n = 3$												
λ	0.9	0.5	0.1	0.01	0.001	10^{-4}	10^{-5}	10^{-6}	10^{-7}	10^{-8}	10^{-9}	10^{-10}
$d(\lambda)$	0.000	0.000	0.500	0.500	0.500	0.308	0.247	0.212	0.188	0.170	0.155	0.143
eff(ξ_3)	0.997	0.994	1.0	1.0	1.0	0.995	0.983	0.972	0.962	0.954	0.947	0.941
eff(ξ^*_{uc})	1.0	1.0	0.950	0.867	0.833	0.818	0.805	0.794	0.786	0.779	0.773	0.768
$n = 4$												
λ	0.9	0.5	0.1	0.01	0.001	10^{-4}	10^{-5}	10^{-6}	10^{-7}	10^{-8}	10^{-9}	10^{-10}
$d(\lambda)$	.000	0.000	0.334	0.312	0.288	0.253	0.219	0.193	0.174	0.159	0.147	0.136
eff(ξ_4)	0.986	0.977	1.0	0.999	0.994	0.983	0.967	0.948	0.930	0.914	0.900	0.888
eff(ξ^*_{uc})	1.0	1.0	0.950	0.813	0.734	0.690	0.662	0.642	0.627	0.614	0.604	0.596
$n = 5$												
λ	0.9	0.5	0.1	0.01	0.001	10^{-4}	10^{-5}	10^{-6}	10^{-7}	10^{-8}	10^{-9}	10^{-10}
$d_1(\lambda)$	0.000	0.000	0.000	0.216	0.216	0.207	0.194	0.183	0.167	0.154	0.142	0.133
$d_2(\lambda)$	0.000	0.000	0.500	0.500	0.500	0.500	0.500	0.433	0.348	0.307	0.278	0.256
eff(ξ_5)	0.975	0.961	0.978	0.997	0.996	0.991	0.985	0.976	0.963	0.947	0.932	0.918
eff(ξ^*_{uc})	1.0	1.0	0.941	0.795	0.690	0.630	0.595	0.573	0.556	0.542	0.531	0.521
$n = 6$												
λ	0.9	0.5	0.1	0.01	0.001	10^{-4}	10^{-5}	10^{-6}	10^{-7}	10^{-8}	10^{-9}	10^{-10}
$d_1(\lambda)$	0.000	0.000	0.000	0.135	0.164	0.165	0.159	0.149	0.137	0.125	0.116	0.108
$d_2(\lambda)$	0.000	0.402	0.339	0.387	0.388	0.380	0.368	0.346	0.315	0.286	0.263	0.244
eff(ξ_6)	0.966	0.946	0.951	0.992	0.995	0.993	0.989	0.982	0.971	0.958	0.943	0.928
eff(ξ^*_{uc})	1.0	0.997	0.929	0.788	0.668	0.595	0.550	0.521	0.500	0.483	0.470	0.459

regression is $\{0, 0.290, 0.413, 0.587, 0.710, 1\}$. We finally note that the equally spaced design is very efficient for ordinary least squares estimation. These observations are in accordance with the results of Bickel, Herzberg and Schilling (1981), who argued by asymptotic arguments that for a large sample size the equally spaced design should be nearly optimal for estimating the slope or intercept in a linear regression with autocorrelation structure (2.2) by ordinary least squares.

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Table 6.2. The non-trivial points of the exact D-optimal designs for ordinary least squares estimation in the quadratic regression model (5.1) with correlation structure (2.2) and $n = 4$ (first row), $n = 5$ (second row) and $n = 6$ (third row) observations. The exact D-optimal design is given by (4.2) or (4.3) if n is even or odd, respectively. The table also shows the D-efficiency of the exact D-optimal design ξ^*_{uc} for uncorrelated observations and the efficiency of the equally spaced design.

