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Equidistant and D-optimal designs for parameters of Ornstein-Uhlenbeck process

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Abstract: In the present paper we provide a thorough study of small sample and asymptotical comparisons of the efficiencies of equidistant designs with taking into account both the parameters of trend θ, as well as the parameters of covariance function r. We concentrate especially to Ornstein-Uhlenbeck processes. If only trend parameters are of interest, the designs covering more-less uniformly the whole design space are rather efficient. We are showing that for all possible combinations of parameters of interest, i.e. $\{\theta\}, \{r\}$ and $\{\theta, r\}$, the interval over which observations are to be made should be extended as far as possible. However doubling the number of observation points in a given interval, when the only parameter θ is of interest and there are already a large number of such points, gives practically no additional estimation information. When $\{r\}$ or $\{\theta, r\}$ are the sets of interest, doubling gives the double information, which is also case of the D-optimal design for r tending to 0. Finally we are proving analytically that n-point equidistant design for parameter θ is D-optimal. Such a result justifies the practise of equidistantly measured returns derived from time series of stock exchange indexes.

Key words and phrases: D-optimal, efficiency, equidistant design, Ornstein-Uhlenbeck process.

1 Introduction

In the present paper we consider the isotropic stationary process

$$Y(x) = \theta + \varepsilon(x)$$

with the design points $x_1, ..., x_N$ taken from a compact design space $\mathcal{X} = [0, l],\ l > 0$. The mean parameter $E(Y(x)) := \theta$ is unknown, the variance-covariance structure $C(d, r)$ depends on another unknown parameter r and d is the distance of a particular design points. Let us define $2\gamma(d) = \mathrm{Var}(Y(s+d) - Y(s))$. The function $2\gamma(d)$ is called *variogram* and $\gamma(d)$ is called *semivariogram* (for more see Banerjee, Carlin and Gelfand (2004, p. 22)). Such process is called in the literature also weak stationary (or second-order stationary), see Cressie (1993, p. 53). We assume that the errors $\varepsilon(x)$ are correlated and the correlation between two measurements depends on the distance through the exponential semivariogram structure $\gamma(d) = 1 - e^{-rd}$. An exact design $\xi = \{x_1, ..., x_n\}$ allows the experimenter to plan where to measure the process to optimize a certain measure of variance of estimators. For optimal design in spatial case see Müller (2001, Chap. 5). In this paper we consider entirely 1-dimensional design space.

We can find applications of various criteria of design optimality for second-order models in the literature. Here we consider D-optimality, which corresponds to the maximization of criteria function $\Phi(M) = \det M$, the determinant of a standard Fisher information matrix. This method, "plugged" from the widely developed uncorrelated setup, is offering considerable potential for automatic implementation, although further development is needed before it can be applied routinely in practice. Theoretical justifications for using the Fisher information for D-optimal designing under correlation can be found in Abt and Welch (1998) and Pázman (2004). Abt and Welch (1998) considered a design space $\mathcal{X} = [0, 1]$ with the correlation function of the form $cov(Y(x), Y(x + d)) = \sigma^2 e^{-rd}$. They shown that $\lim_{n\to+\infty} (M^{-1}(r, \sigma^2))_{1,1} = 0$ and $\lim_{n\to+\infty} n\, (M^{-1}(r, \sigma^2))_{1,1} = 2(r\sigma^2)^2$. These results obtained from the information matrix coincide with the variance of the asymptotic distribution of $\sqrt{n}(\hat{r}\hat{\sigma}^2 - r\sigma^2)$ found in Ying (1993), based on approximations of the log-likelihood function.

