Biometrical Letters
Vol. 44 (2007), No. 2, 85-96

A-optimal designs under a quadratic growth curve model in the transformed time interval

Katarzyna Filipiak, Anna Szczepańska

Department of Mathematical and Statistical Methods, Agricultural University,
Wojska Polskiego 28, 60-637 Poznań, e-mail: kasfil@au.poznan.pl, e-mail: sanna6@wp.pl

SUMMARY

In this paper the quadratic growth curve model with correlated observations is considered. For a symmetric experimental domain we determine a scale $\alpha > 0$ and a correlation structure $\mathbf{V}$ such that the A-optimal design over the time interval $[-1, 1]$ is also optimal over $[-\alpha, \alpha]$. For some correlation structures the design $d^* = \{-\alpha, 0, \alpha\}$ is A- and D-optimal over $[-\alpha, \alpha]$. Therefore the second aim of this paper is to determine an asymmetric experimental domain $[\alpha, \beta]$ and correlation structure $\mathbf{V}$ such that the design $d = \{\alpha, (\alpha+\beta)/2, \beta\}$ which is D-optimal over $[\alpha, \beta]$ is also A-optimal.

Key words: growth curve model, A-optimal design.

1. Introduction

In experiments where some individuals are observed repeatedly in time, growth curve models are often used. Recently some results on optimality concerning approximated designs in polynomial models have been published. Luoma et al. (2001) examined the nature of A-optimal approximated designs in quartic and cubic regression models with uncorrelated observations and the experimental domain $[0,1]$. Mandal (2002) determined optimal approximated designs in a quadratic regression model on the experimental symmetric domain $[-1,1]$ and in an m-factor first-degree polynomial fit model over two extensions of $[-1,1]$: an Euclidean ball of radius $\sqrt{m}$ and a symmetric m-dimensional hypercube $[-1,1]^m$ with half side length 1. Liski et al. (2002) presented the theory of optimal approximated designs in symmetric and asymmetric domains. They showed that a general criterion-specific optimal design constructed with respect to the experimental domain $[-1,1]$ does not lead to the corresponding optimal design over $[0,1]$, obtained by transformation of the experimental domain. Only the D-optimality criterion enjoys this nice property. The authors studied mainly univariate polynomial regression models with k degrees of the polynomial. In the multivariate case, they considered first degree growth curves. In the all papers mentioned, models with uncorrelated errors were studied. Growth curve models with correlated observations were analyzed in Moerbeek (2005). She considered linear, quadratic and cubic growth with autocorrelated errors, and studied the robustness properties of A-, D- and E-optimal designs over the time interval $[0, 2]$. Filipiak and Szczepańska (2005) extended the results of Moerbeek to the case of nearest-neighbor structure (NN(1)), moving average structure (MA(2)) and unstructured antedependence (UAD(1)). Moreover, they showed that the D-optimal design does not depend on the correlation structure.

In this paper we consider the quadratic growth curve model with correlated errors. By a design we mean an allocation of time points, in which the characteristics are measured, in the experimental domain $[\alpha, \beta]$. We assume that the first and the last time points are fixed and defined by the ends of the time interval. We denote a design d by a triple $\{\alpha, x, \beta\}$, where $x \in (\alpha, \beta)$, $\alpha < \beta$. Our aim is to determine such x^* that the design $d^* = \{\alpha, x^*, \beta\}$ is A-optimal over all designs $d = \{\alpha, x, \beta\}$. This means that we determine the design which minimizes the average-variance of the least squares estimator of regression coefficients.

The aim of this paper is to study the robustness of A-optimality with respect to the scaling of a symmetric domain for quadratic growth curve models with arbitrary correlation structures. For a symmetric experimental domain we determine a scale $\alpha > 0$ and a correlation structure $\mathbf{V}$ such that the A-optimal design over the time interval $[-1, 1]$ is also optimal over $[-\alpha, \alpha]$. For some correlation structures the design $d^* = \{-\alpha, 0, \alpha\}$ is A- and D-optimal over $[-\alpha, \alpha]$. It is easy to see that 0 is the average of the ends of the time interval. Therefore the second aim of this paper is to determine an asymmetric experimental domain $[\alpha, \beta]$ and correlation structure $\mathbf{V}$ such that the A-optimal design and the D-optimal design are the same, i.e. $d^* = \{\alpha, (\alpha + \beta)/2, \beta\}$. For the analysis and the determination of optimal designs we use the *Mathematica* 5.0 software.

