Optimal designs for parameters of shifted Ornstein-Uhlenbeck sheets measured on monotonic sets

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Abstract

Measurement on sets with a specific geometric shape can be of interest for many important applications (e.g., measurement along the isotherms in structural engineering). The properties of optimal designs for estimating the parameters of shifted Ornstein-Uhlenbeck sheets are investigated when the processes are observed on monotonic sets. For Ornstein-Uhlenbeck sheets monotonic sets relate well to the notion of non-reversibility. Substantial differences are demonstrated between the cases when one is interested only in trend parameters and when the whole parameter set is of interest. The theoretical results are illustrated by simulated examples from the field of structure engineering. From the design point of view the most interesting finding of the paper is the possible loss of efficiency of the regular grid design compared to the optimal monotonic design.

Keywords: D-optimality, equidistant design, monotonic sets, optimal design, Ornstein-Uhlenbeck sheet.

1. Introduction

Measurement on sets with a specific geometric shape is of interest for many important applications, e.g., measurement along the isotherms. Starting with the fundamental work of Hoel (1958), the central importance of equidistant designs for the estimation of parameters of correlated processes has been realized. Hoel (1958) compared the efficiencies of equally spaced designs for one-dimensional polynomial models for several design regions and correlation structures. In this context by a design we mean a set $\boldsymbol{\xi} = \{x_1, x_2, \ldots, x_n\}$ of locations where the investigated process is observed. A comparison in a multi-dimensional setup including correlations can be found, e.g., in Herzberg and Huda (1981). Later Kiseľák and Stehlík (2008) proved that equidistant design is optimal for estimating the unknown mean parameter of an Ornstein-Uhlenbeck (OU) process, whereas Zagoraiou and Baldi Antognini (2009) also studied shifted stationary OU

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processes. However, in all above mentioned papers on optimal design for OU processes the design regions were intervals of the real line, but a one-dimensional interval is naturally a directed set induced by the total ordering of the real numbers. Obviously, there is a big difference in geometry between a plane and a line and thus OU sheets sampled on two-dimensional intervals provide much more delicate design strategies. In the present work we derive optimal exact designs for parameters of a shifted OU sheet measured in the points constituting a *monotonic set.* A monotonic set can be defined in arbitrary Hilbert space H, with real or complex scalars. For $x, y \in H$, we denote by $\langle x, y\rangle$ the real part of the inner product. A set $E \subset H \times H$ is called monotonic (see Minty (1963) and references therein) if for all $(x_1, y_1), (x_2, y_2) \in E$ we have $\langle x_1 - x_2, y_1 - y_2\rangle \geq 0$. A practical example of such a set are measurements on isotherms of a stationary temperature field with several applications in thermal slab modelling (see, e.g., Babiak et al. (2005)). Another important example in which monotonic measurements appear is motivated by measuring of methane adsorption (Lee and Weber, 1969) where keeping all measurements at isotherm decreases the problems connected to stability. Here we consider the following version of a monotonic set:

Condition D *The potential design points* $\big\{(s_1, t_1), (s_2, t_2), \ldots, (s_n, t_n)\big\} \subset \mathcal{X},\ n \in \mathbb{N}$*, where* $\mathcal{X}$ *denotes a compact design space, satisfy* $0 < s_1 < s_2 < \ldots < s_n$ *and* $0 < t_1 < t_2 < \ldots < t_n$*.*

We remark that the same observation scheme is used in Baran et al. (2013) where the authors deal with prediction of OU sheets and derive optimal designs with respect to integrated mean square prediction error and entropy criteria. *Condition D* relates the geometry of the underlying set of points to the Markovian properties of OU sheets and corresponding Fisher information matrices. This geometry has direct connection with the interpretation of OU sheet diffusion. Standard diffusion is *non-reversible*, and the heat partial differential equation is not time-reversible. Thus, in some realistic physical situations we cannot step back in time. In thermodynamics, a reversible process is a process that can be “reversed” by means of infinitesimal changes in some property of the system without entropy production (i.e., dissipation of energy, see, e.g., Sears and Salinger (1986)). There exists a “reversible diffusion”, which is a specific example of a reversible stochastic process, having an elegant characterization due to Kolmogorov (1937). Thus, statistician shall decide, whether the process to be modelled is reversible. If not, for estimating parameters of an OU sheet it is better to consider a design satisfying *Condition D.* We understand that this does not necessarily cover all applications, but it is interesting for some of them.