Zhu and Stein (2005) use the simulations (under Gaussian random field and Matérn covariance) to study whether the inverse Fisher information matrix is a reasonable approximation of the covariance matrix of maximal likelihood (ML) estimators as well as a reasonable design criterion. For more references on the Fisher information as design criterion in the correlated setup see e.g. Stehlík (2007). Therein is studied the structure of the Fisher's information matrices for stationary process. Stehlík (2007) showed that under the mild conditions given on covariance structures the lower bound for $M_\theta(k)$ is an increasing function of the distances between the design points. Particularly this supports the idea of increasing domain asymptotics. If only trend parameters are of interest, the designs covering uniformly the whole design space are very efficient. The similar observation has been made by recent paper by Dette, Kunert and Pepelyshev in a more general framework. They proved that if $r \to 0$, then any exact n-point D-optimal design in the linear regression model with exponential semivariogram converges to the equally spaced design. A recurring topic in the recent literature is that uniform or equi-spaced designs perform well in terms of model-robustness when a Bayesian approach is adopted, when the maximum bias is to be minimized or when the minimum power of the lack-of-fit test is to be maximized (see Goos, Kobilinsky, O'Brien and Vandebroek (2005)). However, the equidistant design is easy to construct in the case of a single experimental variable. When more than one variable is involved in an experiment and the number of observations available is small, it becomes much more difficult to construct these type of designs. Uniform design is a kind of space-filling design whose applications in industrial experiments, reliability testing and computer experiments is a novel endeavor. The concept of uniform designs was introduced by Fang (1978) and has now gained popularity and proven to be very successful in industrial applications (see Pham (2006, Chap. 13)).

Hoel (1958) considered the weighted least square estimates and using the generalized variance as criterion for the efficiency of estimation. Some results are obtained on the increased efficiency arising from doubling the number of equally spaced observation points when the total interval is fixed or when it is doubled. The asymptotical comparison is made for three cases of covariance structures. As is pointed out the asymptotic measures of estimation efficiency obtained may not be very realistic for small samples. However, Hoel (1958) is considering the only trend parameters as the parameters of interest. In principle one can identify two sets of parameters of interest: one describing the trend and the second one describing the covariance functions.

In the present paper we provide a thorough study of small sample and asymptotical comparisons of the efficiencies with taking into account both the parameters of trend as well as the parameters of covariance function. We will demonstrate the substantial differences between the cases when only trend parameters are of interests and when the whole parameter set is of interest. The paper is organized as follows. In the section 2 the recurrent relations for the Fisher information $M_\theta(n)$ about the trend parameter θ and for the Fisher information $M_r(n)$ about the covariance parameter r are derived. These formulas are used to establish the small and large sample comparisons of the efficiencies. In the section 3 D-optimal designs are derived. Therein we are proving that an equidistant design is D-optimal for the trend parameter θ. To maintain the continuity of the explanation the proofs are included into the Appendix.

2 Equidistant designs

2.1 Recurrent relations for $M_\theta(n)$ and $M_r(n)$

In the proposed model we have Fisher information matrices

$$M_\theta(n) = 1^T C^{-1}(r)\, 1$$

and (see Pázman (2004) and Xia, Miranda and Gelfand (2006))

$$M_r(n) = \frac{1}{2} tr \left\{ C^{-1}(r) \frac{\partial C(r)}{\partial r} C^{-1}(r) \frac{\partial C(r)}{\partial r^T} \right\}.$$

So for both parameters of interest we have $M(n)(\theta, r) = \begin{pmatrix} M_\theta(n) & 0 \\ 0 & M_r(n) \end{pmatrix}$.

Theorem 1 *Let us consider an equidistant n-point design with $d = x_{i+1} - x_i$. Then*

$$M_\theta(n) = \frac{2 - n + ne^{rd}}{1 + e^{rd}}$$

and

$$(n-1)M_r(2) = M_r(n), \;\; M_r(2) = d^2 \frac{e^{2rd} + 1}{(e^{2rd} - 1)^2} \tag{1}$$

holds. The D-criterion $\Phi(M) = \det M$ for both parameters r, θ has the form

$$\Phi_n(M) = \frac{(n-1)(ne^{rd} + 2 - n)d^2(1 + e^{2rd})}{(1 + e^{rd})(e^{2rd} - 1)^2}.$$