We organize the paper as follows. In Section 2 we introduce some definitions and notations. We present a polynomial growth curve model with correlated observations over the experimental domain $[\alpha, \beta]$ and over the transformed time interval of the form $[a\alpha + b,\ a\beta + b]$. For these time intervals we give the forms of information matrices for estimating the unknown regression coefficients and we show the connection between these matrices. In Section 3 we give some optimality results. First we consider A-optimal designs over a symmetric time interval, and finally we formulate conditions of A-optimality of the design on $\{\alpha, (\alpha + \beta)/2, \beta\}$, $\alpha < \beta$.

2. Growth curve model

Consider an experiment where r individuals are assigned to N units. Suppose that the same characteristic is measured at q time points in the time interval $[\alpha, \beta]$, which are denoted by t_j, $j = 1, 2, \ldots, q$. Assume that each individual in the unit is observed once at each time point, and all individuals are measured at the same time points. By p we denote the degree of a polynomial describing an individual's responses at time points on each unit; in every unit the polynomial coefficients are allowed to be different.

The polynomial growth curve model of such an experiment has the form

$$\mathbf{Y} = \mathbf{A}\mathbf{B}\mathbf{X}'_d + \mathbf{E}, \tag{1}$$

where $\mathbf{Y}$ is an $N \times q$ matrix of observations, the $N \times r$ matrix $\mathbf{A}$ is the design matrix of individuals, the $r \times (p+1)$ matrix $\mathbf{B}$ is the matrix of unknown parameters (regression coefficients), the $q \times (p+1)$ matrix $\mathbf{X}_d$ is the design matrix of time points, and $\mathbf{E}$ is an $N \times q$ matrix of random errors with zero mean. We assume that the observations of individuals on the different units measured at the same time points are uncorrelated, while the correlation between observations of individuals at different time points is described by the matrix $\mathbf{V}$. Hence, the dispersion matrix of errors has the form $\mathrm{D}(\mathrm{vec}(\mathbf{E})) = \sigma^2 \mathbf{V} \otimes \mathbf{I}_N$, where $\mathrm{vec}(\mathbf{E})$ denotes the Nq-dimensional vector formed by writing the columns of $\mathbf{E}$ one under another in sequence, $\mathbf{V}$ is a known $q \times q$ positive definite matrix, $\mathbf{I}_N$ is the $N \times N$ identity matrix, and the symbol $\otimes$ denotes the Kronecker product.

In the considered model the design matrix of time points, $\mathbf{X}_d$, is of the form:

$$\mathbf{X}_d = \begin{pmatrix} 1 & t_1 & t_1^2 & \dots & t_1^p \\ 1 & t_2 & t_2^2 & \dots & t_2^p \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & t_q & t_q^2 & \dots & t_q^p \end{pmatrix}.$$

Since we assume that the assignment of observations on units is fixed, observe that the design matrix $\mathbf{A}$ does not depend on the allocation of time points and therefore it is not indexed by d.

If we change the time interval to the form $\left[a\alpha + b, a\beta + b\right]$ then model (1) can be rewritten as

$$\mathbf{Y} = \mathbf{A}\boldsymbol{\Gamma}\mathbf{U}'_d + \mathbf{E}, \tag{2}$$

where

$$\mathbf{U}_d = \begin{pmatrix} 1 & u_1 & u_1^2 & \dots & u_1^p \\ 1 & u_2 & u_2^2 & \dots & u_2^p \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & u_q & u_q^2 & \dots & u_q^p \end{pmatrix}, \qquad \begin{array}{l} u_i = at_i + b, \\ i = 1, 2, \dots, q, \end{array}$$

with $\boldsymbol{\Gamma} = \mathbf{B}\mathbf{K}'^{-1}$ and $\mathbf{U}_d = \mathbf{X}_d\mathbf{K}$,

$$\mathbf{K} = \begin{pmatrix} 1 & b & b^2 & \dots & b^{p-1} & b^p \\ 0 & a & \binom{2}{1}ab & \dots & \binom{p-1}{p-2}ab^{p-2} & \binom{p}{p-1}ab^{p-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & \dots & \binom{p}{0}a^p \end{pmatrix}.$$