We do not claim that monotonic set designs should be used routinely in engineering practice. The aim of our paper is merely to show that for an OU sheet, in some scenarios, monotonic curve could provide better efficiency than simple grid designs. Therefore, the experimenter is advised to integrate carefully the monotonic set design into his/her portfolio of candidate designs – especially in cases when there is a strong intuition/justification of the Markovian nature of the process. Being more particular, it is often overseen in practice, that information increases with the number of points only in the case of independence (or specific form of dependence). Thus, general filling designs, generated without further caution, may increase the variance instead of information. For a classical example see, e.g., Smit (1961). Another discussion of designing for correlated processes in the context of space filling and its limitations can be found in Müller and Stehlík (2009) and Pronzato and Müller (2012).

The paper is organized as follows. In this section we introduce the model to be studied and our notations. We also deal with an example which motivates the present study, namely, a design experiment for measuring on isotherms of a stationary thermal field. Sections 2, 3, and 4 deal with the optimal designs for the estimation of parameters of our model. We demonstrate the substantial differences between the cases when one is interested only in the trend parameter and when the whole parameter set is of interest. Section 5 contains an application, whereas to maintain the continuity of the explanation, the proofs are given in the Appendix.

1.1. Statistical Model

Consider the stationary process

$$Y(s,t) = \theta + \varepsilon(s,t) \tag{1.1}$$

with design points taken from a compact design space $\mathcal{X} = [a_1, b_1] \times [a_2, b_2]$, where $b_1 > a_1$ and $b_2 > a_2$ and $\varepsilon(s,t),\ s,t \in \mathbb{R}$, is a stationary Ornstein-Uhlenbeck sheet, that is a zero mean Gaussian process with covariance structure

$$\mathsf{E}\,\varepsilon(s_1,t_1)\varepsilon(s_2,t_2) = \frac{\widetilde{\sigma}^2}{4\alpha\beta}\exp\big(-\alpha|t_1-t_2| - \beta|s_1-s_2|\big), \tag{1.2}$$

where $\alpha > 0,\ \beta > 0,\ \widetilde{\sigma} > 0$. We remark that $\varepsilon(s,t)$ can also be represented as

$$\varepsilon(s,t) = \frac{\widetilde{\sigma}}{2\sqrt{\alpha\beta}}\mathrm{e}^{-\alpha t - \beta s}\mathcal{W}\big(\mathrm{e}^{2\alpha t}, \mathrm{e}^{2\beta s}\big),$$

where $\mathcal{W}(s,t),\ s,t \in \mathbb{R}$, is a standard Brownian sheet (Baran et al., 2003; Baran and Sikolya, 2012), i.e., a centered Gaussian random field with covariances $\mathsf{E}\,\mathcal{W}(s_1,t_1)\mathcal{W}(s_2,t_2) = \min(s_1,s_2)\cdot\min(t_1,t_2)$. Covariance structure (1.2) implies that for $\mathbf{d} = (d,\delta),\ d \geq 0,\ \delta \geq 0$, the variogram $2\gamma(\mathbf{d}) := \mathsf{Var}\big(\varepsilon(s_1,t_1) - \varepsilon(s_2,t_2)\big) = \frac{\widetilde{\sigma}^2}{2\alpha\beta}\Big(1 - \mathrm{e}^{-\alpha d - \beta\delta}\Big)$, where now $|s_1 - s_2| = d,\ |t_1 - t_2| = \delta$, and the correlation between two measurements depends on the distance through the semivariogram $\gamma(\mathbf{d})$.