One can find a nice geometrical interpretation of (1) firstly proposed as conjecture in Stehlík (2006). Let us imagine that design points (vertexes) are connected with edges and constitute a simple tree (from Graph Theory, see e.g. Foulds (1992, Chap. 3)), such that all vertices besides the first one and the last one have the degree two. Then adding another design point adds one edge. So the information relation (1) has a direct graphical representation and interpretation. However, we did not find any simple interpretation of behavior of the ratios $\frac{M_\theta(n)}{M_\theta(n-1)}$ and $\frac{\Phi_n(M)}{\Phi_{n-1}(M)}$. We see, that for $r \to 0$ we have

$$\frac{\Phi_n(M)}{\Phi_{n-1}(M)} = \frac{n-1}{n-2} = \frac{M_r(n)}{M_r(n-1)}$$

and $\frac{M_\theta(n)}{M_\theta(n-1)} = 1$. This supports the observed fact that the D-optimal designs are mainly influenced by the parameters of covariance functions, at least when the trend has a linear form. In fact, the limit $r \to 0$ is modeling the maximally correlated case and Dette, Kunert and Pepelyshev (see Theorem 3.6 therein) were proved that in such a case the exact n-point D-optimal design in the linear regression model with exponential covariance converges to the equally spaced design. For $d \to +0$ we obtain the same behavior.

When $n \to +\infty$ we obtain the intuitive convergence of all three fractions to 1, since no more information is added in these cases by additional observation when the number of observations becomes infinite.

We can see the limits of increasing domain asymptotics under the equidistant design for $d \to +\infty$. The highest rate of increase of information has $\Phi_n(M)$,

$$\frac{\Phi_n(M)}{\Phi_{n-1}(M)} = \frac{n}{n-2},$$

since the both information on θ and r are increasing with n,

$$\frac{M_r(n)}{M_r(n-1)} = \frac{n-1}{n-2}, \; \frac{M_\theta(n)}{M_\theta(n-1)} = \frac{n}{n-1}.$$

The interesting feature of the estimation of both of the parameters $\{\theta, r\}$ is that there exist D-optimal equidistant design with finite $d^\star > 0$ when $n > 3$. This is not a case when the only r is estimated parameter, since the function $d \to M_r(2)$ is strictly decreasing and thus the D-optimal design is collapsing. However for $n = 2, 3$ the collapsing should be compensated by a so called nugget effect (see Stehlík, Rodríguez-Díaz, Müller and López-Fidalgo). The following Theorem gives the procedure how to compute the D-optimal distance $d^\star$ numerically when $n > 3$.

Theorem 2 *In the case when both parameters θ, r are of interest and $n > 3$, the D-optimal distance $d^\star > 0$ is the positive solution of the equation*

$$-rd = \frac{-e^{-5rd}(n-2) + ne^{-4rd} - e^{-rd}(2-n) - n}{e^{-4rd}(n-1) + e^{-3rd}(7-4n) + e^{-2rd}(4n-1) + e^{-rd}(3-2n) + n}. \tag{2}$$

2.2 Comparisons of equally spaced designs

Hoel (1958) provided asymptotical comparisons made for equally spaced sets of points. The sets of points that he selected for consideration were the following:

(a) n equally spaced points in the interval $(0, l)$
(b) $2n$ equally spaced points in the interval $(0, l)$
(c) $2n$ equally spaced points in the interval $(0, 2l)$
(d) two sets of observations of type (a)