The elements of the inverse of this matrix are of the form:

$$\mathbf{K'}^{-1} = \begin{cases} \dfrac{1}{k_{ii}} & \text{if} \quad i = j \\ \dfrac{(-1)^{i+1} k_{ji}}{a^{i+j-2}} & \text{if} \quad i > j \\ 0 & \text{otherwise.} \end{cases}$$

To determine the optimal allocation of time points we need the information matrix of a design. Under model (1) the information matrix for estimating the matrix of regression coefficients, $\mathbf{B}$, has the form

$$\mathbf{M}_d = \left(\mathbf{X'}_d \mathbf{V}^{-1}\mathbf{X}_d\right) \otimes \left(\mathbf{A'A}\right)$$

(for more details see e.g. Markiewicz and Szczepańska, 2006). Under model (2) the information matrix for estimating the matrix $\mathbf{\Gamma}$ can be written as

$$\mathbf{N}_d = \left(\mathbf{U'}_d \mathbf{V}^{-1}\mathbf{U}_d\right) \otimes \left(\mathbf{A'A}\right).$$

From the form of the matrix $\mathbf{\Gamma}$ it follows that

$$\mathbf{N}_d = (\mathbf{K'} \otimes \mathbf{I})\mathbf{M}_d (\mathbf{K} \otimes \mathbf{I}).$$

Since we assumed that in a design each individual is measured at least once, the matrix $\mathbf{A'A}$ is diagonal with the numbers of replications of each individual on the diagonal. Moreover, this matrix does not depend on the allocation of time points. Hence to determine optimal design in growth curve model (1) it is enough to consider the properties of the matrix

$$\mathbf{C}_d = \mathbf{X'}_d \mathbf{V}^{-1}\mathbf{X}_d, \tag{3}$$

and for model (2)

$$\mathbf{F}_d = \mathbf{U'}_d \mathbf{V}^{-1}\mathbf{U}_d.$$

The matrices $\mathbf{C}_d$ and $\mathbf{F}_d$ are the information matrices for estimating the unknown regression coefficients $\mathbf{B}$ and $\mathbf{\Gamma}$, respectively, in a univariate polynomial regression model.

The following relation between matrices $\mathbf{C}_d$ and $\mathbf{F}_d$ holds:

$$\mathbf{F}_d = \mathbf{K}'\mathbf{C}_d\mathbf{K}. \tag{4}$$

In general, following Liski et al. (2002), optimal designs over a given experimental domain do not correspond to the optimal designs over the transformed domain.

Filipiak and Szczepańska (2005) showed that D-optimality of the design does not depend on the correlation structure. From formula (4) it is easy to see that such a design does not depend on the scaling and moving time interval. Indeed, observe

$$\max_{d\in\mathcal{D}} \det \mathbf{F}_d = \max_{d\in\mathcal{D}} \det(\mathbf{K}'\mathbf{C}_d\mathbf{K}) = (\det \mathbf{K})^2 \max_{d\in\mathcal{D}} \det \mathbf{C}_d,$$

where D is the class of designs. Following e.g. Moerbeek (2005), the D-optimal design under the quadratic growth curve model with the time interval $[\alpha, \beta]$ has the form $d^* = \{\alpha, (\alpha+\beta)/2, \beta\}$.

In this paper we study the robustness of A-optimality over the scaled time interval.

We assume that the number of time points, q, is equal to the number of regression coefficients $p+1$ in the polynomial growth curve models (c.f. Garza, 1954, Pukelsheim, 1993, Mandal, 2002). Moerbeek (2005) showed that the efficiency of the design decreases when the number of time points increases.