In order to apply the usual approach for design in spatial modeling (Kiseľák and Stehlík, 2008) we introduce $\sigma := \widetilde{\sigma}/(2\sqrt{\alpha\beta})$ and instead of (1.2) we investigate

$$\mathsf{E}\,\varepsilon(s_1,t_1)\varepsilon(s_2,t_2) = \sigma^2\exp\big(-\alpha|t_1-t_2| - \beta|s_1-s_2|\big), \tag{1.3}$$

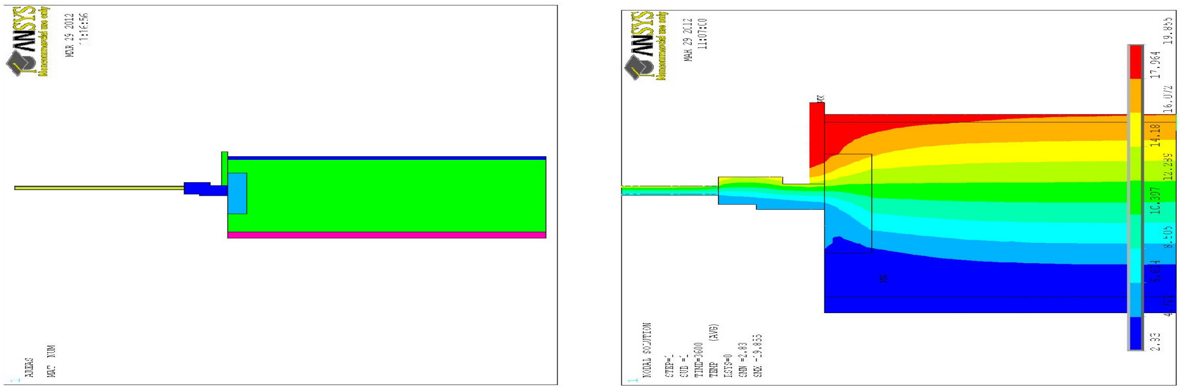
where σ is considered as a nuisance parameter. In an uncorrelated model the parameter σ influences neither the estimation of the mean value parameters, nor the optimal design. In the present paper we assume σ to be known but a valuable direction for the future research will be the investigation of models with unknown nuisance parameter σ. Moreover, the assumption of known σ is reasonable when α and β are known as well. For most of the realistic situations, where the parameters of the correlation structure are not known, there is no optimal design, as we show, e.g., in Sections 3 and 4. However, we think that all recent developments on optimal design strategies for estimation of parameters should mostly be considered as benchmarks in more realistic setups for optimal design (e.g., like geometric progression ones, as discussed in Section 4, or in Zagoraiou and Baldi Antognini (2009) for a one-dimensional design space). These benchmarks should always be confronted directly with a subject science, e.g., with methane modelling with the help of the modified Arrhenius model in Rodríguez-Díaz et al. (2012). Nevertheless, form (1.3) of the covariance structure is more suitable for statistical applications, while (1.2) fits better to probabilistic modelling. Further, we require *Condition D* to be hold on the design points because under this condition we may use the construction of Kiseľák and Stehlík (2008) to obtain the inverse of the covariance matrix of observations which is tridiagonal. Moreover, in case of an equidistant design the covariance matrix is Toeplitz.

Here we consider D-optimality, which corresponds to the maximization of objective function $\Phi(M) := \det(M)$, the determinant of the standard Fisher information matrix. This criterion, "plugged" from the widely developed uncorrelated setup, offers considerable potential for automatic implementation, although further development is needed before it can be applied routinely in practice. Theoretical justifications for using Fisher information for D-optimal designing under correlation can be found in Abt and Welch (1998) and Pázman (2007). The concept of uniform designs has now gained popularity and proved to be very successful in industrial applications and in computer experiments (Müller and Stehlík, 2009; Santner et al., 2003). It has become standard practice to select the design points such as to cover the available space as uniformly as possible, e.g., to apply the so called space-filling designs. In higher dimensions there are several ways to produce such designs. In this paper we illustrate that for the OU sheet the design satisfying monotonicity *Condition D* could be possibly superior to the space filling grid designs. The idea of choosing a monotonic set is mainly motivated by Markovian properties of the OU sheet.