A comparison of the relative advantage of choices (b), (c) and (d) over (a) were made by comparing their generalized variances. Letting d denote the interval length between the consecutive x values, i.e. $d = x_{i+1} - x_i$, these generalized variances will be denoted by $M_\theta^{-1}(n, d), M_\theta^{-1}(2n, d/2), M_\theta^{-1}(2n, d)$ and $M_\theta^{-1}(2\ runs)$, respectively. For comparison purposes we use the ratios introduced by Hoel (1958), i.e. in our notation they are:

$$R_1 = \left[\frac{M(n,d)}{M(2n,d/2)}\right]^{-1}$$
$$R_2 = \left[\frac{M(n,d)}{M(2n,d)}\right]^{-1}$$
$$R_3 = \left[\frac{M(n,d)}{M(m\ runs)}\right]^{-1}.$$

These ratios are used in the three cases,

(A) when the only trend parameter θ is estimated

(B) when the only correlation parameter r is estimated

(C) when the both parameters (θ, r) are estimated. Thus the ratios are denoted by $R_i(\theta), R_i(r)$ and $R_i(\theta, r)$, respectively. We denote by $R_i^*(\theta), R_i^*(r), R_i^*(\theta, r)$ the limits of $R_i(\theta), R_i(r)$ and $R_i(\theta, r)$ for $n \to +\infty$.

The comparison of efficiencies is in a good coherence with two main current asymptotical frameworks, increasing domain asymptotics and infill asymptotics, for obtaining limiting distributions of maximum likelihood estimators of covariance parameters in Gaussian spatial models with or without a nugget effect. These limiting distributions differ in some cases. Zhang and Zimmerman (2005) have investigated the quality of these approximations both theoretically and empirically. They have found, that for certain consistently estimable parameters of exponential covariograms approximations corresponding to these two frameworks perform about equally well. For those parameters that cannot be estimated consistently, however, the infill asymptotics is preferable. They have also observed, that the Fisher information appears to be a compromise between the infill asymptotic variance and the increasing domain asymptotic variance. For exponential variogram some infill asymptotic justification can be found in Zhang and Zimmerman (2005). In our comparison, doubling the design points in the fixed-length interval corresponds to the infill asymptotics whereas doubling the design points with the fixed neighbor distances corresponds to the increasing domain asymptotics.

Theorem 3 *We have*

$$R_1(\theta) = \frac{(1+e^{rd})}{(1+e^{\frac{rd}{2}})} \frac{(2+2n(-1+e^{\frac{rd}{2}}))}{(2+n(-1+e^{rd}))}, \ R_1^*(\theta) = \frac{2(1+e^{rd})}{(1+e^{\frac{rd}{2}})^2}. \tag{3}$$

$$R_2(\theta) = \frac{2(1-n+ne^{rd})}{2-n+ne^{rd}}, \ R_2^*(\theta) = 2. \tag{4}$$

$$R_1(r) = \frac{(2n-1)(1+e^{-rd})^3}{4(n-1)(1+e^{-2rd})e^{-rd}}, \ R_1^*(r) = \frac{(1+e^{rd})^3}{2(1+e^{2rd})}. \tag{5}$$

$$R_2(r) = \frac{2n-1}{n-1}, \ R_2^*(r) = 2. \tag{6}$$

$$R_1(\theta, r) = \frac{(2n-1)(1+e^{-rd})^3(1-n+ne^{\frac{rd}{2}})(1+e^{rd})}{2(n-1)(1+e^{-2rd})(1+e^{\frac{rd}{2}})e^{-rd}(2-n+ne^{rd})}, \tag{7}$$

$$R_1^*(\theta, r) = \frac{(1+e^{rd})^4}{e^{3rd}+2e^{\frac{5rd}{2}}+e^{2rd}+e^{rd}+2e^{\frac{rd}{2}}+1}. \tag{8}$$

$$R_2(\theta, r) = \frac{(2-n+ne^{rd})(n-1)}{(1-n+ne^{rd})(2n-1)}, \; R_2^*(\theta, r) = 4. \tag{9}$$