$n = 4$												
λ	0.9	0.5	0.1	0.01	0.001	10^{-4}	10^{-5}	10^{-6}	10^{-7}	10^{-8}	10^{-9}	10^{-10}
$d(\lambda)$	0.352	0.356	0.359	0.359	0.363	0.369	0.378	0.386	0.393	0.400	0.407	0.412
eff(ξ_4)	0.999	0.999	0.998	0.996	0.994	0.992	0.988	0.984	0.981	0.978	0.975	0.973
eff(ξ^*_{uc})	0.951	0.950	0.933	0.894	0.861	0.840	0.828	0.820	0.815	0.811	0.809	0.807
$n = 5$												
λ	0.9	0.5	0.1	0.01	0.001	10^{-4}	10^{-5}	10^{-6}	10^{-7}	10^{-8}	10^{-9}	10^{-10}
$d_1(\lambda)$	0.304	0.310	0.305	0.288	0.279	0.278	0.280	0.286	0.294	0.304	0.315	0.325
$d_2(\lambda)$	0.500	0.500	0.500	0.500	0.500	0.500	0.500	0.500	0.500	0.500	0.500	0.500
eff(ξ_5)	0.996	0.995	0.994	0.996	0.997	0.997	0.997	0.996	0.995	0.993	0.992	0.990
eff(ξ^*_{uc})	0.944	0.943	0.920	0.861	0.805	0.768	0.744	0.730	0.722	0.716	0.712	0.710
$n = 6$												
λ	0.9	0.5	0.1	0.01	0.001	10^{-4}	10^{-5}	10^{-6}	10^{-7}	10^{-8}	10^{-9}	10^{-10}
$d_1(\lambda)$	0.290	0.301	0.289	0.250	0.228	0.215	0.206	0.197	0.186	0.168	0.144	0.126
$d_2(\lambda)$	0.413	0.422	0.425	0.415	0.410	0.409	0.408	0.408	0.409	0.411	0.415	0.419
eff(ξ_6)	0.991	0.989	0.990	0.994	0.998	0.999	0.999	0.999	0.998	0.996	0.993	0.987
eff(ξ^*_{uc})	0.945	0.945	0.921	0.850	0.780	0.727	0.691	0.668	0.653	0.643	0.635	0.627

References

Abt, M., Liski, E. P., Mandal, N. K. and Sinha, B. K. (1997). Optimal designs in growth curve models: Part I Correlated model for linear growth: Optimal designs for slope parameter estimation and growth prediction. *J. Statist. Plann. Inference* **64**, 141-150.

Abt, M., Liski, E. P., Mandal, N. K. and Sinha, B. K. (1998). Optimal designs in growth curve models: Part II Correlated model for quadratic growth: Optimal designs for parameter estimation and growth prediction. *J. Statist. Plann. Inference* **67**, 287-296.

Bickel, P. J. and Herzberg, A. M. (1979). Robustness of design against autocorrelation in time I: Asymptotic theory, optimality for location and linear regression. *Ann. Stat.* **7**, 77-95.

Bickel, P. J., Herzberg, A. M. and Schilling, M. F. (1981). Robustness of design against autocorrelation in time II: Optimality, theoretical and numerical results for the first-order autoregressive process. *J. Amer. Statist. Assoc.* **76**, 870-877.

Bischoff, W. (1995). Lower bounds for the efficiency of designs with respect to the D-criterion when the observations are correlated. *Statistics* **27**, 27-44.

Gaffke, N., and Krafft, O. (1982). Exact D-optimum designs for quadratic regression. *J. Roy. Statist. Soc. Ser. B* **44**, 394-397.

Hoel, P. G. (1958). Efficiency problems in polynomial estimation. *Ann. Math. Statist.* **29**, 1134-1145.

Hohmann, G. and Jung, W. (1975). On sequential and nonsequential D-optimal experimental design. *Biometr. Z.* **17**, 329-336.

Imhof, L. (1998). A-optimum exact designs for quadratic regression. *J. Math. Anal. Appl.* **228**, 157-165.

Imhof, L. (2000). Exact designs minimizing the integrated variance in quadratic regression. *Statistics* **34**, 103-115.

Imhof, L., Krafft, O. and Schaefer, M. (2000). D-optimal exact designs for parameter estimation in a quadratic model. Sankhya B **62**, 266-275.

Karlin, S. and Studden, W. J. (1966). *Tchebycheff Systems: With Applications in Analysis and Statistics.* Interscience, New York.

Kunert, J. (1985). Optimal repeated measurements designs for correlated observations and analysis by weighted least squares. *Biometrika* **72**, 375-389.

Martin, R. J. (1996). Spatial Experimental Design. In *Handbook of Statistics* **13** (Edited by S. Ghosh and C. R. Rao), 477-514. North-Holland, Amsterdam.

Müller, W. and Pazman, A. (2003). Measures for designs in experiments with correlated errors. *Biometrika* **90**, 423-434.

Potthoff, R. F., and Roy, S. N. (1964). A generalized multivariate analysis of variance model useful especially for growth curve problems. *Biometrika* **51**, 313-326.

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