1.2. Motivating example: measurement of a stationary thermal field

Temperature distribution calculations during the process of designing a building is a necessary part of testing the critical places at the building envelope. The aim is to increase the minimal surface temperature, and to predict the possible thermal bridges which are possible locations of mould growth in the building. Figure 1a displays the composition of materials of the 2D section of a thermal bridge within the building construction. Data are taken from Minárová (2005), where a finite element method for computation of the temperature field is applied using software package ANSYS. Figure 1b illustrates the isotherms of the thermal field which fit well to measurements forming a monotonic set satisfying *Condition D.*

Data points in which we measure the temperature are plotted on Figure 2. We assume that the covariance parameters α and β are given and we are interested in the estimation of the trend parameter θ of the model



(a)

(b)

Figure 1: 2D section of a fragment of the building envelope near the thermal bridge (Minárová, 2005). (a) Composition of a material; (b) Isoterms of the thermal field.

(1.1). Table 1 lists the relative efficiency, the information M_θ gained in the data points and the optimal information gain ($\max M_\theta$) of the data from Figure 2 for three choices of known correlation parameters α, β. Here M_θ is evaluated on the given observations and $\max M_\theta$ is the theoretical maximal value reachable at the given number of points, trajectory length and given values of parameters. Obviously, the relative efficiency of the given data points varies with these parameters.

2. Estimation of trend parameter only

Assume first that parameters α, β and σ of the covariance structure (1.3) of the OU sheet ε are given and we are interested in the estimation of the trend parameter θ. In this case the Fisher information on θ based on observations $\{Y(s_i, t_i),\ i = 1, 2, \ldots, n\}$ equals $M_\theta(n) = \mathbf{1}_n^\top C^{-1}(n, r)\mathbf{1}_n$, where $\mathbf{1}_n$ is the column vector of ones of length n, $r = (\alpha, \beta)^\top$, and $C(n, r)$ is the covariance matrix of the observations (Pázman, 2007; Xia et al., 2006). Further, let $d_i := s_{i+1} - s_i$ and $\delta_i := t_{i+1} - t_i,\ i = 1, 2, \ldots, n-1$, be the distances between two adjacent design points. With the help of this representation one can prove the following theorem.

Correlation Parameters	M_θ	$\max M_\theta$	Efficiency ($M_\theta / \max M_\theta$)
$\alpha = 1,\ \beta = 1$	1.4816	1.4817	0.990
$\alpha = 1,\ \beta = 10$	4.9726	5.0813	0.978
$\alpha = 10,\ \beta = 1$	2.2124	2.2129	0.999

Table 1: Efficiency depending on correlation parameters.

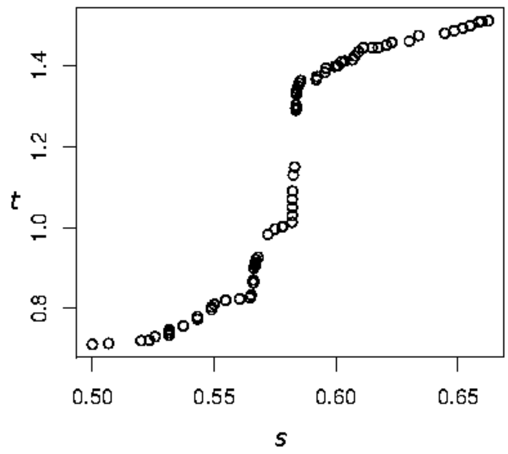


Figure 2: Observation points on Isotherms.