Results (3) and (4) correspond to the results in Hoel (1958, p. 1141). For instance, considering the numerical value $e^{-rd} = 0.64$ (i.e. correlation coefficient between neighboring y values is 0.64) we have $R_1^*(\theta) = 1.01$. Thus doubling the number of observation points in a given interval, when the only parameter θ is of interest and there are already a large number of such points, gives practically no additional estimation information, which is in accord with the conclusions of Hoel (1958). However, doubling the number of observation points in a given interval gives two times higher information in the case when r or $\{\theta, r\}$ are the parameters of interest and $r \to +0$, since $R_1^*(r) = R_1^*(\theta, r) \to 2$ for $r \to +0$. This is the case when any exact n-point D-optimal design in the linear regression model with exponential semivariogram converges to the equally spaced design. Thus we can conclude that also for the D-optimal design (for $r \to +0$) doubling the number of observation points in a given interval gives a double information. The value of $R_2^*(\theta)$ shows that the same asymptotic efficiency is gained here as in the case of uncorrelated variables. It is clear, that for all possible combinations of parameters of interest, i.e. $\{\theta\}, \{r\}$ and $\{\theta, r\}$, the interval over which observations are to be made should be extended as far as possible, since $R_2^*(\theta) = R_2^*(r) = 2$ and $R_2^*(\theta, r) = 4$.

Let us derive the limits of increasing domain asymptotics under the equidistant design for $d \to +\infty$. We have

$$\lim_{d\to+\infty} R_1^*(\theta) = \lim_{d\to+\infty} R_1(\theta) = \lim_{d\to+\infty} R_2^*(\theta) = \lim_{d\to+\infty} R_2(\theta) = 2$$

which again justifies that the interval over which observations are to be made should be extended as far as possible.

3 D-optimal designs

The information matrix $M_\theta(2)$ has the form $\frac{2e^{rd}}{1+e^{rd}}$ and this is increasing function of d. Thus the optimal design is the maximal distant. If we consider three-point-design in Stehlík (2004) is proved, that the design $\{-1, 0, 1\}$ is D-optimal, when the design space is $[-1, 1]$. However the proof is more general and actually is proving that for general design space $[a, b]$ is an equidistant three point design D-optimal. Let us consider 4-point design. Employing the exchange algorithm Stehlík (2004) has checked that the D-optimum design is the equidistant one (on the design space $[-1, 1]$) and the D-optimum design information is $M = 1.964538$. Due to the knowledge of the analytical form of the information one can employ also Lipschitz and continuous optimization (see Horst and Tuy (1996)), which can be implemented like a net-searching algorithm. The only problem of such an algorithm is its time complexity.

The Fisher information in the case of 5-point design has much more complicated form and can be found in Stehlík (2006). Therein we have computationally obtained that the D-optimal design is equidistant with $d_1 = d_2 = d_3 = d_4 = 1/2$ and has information $M = 1.979674635$ (note, that information is increasing with number of design points). The following theorem provides analytical verification of obtained numerical observations.

Theorem 4 *The equidistant design for parameter θ is D-optimal.*

This theorem is extension of the Theorem 3.6 in Dette, Kunert and Pepelyshev. Therein is proved, that for $r \to 0$ the exact n-point D-optimal design in the linear regression model with exponential covariance converges to the equally spaced design.

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4 Appendix

Proof of Theorem 1 The covariance matrix and its inverse have the forms (here $x = e^{-rd}$, see also Hoel (1958, p. 1140)

$$C(n,r) = \begin{pmatrix} 1 & x & x^2 & \dots & x^{n-1} \\ x & 1 & x & \dots & x^{n-2} \\ \vdots & \vdots & \vdots & & \vdots \\ x^{n-1} & x^{n-2} & x^{n-3} & \dots & 1 \end{pmatrix},$$

$$C(n,r)^{-1} = \frac{1}{1-x^2} \begin{pmatrix} 1 & -x & 0 & \dots & 0 & 0 \\ -x & 1+x^2 & -x & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \dots & -x & 1 \end{pmatrix}.$$