We are interested in a quadratic growth curve model, so we have $q = 3$ and $p = 2$. Since we assume that the first and the last time points are fixed and are defined by the ends of the time interval, the matrix $\mathbf{X}_d$ has the following form:

$$\mathbf{X}_d = \begin{pmatrix} 1 & \alpha & \alpha^2 \\ 1 & x & x^2 \\ 1 & \beta & \beta^2 \end{pmatrix}, \qquad x \in (\alpha, \beta).$$

In this paper we are interested in determining an A-optimal design $d^* = \{\alpha, x^*, \beta\}$ over designs $d = \{\alpha, x, \beta\}$, $x \in (\alpha, \beta)$, which minimizes the trace of the inverse of the information matrix of d^*. This criterion is equivalent to minimizing the average variance of the least squares estimator of $\mathbf{B}$.

3. Results

In this section we determine a scale α and a correlation structure $\mathbf{V}$ such that the A-optimal design over the time interval $[-1,1]$ is also optimal over $[-\alpha,\alpha]$. In the second part of this section we determine the time interval $[\alpha,\beta]$ and the correlation structure $\mathbf{V}$, such that the A-optimal design has the form $d^* = \{\alpha, (\alpha+\beta)/2, \beta\}$.

3.1. A-optimal design over the symmetric time interval

The following theorem gives the conditions for the A-optimality of a design in the quadratic growth curve model with correlated observations over the symmetric experimental domain.

Theorem 1.
In the quadratic growth curve model with the correlation structure

$$\mathbf{V} = \begin{pmatrix} 1 & \rho_1 & \rho_3 \\ \rho_1 & 1 & \rho_2 \\ \rho_3 & \rho_2 & 1 \end{pmatrix},$$

where $\rho_i \in (-1,1)$, $i = 1,2,3$, *and* $\mathbf{V}$ *is positive definite, the design* $d^* = \{-\alpha, x^*, \alpha\}$ *with*

$$x^* = \frac{2\left(\sqrt[3]{(1-\rho_2)(1-\rho_1)^2}\right)^2 + (\rho_1-\rho_2)\sqrt[3]{(1-\rho_2)(1-\rho_1)^2} - 2(1-\rho_1)(1-\rho_2)}{(\rho_1+\rho_2-2)\sqrt[3]{(1-\rho_2)(1-\rho_1)^2}}, \tag{5}$$

is A-optimal for each $\alpha > 0$ *if and only if one of the following conditions is satisfied:*

(i) $\rho_3 = \rho_1 + \rho_2 - 1$ *and* $\rho_2 > -\rho_1$,

(ii) $\rho_1 = \rho_2$ *and* $\rho_3 > 2\rho_1^2 - 1$.

Proof. Consider the quadratic growth curve model with time points from the interval $[-1,1]$ and the correlation structure assumed in the theorem. Then the A-optimal design has the form $d^{\#}=\{-1, x^*, 1\}$, with x^* given in (5). We are interested in determining such scale $\alpha>0$ that the design $d^*=\{-\alpha, x^*, \alpha\}$ is also A-optimal. Using the matrix (4) we obtain

$$\operatorname{tr}\left(\mathbf{F}_d^{-1}\right)=\frac{x^4\alpha^2\left[\alpha^2(\rho_3+1)-(\rho_3-1)\right]+x^2\left[(2\alpha^2-1)(\rho_3-1)+\alpha^4(1-2\rho_1-2\rho_2-\rho_3)\right]}{2\alpha^4\left(x^2-1\right)^2}+$$

$$+\frac{2x(\alpha^4+1)(\rho_1-\rho_2)+2\alpha^4-\alpha^2(\rho_3-1)-2\rho_1-2\rho_2+\rho_3+3}{2\alpha^4\left(x^2-1\right)^2}$$

and

$$\frac{d}{dx}\operatorname{tr}\left(\mathbf{F}_d^{-1}\right)=\frac{x^3\left[2\alpha^2(\rho_1+\rho_2)+1+3\alpha^4+(\alpha^4-1)\rho_3\right]+3x^2(\alpha^4+1)(\rho_2-\rho_1)}{\alpha^4\left(x^2-1\right)^3}+$$

$$+\frac{x\left[2(\alpha^4+2)(\rho_1+\rho_2)+7+5\alpha^4-(\alpha^4-1)\rho_3\right]+(\alpha^4+1)(\rho_2-\rho_1)}{\alpha^4\left(x^2-1\right)^3}.$$