Theorem 1. *Consider the model* (1.1) *with covariance structure* (1.3) *observed in points* $\big\{(s_i,t_i),\ i = 1,2,\ldots,n\big\}$ *satisfying Condition D and assume that the only parameter of interest is the trend parameter* θ*. In this case, the equidistant design satisfying* $\alpha d_1+\beta\delta_1 = \alpha d_2+\beta\delta_2 = \ldots = \alpha d_{n-1}+\beta\delta_{n-1}$ *is optimal for estimation of* θ*.*

According to Theorem 1 the optimality holds for $\alpha d_i + \beta\delta_i = \frac{\lambda}{n-1}$, where λ is the "skewed size" of the design region, i.e., $\lambda := \alpha\sum_{i=1}^{n-1} d_i + \beta\sum_{i=1}^{n-1}\delta_i$ and $\sum_{i=1}^{n-1} d_i < b_1 - a_1,\ \sum_{i=1}^{n-1}\delta_i < b_2 - a_2$. Several situations may appear in practice. As now we consider the covariance parameters α,β to be fixed and make inference only on the unknown trend parameter θ, from the proof of Theorem 1 we obtain

$$M_\theta(n) = 1 + \sum_{i=1}^{n-1}\frac{1-q_i}{1+q_i}, \tag{2.1}$$

where $q_i := \exp(-\alpha d_i - \beta\delta_i)$. Thus, for an optimal design we have

$$M_\theta(n) = M_\theta(n;\lambda) = 1 + (n-1)\frac{1-\exp(-\lambda/(n-1))}{1+\exp(-\lambda/(n-1))},$$

which is an increasing function of both the number of design points n and the "skewed size" λ. Further, $M_\theta(n;\lambda) \to \lambda/2+1$ as $n\to\infty$ and $M_\theta(n;\lambda)\to n$ as $\lambda\to\infty$, which values are bounds for information increase in experiments.

To illustrate the latter fact let us consider the design region $\mathcal{X} = [0,1]^2$ and a four-point design, and assume that the correlation parameters are $\alpha=\beta=1$. As a comparison we consider a regular grid design which puts the four points into the vertices of the rectangle $\mathcal{X}$ (this design does not satisfy *Condition D*). The information corresponding to this latter design is $M_\theta = 2.13$. Having the same design region we cannot reach such an efficiency, because $\lambda = 2$ and $M_\theta(n;\lambda) < \lambda/2+1$. Indeed, the maximal information gain can be $M_\theta(4;2) = 1.965$ which gives us an efficiency of 0.919. If we allow the growth of the design region, e.g. $\mathcal{X} = [0,x]^2$, for a four-point design, under the above conditions we obtain $M_\theta = \frac{4}{1+\exp(-2x)+\exp(-x)} \to 4$ for $x \to \infty$ at a regular grid design with vertices.

3. Estimation of covariance parameters only

Assume now that we are interested only in the estimation of the parameters α and β of the OU sheet. According to the results of Pázman (2007) and Xia et al. (2006) the Fisher information matrix on $r = (\alpha,\beta)^\top$ has the form

$$M_r(n) = \begin{bmatrix} M_\alpha(n) & M_{\alpha,\beta}(n) \\ M_{\alpha,\beta}(n) & M_\beta(n) \end{bmatrix}, \tag{3.1}$$

where

$$\begin{aligned} M_\alpha(n) &:= \frac{1}{2}\mathrm{tr}\left\{ C^{-1}(n,r)\frac{\partial C(n,r)}{\partial \alpha} C^{-1}(n,r)\frac{\partial C(n,r)}{\partial \alpha} \right\}, \\ M_\beta(n) &:= \frac{1}{2}\mathrm{tr}\left\{ C^{-1}(n,r)\frac{\partial C(n,r)}{\partial \beta} C^{-1}(n,r)\frac{\partial C(n,r)}{\partial \beta} \right\}, \\ M_{\alpha,\beta}(n) &:= \frac{1}{2}\mathrm{tr}\left\{ C^{-1}(n,r)\frac{\partial C(n,r)}{\partial \alpha} C^{-1}(n,r)\frac{\partial C(n,r)}{\partial \beta} \right\}, \end{aligned}$$

and $C(n,r)$ denotes the covariance matrix of the observations $\{Y(s_i,t_i),\ i=1,2,\ldots,n\}$. Note, that here $M_\alpha(n)$ and $M_\beta(n)$ are Fisher information on parameters α and β, respectively, taking the other parameter as a nuisance.

The following theorem gives the exact form of $M_r(n)$ for the model (1.1).