Furthermore, we have

$$\frac{\partial C(n,r)}{\partial r} = \begin{pmatrix} 0 & -xd & -2x^2d & \dots & (1-n)x^{n-1}d \\ -xd & 0 & -xd & \dots & (2-n)x^{n-2}d \\ \vdots & \vdots & \vdots & & \vdots \\ (1-n)x^{n-1}d & (2-n)x^{n-2}d & (3-n)x^{n-3}d & \dots & 0 \end{pmatrix}.$$

Finally we have

$$M_r(n) = (n-1)d^2 \frac{e^{2rd}+1}{(e^{2rd}-1)^2} = (n-1)M_r(2),$$

since $M_r(2) = d^2 \frac{e^{2rd}+1}{(e^{2rd}-1)^2}$ (see Stehlík (2007)) and

$$M_\theta(n) = 1^T C^{-1}(n,r)\,1 = \frac{2-n+ne^{rd}}{1+e^{rd}}.$$

□

Proof of Theorem 2 Let us have $n = 2$. Then in Stehlík (2004) is proved that the two-point design for both parameters θ, r is collapsing, i.e. the maximal information is gained for $d = 0$.

Let us consider $n = 3$. Then

$$\frac{\partial M_{r,\theta}(3)}{\partial d} = \frac{-4d\left(rd\left[3e^{5rd} - 3e^{4rd} + 11e^{3rd} - 5e^{2rd} + 2e^{rd}\right] - 3e^{5rd} + 3e^{rd} + e^{4rd} - 1\right)}{(1+e^{rd})(e^{2rd}-1)^3}.$$

Thus we have to solve $4d = 0$ or

$$rd\left[3e^{5rd} - 3e^{4rd} + 11e^{3rd} - 5e^{2rd} + 2e^{rd}\right] - 3e^{5rd} + 3e^{rd} + e^{4rd} - 1 = 0.$$

We have the only solution $d = 0$.

Finally, let us consider $n > 3$. For all $r > 0$ is the function $d \to \det M(n)(\theta, r)$ continuous and differentiable at $(0, +\infty)$. Let us consider the solutions

$$d \in [0, +\infty) : \frac{\partial \det M(n)(\theta, r)}{\partial d} = \frac{2(n-1)de^{-rd}V(d)}{(e^{rd}+1)^2(e^{-2rd}-1)^3} = 0. \tag{1}$$

A thorough analysis of (1) shows, that there exist one trivial solution $d = 0$ and the nontrivial $d^* \in (0, +\infty)$ one, such that $V(d^*) = 0$. Finally we obtain the implicit equation (2) to compute the d^*.

Now let us prove that there exist a non-trivial solution of implicit equation (2) for each $n > 3$. Indeed, $V(d) = rd - T(rd)$, where

$$T(x) = \frac{(e^x+1)(e^x-1)(e^{2x}+1)(ne^x+2-n)}{e^x\left(ne^{4x} + e^{3x}(3-2n) + e^{2x}(4n-1) + e^x(7-4n) + n - 1\right)}.$$

Thus $V(x)$ is vanishing iff $T(x)$ has a fixed point, or equivalently $T(x) - x = 0$. We have $T(0) = 0$, $T(x)$ is continuous and for all $n > 3$ we have $\lim_{x\to+\infty} -T(x) + x = +\infty$. It is sufficient to find x_n for every $n > 3$ such that $-T(x_n) + x_n < 0$. Let us take $x_n = 0.1, n > 3$. Then we have

$$-T(x_n) + x_n = -\frac{10^{-10}\,(0.1054993192\,10^{18}\,n - 0.3319711520\,10^{18})}{0.128517221\,10^9\,n + 0.4782185045\,10^{10}} < 0$$

for $n > 3$. This completes the proof.

□

Proof of Theorem 3 It is easy to see that $R_1^{\star}(\theta) = \frac{2(1+e^{rd})}{(1+e^{\frac{rd}{2}})^2}$ is strictly increasing at $d \in (0, +\infty)$, and $\lim_{d\to0} R_1^*(\theta) = \lim_{d\to0} R_1(\theta) = 1$.