We want the design d^* from the theorem to be optimal, so the last expression in the point x^* must be zero. Hence we obtain the condition

$$4(\alpha^4-1)(\rho_1+\rho_2-\rho_3-1)(\rho_1-\rho_2)\cdot W_1(\rho_1,\rho_2)=0,$$

where $W_1(\rho_1,\rho_2)$ is a non-zero expression for each $\rho_i\in(-1,1)$, $i=1,2$, and it holds for each $\alpha\in IR$ if and only if

$$\text{(i) } \rho_3=\rho_1+\rho_2-1 \qquad \text{or (ii) } \rho_1=\rho_2.$$

Thus we have shown that under these conditions there exists an extremum at the point x^*.

(i) Let $\rho_3 = \rho_1 + \rho_2 - 1$. The second derivative of the trace of the inverse of $\mathbf{F}_d$ in x^* can be written as

$$\frac{-3(1+\alpha^4)(\rho_1 - 1)(\rho_1 + \rho_2 - 2)^5 \cdot W_2(\rho_1, \rho_2)}{16\alpha^4(\rho_2 - 1)}$$

with the positive expression $W_2(\rho_1, \rho_2)$, $\rho_i \in (-1, 1)$, $i = 1, 2$, and it can be observed that this second derivative is positive. Thus we have obtained the minimum in x^*.
From the positive-definiteness of $\mathbf{V}$ we obtain $\rho_2 > -\rho_1$.

(ii) Let $\rho_1 = \rho_2$. The second derivative of the trace of the inverse of $\mathbf{F}_d$ in x^* can be written as

$$\frac{7 - 8\rho_1 + \rho_3 + \alpha^4(5 - 4\rho_1 - \rho_3)}{\alpha^4}.$$

Under the assumption of positive-definiteness of $\mathbf{V}$, i.e. $\rho_3 > 2\rho_1^2 - 1$, the positivity of the second derivative can be observed. Hence we have a minimum at the point x^*. ■

Remark 1. *In case (ii) the A-optimal design reduces to the form* $d^* = \{-\alpha, 0, \alpha\}$.

Remark 2. *If neither condition (i) nor (ii) holds, the design* $d^* = \{-\alpha, x^*, \alpha\}$ *is A-optimal if and only if* $\alpha = 1$.

Now we give some examples of correlation structures which satisfy the conditions of Remark 1 and Remark 2. More details about the given correlation structures can be found in Zimmerman and Núñez-Antón (2001) or Filipiak and Szczepańska (2005).

Example

a) For the following correlation structures:

- the nearest neighbor structure NN(1): $\mathbf{V} = \begin{pmatrix} 1 & \rho & 0 \\ \rho & 1 & \rho \\ 0 & \rho & 1 \end{pmatrix}$,

- the first-order autoregression AR(1): $\mathbf{V} = \begin{pmatrix} 1 & \rho & \rho^2 \\ \rho & 1 & \rho \\ \rho^2 & \rho & 1 \end{pmatrix}$,

- the second-order moving average MA(2): $\mathbf{V} = \begin{pmatrix} 1 & \rho_1 & \rho_2 \\ \rho_1 & 1 & \rho_1 \\ \rho_2 & \rho_1 & 1 \end{pmatrix}$,

the A-optimal design has the form $d^* = \{-\alpha, 0, \alpha\}$.

b) For the unstructured antedependence UAD(1):

$$\mathbf{V} = \begin{pmatrix} 1 & \rho_1 & \rho_1\rho_2 \\ \rho_1 & 1 & \rho_2 \\ \rho_1\rho_2 & \rho_2 & 1 \end{pmatrix},$$

the A-optimal design is of the form $d^* = \{-1, x^*, 1\}$ with x^* given in (5).