Theorem 2. *Consider the model* (1.1) *with covariance structure* (1.3) *observed in points* $\{(s_i,t_i),\ i = 1,2,\ldots,n\}$ *satisfying Condition D. Then*

$$M_\alpha(n) = \sum_{i=1}^{n-1} \frac{d_i^2 q_i^2(1+q_i^2)}{(1-q_i^2)^2}, \qquad M_\beta(n) = \sum_{i=1}^{n-1} \frac{\delta_i^2 q_i^2(1+q_i^2)}{(1-q_i^2)^2}, \qquad M_{\alpha,\beta}(n) = \sum_{i=1}^{n-1} \frac{d_i\delta_i q_i^2(1+q_i^2)}{(1-q_i^2)^2}, \tag{3.2}$$

where d_i, δ_i *and* q_i *denote the same quantities as in the previous section, i.e.* $d_i := s_{i+1} - s_i,\ \delta_i := t_{i+1} - t_i$ *and* $q_i := \exp(-\alpha d_i - \beta\delta_i),\ i = 1,2,\ldots,n-1$.

Using Theorem 2 one can formulate the following statement on the optimal design for the parameters of the covariance structure of the OU sheet.

Theorem 3. *The design which is optimal for estimation of the covariance parameters* $\alpha,\ \beta$ *does not exist within the class of admissible designs.*

4. Estimation of all parameters

Consider now the most general case, when both α, β and θ are unknown and the Fisher information matrix on these parameters equals $M(n) = \begin{bmatrix} M_\theta(n) & 0 \\ 0 & M_r(n) \end{bmatrix}$, where $M_\theta(n)$ and $M_r(n)$ are Fisher information matrices on θ and $r = (\alpha, \beta)^\top$, respectively, see (2.1) and (3.1).

Theorem 4. *The design which is optimal for estimation of the covariance parameters α, β and of the trend parameter θ does not exist within the class of admissible designs.*

Loosely speaking, the optimal designs for the trend have the tendency to move the design points as far as possible, while the optimal designs for the covariance structure have the tendency to shrink the set of design points. However, we can choose a compromise between estimating the trend and correlation parameters. Therefore, similarly to Zagoraiou and Baldi Antognini (2009), we may consider the so-called geometric progression design, which is generated by the vectors of distances

$$\boldsymbol{d}_{n,r_1} := (k, kr_1, kr_1^2, \ldots, kr_1^{n-2}), \qquad \boldsymbol{\delta}_{n,r_2} := (\ell, \ell r_2, \ell r_2^2, \ldots, \ell r_2^{n-2}),$$

where $0 < r_1, r_2 \leq 1$.

Assume $\sum_{i=1}^{n-1} d_i = 1$ and $\sum_{i=1}^{n-1} \delta_i = 1$, for $r_1 = 1,\ r_2 = 1$ both constants k and ℓ are equal to $(n-1)^{-1}$, while for $r_1 < 1$ and $r_2 < 1$ we get $k = \frac{1-r_1}{1-r_1^{n-1}}$ and $\ell = \frac{1-r_2}{1-r_2^{n-1}}$, respectively. The tuning parameters $r_1,\ r_2$ can be varied according to the desired efficiency for the estimation of the trend or correlation parameters.

Note, that case $r_1 = 1,\ r_2 = 1$ corresponds to the equidistant design, which we have proved to be optimal for estimation of the trend parameter, whereas for $r_1 \to 0$, $r_2 \to 0$, vectors $\boldsymbol{d}_{n,r_1}$ and $\boldsymbol{\delta}_{n,r_2}$ tend to the best design for the estimation of α and β. The following theorem describes the behaviors of $M_\theta(n)$ and $\det\big(M_r(n)\big)$ as functions of the tuning parameters r_1 and r_2.

Theorem 5. *For any fixed $n > 2$, $\alpha > 0$, $\beta > 0$, the information $M_\theta(n)$ of the trend is increasing with respect to r_1, r_2, while the determinant of the Fisher information $M_r(n)$ of covariance parameters has a global minimum at $r_1 = r_2$.*

We remark that the first statement of Theorem 5 is a straightforward extension of the corresponding part of Theorem 5.1 of Zagoraiou and Baldi Antognini (2009). Further, observe that Theorem 5 obviously implies that the total information $\det\big(M(n)\big)$ has the same behavior as $\det\big(M_r(n)\big)$, that is it has a global minimum at $r_1 = r_2$.