We have $\lim_{d\to0} R_2(\theta) = 1$, $\lim_{d\to+\infty} R_2^*(\theta) = \lim_{d\to+\infty} R_2(\theta) = 2$.

We have $\lim_{d\to0} R_1(r) = \frac{2n-1}{n-1}$, $\lim_{d\to\infty} R_1(r) = \infty$, $\lim_{d\to0} R_1^*(r) = 2$, $\lim_{d\to\infty} R_1^*(r) = \infty$. The both functions, $R_1(r), R_1^*(r)$ are strictly increasing at $d \in (0, +\infty)$.

Function $R_2(\theta, r)$ is strictly increasing at $d \in (0, +\infty)$ and $\lim_{d\to\infty} R_2(\theta, r) = \frac{4n-2}{n-1}$, $\lim_{d\to0} R_2(\theta, r) = \frac{2n-1}{n-1}$. We have $\lim_{d\to+\infty} R_1(\theta, r) = \lim_{d\to+\infty} R_1^*(\theta, r) = +\infty$.

□

Proof of Theorem 4

Let us consider $n \leq 5$. Denote $d_i = x_{i+1} - x_i, q_i = e^{-rd_i}$. We have

$$C(n,r) = \begin{pmatrix} 1 & q_1 & q_1q_2 & q_1q_2q_3 & \dots & \dots & \prod_{i=1}^{n-1} q_i \\ q_1 & 1 & q_2 & q_2q_3 & \dots & \dots & \prod_{i=2}^{n-1} q_i \\ q_1q_2 & q_2 & 1 & q_3 & \dots & \dots & \prod_{i=3}^{n-1} q_i \\ q_1q_2q_3 & q_2q_3 & q_3 & 1 & \dots & \dots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \ddots & & \vdots \\ \vdots & \vdots & \vdots & \vdots & & \ddots & q_{n-1} \\ \prod_{i=1}^{n-1} q_i & \prod_{i=2}^{n-1} q_i & \prod_{i=3}^{n-1} q_i & \dots & \dots & q_{n-1} & 1 \end{pmatrix}$$

and

$$C(n,r)^{-1} = \begin{pmatrix} \frac{1}{1-q_1^2} & \frac{q_1}{q_1^2-1} & 0 & 0 & \dots & \dots & 0 \\ \frac{q_1}{q_1^2-1} & V_2 & \frac{q_2}{q_2^2-1} & 0 & \dots & \dots & 0 \\ 0 & \frac{q_2}{q_2^2-1} & V_3 & \frac{q_3}{q_3^2-1} & \dots & \dots & 0 \\ 0 & 0 & \frac{q_3}{q_3^2-1} & V_4 & \dots & \dots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \ddots & & \vdots \\ \vdots & \vdots & \vdots & \vdots & & V_{n-1} & \frac{q_{n-1}}{q_{n-1}^2-1} \\ 0 & 0 & 0 & \dots & \dots & \frac{q_{n-1}}{q_{n-1}^2-1} & \frac{1}{1-q_{n-1}^2} \end{pmatrix},$$

where $V_k = \frac{1-q_k^2q_{k-1}^2}{(q_k^2-1)(q_{k-1}^2-1)}$, $k = 2, \dots, n-1$. Thus we have

$$-M_\theta(n) = \frac{2q_1 - 1}{1 - q_1^2} + \frac{-1}{1 - q_{n-1}^2} - \sum_{i=2}^{n-1} \left[\frac{2q_i}{q_i^2 - 1} + \frac{1 - q_i^2 q_{i-1}^2}{(q_i^2 - 1)(q_{i-1}^2 - 1)} \right].$$

The minus of gradient is

$$-\nabla\Phi_\theta(M) = (2/(q_1 + 1)^2, ..., 2/(q_i + 1)^2, .., 2/(q_{n-1} + 1)^2).$$

Thus function $\Phi_\theta(M)$ is increasing in all coordinates d_i with the same speed and the maximum condition is $d_i = l/(n-1)$, where l is the length of the design interval. The analysis of Hesse matrices under the optimality condition $d_i = l/(n-1)$ shows that an equidistant design is the D-optimal for the parameter θ.