3.2. A-optimal design of the form $\left\{\alpha, \frac{\alpha+\beta}{2}, \beta\right\}$

In this section we give the form of correlation structure $\mathbf{V}$ and the time interval $[\alpha, \beta]$, for which the design $d^* = \left\{\alpha, \frac{\alpha+\beta}{2}, \beta\right\}$, $\alpha < \beta$, is A-optimal under the quadratic growth curve model.

Proposition 1. *In the quadratic growth curve model with correlation structure*

$$\mathbf{V} = \begin{pmatrix} 1 & \rho_1 & \rho_2 \\ \rho_1 & 1 & \rho_1 \\ \rho_2 & \rho_1 & 1 \end{pmatrix},$$

where $\rho_1 \in (-1, 1)$ *and* $2\rho_1^2 - 1 < \rho_2 < 1$, *the design* $d^* = \left\{\alpha, \frac{\alpha+\beta}{2}, \beta\right\}$ *is A-optimal if and only if* $\beta = -2\alpha$ *or* $\beta = -\alpha$ *(* $\alpha < \beta$ *).*

Proof. Consider the quadratic growth curve model with $\mathbf{V}$ given in Proposition 1 and the time interval $[\alpha, \beta]$. Then the information matrix $\mathbf{C}_d$ has the form (3). The first derivative of the trace of the inverse of the matrix $\mathbf{C}_d$ in $x^* = \frac{\alpha+\beta}{2}$ is of the form

$$\frac{8\left(2\beta + \alpha^2\beta + \alpha\left(2 + \beta^2\right)\right)\left(\rho_2 - 1\right)}{(\alpha - \beta)^4}.$$

It is easy to see that it is equal to zero if and only if $\beta = -2\alpha$ or $\beta = -\alpha$.
The case $\beta = -\alpha$, $\alpha < \beta$, is proved in Theorem 1(ii).
Let $\beta = -2\alpha$, $\alpha < \beta$. Then the second derivative in $x^* = \frac{\alpha+\beta}{2} = -\frac{\alpha}{2}$ is of the form

$$-\frac{64\left[\alpha^4\left(14\rho_1 + 5\rho_2 - 19\right) + \alpha^2\left(8\rho_1 - \rho_2 - 7\right) + 8\rho_1 - \rho_2 - 7\right]}{729\alpha^6}.$$

Since the expression in square brackets is negative for each $\rho_i \in (-1, 1)$, $i = 1, 2$, we have a minimum. ■

Example. For the correlation structures NN(1), AR(1) and MA(2), the design $d^* = \left\{\alpha, -\frac{\alpha}{2}, -2\alpha\right\}$ is A-optimal.

REFERENCES

Filipiak K., A. Szczepańska (2005). A-,D- and E-optimal designs for quadratic and cubic growth curve models with correlated errors. Biom. Lett. 42(1), 43–56.

Garza A. (1954). Spacing of information in polynomial regression. Ann. Math. Statist. 25(1), 123–130.

Liski E.P., Mandal N.K., Shah K.R., B.K. Sinha (2002). Topics in Optimal Designs. Springer, New York.

Luoma A., Mandal N.K., B.K. Sinha (2001). A-optimal cubic and quartic regression designs in asymmetric factor spaces. Stat. Appl. 3, 147–153.

Mandal N.K. (2002). Optimal regression designs in symmetric domains. ISI November 25-29, 23–32.

Markiewicz A. A. Szczepańska (2006). Optimal designs in multivariate linear models. Statist. Probab. Lett. 77, 426–430.

Moerbeek M. (2005). Robustness properties of A-, D-, and E-optimal designs for polynomial growth models with autocorrelated errors. Comput. Statist. Data Anal. 48, 765–778.

Pukelsheim F. (1993). Optimal Designs of Experiments. Wiley, New York.

Zimmerman D.L., V. Núñez-Antón (2001). Parametric modelling of growth curve data: An overview. Test 10, 1–73.