5. Application to Deterioration of highways

Typically, engineers are using regular grids for estimation of the parameters of a random field. E.g., in Mohapl (1997) the deterioration of a highway in New York state is investigated where data were collected in four successive years at distances of 0.2 miles from each other forming a 4×16 table, Based on these data the author estimated the parameters of the underlying stochastic process. What is the efficiency of such a design? The design region has the natural form $[0, 4] \times [0, 3.2]$ and the number of observed points is 64. In the case $\alpha = \beta = 1$ design satisfying *Condition D* and having 64 points in such a region has $M_\theta(64, 7.2) = 4.596$.

Now, let us have 16 time coordinates uniformly generated from time region $[0, 4]$ and 16 location coordinates generated from space region $[0, 3.2]$. Then for time points

1.35, 3.66, 1.86, 0.996, 0.89, 1.56, 3.37, 2.189, 0.5157, 2.58, 0.058, 0.32, 0.58, 1.4, 0.36, 1.82

and lengths

0.64, 0.37, 1.2, 0.91, 1.34, 2.82, 2.56, 2.44, 0.257, 2.568, 2.223, 0.66, 2.298, 2.814, 2.75, 1.61

we obtain $M_\theta = 5.2$ in the case both parameters α and β are equal to 1. According to Section 2 the maximal information gain with *Condition D* for $n = 64, \lambda = 5.12$ equals 3.56, thus the relative efficiency is 0.68. However, there is an open question, how to estimate parameters in case of this particular setting of points, which is far not trivial. Since the observations form a Gaussian random vector, one can derive the likelihood function and find the ML estimates at least numerically. For a regular grid design Ying (1993) proved consistency and asymptotic normality of the ML estimators, but according to the authors best knowledge this is the only result in this direction. The problem is that in the general case the dependence of the likelihood function on the parameters and design points is too complicated to find its asymptotic properties.

When one uses regular grids of Mohapl (1997), then the following situation occurs: time is measured in 16 equispaced moments starting from 0, until 3.75 by 0.25, while the deterioration of the highway is measured in 16 points (by 0.2 miles). Then $M_\theta = 4.32$ (in the case $\alpha = \beta = 1$) with relative efficiency of 0.827. Table 2 is revealing an interesting fact, that regular grid design (with $256 = 16^2$ points) has a lost of efficiency with respect to the optimal design satisfying *Condition D* with the same number of points in the same design region. This loss can be substantial depending on the values the correlation parameters. A simulation comparison between monotonic and Latin hypercube designs (LHS) has been made by Stehlík et al. (2014). For a specific setup, e.g., $\alpha = 1,\ \beta = 10,\ \sigma = 1$ and a small number of design points, i.e., $n < 15$, D-optimal designs have better efficiency than both implementations of LHS designs (i.e., S-optimal and Euclidean distance) and factorial design. However, for $n > 15$ the LHS and factorial designs are more efficient.

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Correlation Parameters	M_θ	$\max M_\theta$	Efficiency $(M_\theta / \max M_\theta)$
$\alpha = 1,\ \beta = 1$	4.3192	4.3748	0.987
$\alpha = 1,\ \beta = 10$	13.1395	17.8504	0.736
$\alpha = 10,\ \beta = 1$	14.1108	21.2075	0.665

Table 2: Efficiency depending on correlation parameters.