□

References

Abt, M. and Welch, W.J. (1998). Fisher information and maximum-likelihood estimation of covariance parameters in Gaussian stochastic processes. *The Canadian Journal of Statistics*, Vol. **26**, No. 1, 127-137.

Banerjee, S., Carlin, B. and Gelfand, A. (2004). *Hierarchical Modeling and Analysis for Spatial Data*, Chapman & Hall/CRC.

Cressie, N.A.C. (1993). *Statistics for Spatial Data*, 2nd ed., New York: Wiley.

Dette, H., Kunert, J. and Pepelyshev, A. Exact optimal designs for weighted least squares analysis with correlated errors, accepted to *Statistica Sinica*.

Fang, K.T. (1978). Uniform design: application of number-theoretic methods in experimental design, *Prob. Stat. Bull.* **1**, 56-97.

Foulds, L.R. (1992). *Graph Theory Applications*, Springer Verlag, New York, Inc., 17-19.

Goos, P., Kobilinsky, A., O'Brien, T. E. and Vandebroek, M. (2005). Model-robust and model-sensitive designs, *Computational Statistics & Data Analysis* **49**, 201-216.

Hoel, P.G. (1958). Efficiency Problems in Polynomial Estimation. *Annals of Math. Statistics* **29**, 1134-1145.

Horst, R. and Tuy, H. (1996). *Global Optimization - Deterministic Approaches*, Springer.

Müller, W.G. (2001). *Collecting Spatial Data*, 2nd edition, Physica Verlag.

Pázman, A. (2004). Correlated optimum design with parametrized covariance function: Justification of the use of the Fisher information matrix and of the method of virtual noise, *Report # 5*, *Research Report Series*, Department of Statistics and Mathematics, Wirtschaftsuniversität Wien.

Pham, H. (Editor) (2006). *Springer Handbook of Engineering Statistics*, Springer Verlag, London, Chapter 13, 229-247.

Stehlík, M. (2004). Some Properties of D-optimal Designs for Random Fields with Different Variograms, *Report #4 Research Report Series*, Department of Statistics and Mathematics, Wirtschaftsuniversität Wien.

Stehlík, M. (2006). Some Properties of Exchange Design Algorithms Under Correlation, Working Paper Nr. 28, WU Wien: *Research Report Series*/ Department of Statistics and Mathematics.

Stehlík, M. (2007). D-optimal designs and equidistant designs for stationary processes, *mODa 8* (Model Oriented Design and Analysis Conference) *Proceedings* (Springer Verlag), Almagro, Spain, 4th-8th June 2007, 205-211.

Stehlík, M., Rodríguez-Díaz, J.M., Müller, W.G. and López-Fidalgo, J. (2008) Optimal allocation of bioassays in the case of parametrized covariance functions: an application in lung's retention of radioactive particles, *TEST* 17: 56–68.

Xia, G., Miranda, M.L. and Gelfand, A.E. (2006). Approximately optimal spatial design approaches for environmental health data, *Environmetrics*, **17**: 363-385.

Ying, Z. (1993). Maximum Likelihood Estimation of Parameters under a Spatial Sampling Scheme, *The Annals of Statistics*, Vol. **21**, No. 3, 1567-1590.

Zhu, Z. and Stein, M.L. (2005). Spatial sampling design for parameter estimation of the covariance function, *Journal of Statistical Planning and Inference*, vol. **134**, no 2, 583-603.

Zhang, H. and Zimmerman, D. (2005). Towards reconciling two asymptotic frameworks in spatial statistics, *Biometrika*, vol. **92**, no 4: 921-936.