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6. Appendix

6.1. Proof of Theorem 1

According to the notations of Section 2 let $d_i := t_{i+1} - t_i,\ \delta_i := s_{i+1} - s_i$ and $q_i := \exp(-\alpha d_i - \beta \delta_i)$. Similarly to the results of Kiselák and Stehlík (2008) we have

$$C(n,r) = \begin{bmatrix} 1 & q_1 & q_1 q_2 & q_1 q_2 q_3 & \cdots & \cdots & \prod_{i=1}^{n-1} q_i \\ q_1 & 1 & q_2 & q_2 q_3 & \cdots & \cdots & \prod_{i=2}^{n-1} q_i \\ q_1 q_2 & q_2 & 1 & q_3 & \cdots & \cdots & \prod_{i=3}^{n-1} q_i \\ q_1 q_2 q_3 & q_2 q_3 & q_3 & 1 & \cdots & \cdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \ddots & & \vdots \\ \vdots & \vdots & \vdots & \vdots & & \ddots & q_{n-1} \\ \prod_{i=1}^{n-1} q_i & \prod_{i=2}^{n-1} q_i & \prod_{i=3}^{n-1} q_i & \cdots & \cdots & q_{n-1} & 1 \end{bmatrix} \tag{6.1}$$

and

$$C^{-1}(n,r) = \begin{bmatrix} \frac{1}{1-q_1^2} & \frac{q_1}{q_1^2-1} & 0 & 0 & \cdots & \cdots & 0 \\ \frac{q_1}{q_1^2-1} & V_2 & \frac{q_2}{q_2^2-1} & 0 & \cdots & \cdots & 0 \\ 0 & \frac{q_2}{q_2^2-1} & V_3 & \frac{q_3}{q_3^2-1} & \cdots & \cdots & 0 \\ 0 & 0 & \frac{q_3}{q_3^2-1} & V_4 & \cdots & \cdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \ddots & & \vdots \\ \vdots & \vdots & \vdots & \vdots & & V_{n-1} & \frac{q_{n-1}}{q_{n-1}^2-1} \\ 0 & 0 & 0 & \cdots & \cdots & \frac{q_{n-1}}{q_{n-1}^2-1} & \frac{1}{1-q_{n-1}^2} \end{bmatrix}, \tag{6.2}$$

where $V_k := \frac{1-q_k^2 q_{k-1}^2}{(q_k^2-1)(q_{k-1}^2-1)} = \frac{1}{1-q_k^2} + \frac{q_{k-1}^2}{1-q_{k-1}^2},\ k = 2, \ldots, n-1$. Hence, for $M_\theta(n) = \mathbf{1}_n^\top C^{-1}(n,r)\mathbf{1}_n$ we obtain

$$M_\theta(n) = \frac{1-2q_1}{1-q_1^2} + \frac{1}{1-q_{n-1}^2} + \sum_{i=2}^{n-1}\left(\frac{2q_i}{q_i^2-1} + \frac{1-q_i^2 q_{i-1}^2}{(q_i^2-1)(q_{i-1}^2-1)}\right) = 1 + \sum_{i=1}^{n-1}\frac{1-q_i}{1+q_i}. \tag{6.3}$$

Now, consider reformulation

$$M_\theta(n) = 1 + \sum_{i=1}^{n-1} g\big(\alpha d_i + \beta\delta_i\big), \qquad \text{where} \qquad g(x) := \frac{1-\exp(-x)}{1+\exp(-x)}.$$

As $g(x)$ is a concave function of x, by Proposition C1 of Marshall and Olkin (1979), $M_\theta(n)$ is a Schur-concave function of $\alpha d_i + \beta\delta_i,\ i = 1, 2, \ldots, n-1$. In this way $M_\theta(n)$ attains its maximum when $\alpha d_i + \beta\delta_i = \lambda/(n-1),\ i = 1, 2, \ldots, n-1$, where λ is the “skewed size” of the design rectangle. Hence, an equidistant design is the D-optimal for the parameter θ. □

6.2. Proof of Theorem 2

By symmetry it suffices to prove

$$M_\alpha(n) = \frac{1}{2}\mathrm{tr}\left\{C^{-1}(n,r)\frac{\partial C(n,r)}{\partial\alpha}C^{-1}(n,r)\frac{\partial C(n,r)}{\partial\alpha}\right\} = \sum_{i=1}^{n-1}\frac{d_i^2 q_i^2(1+q_i^2)}{(1-q_i^2)^2}. \tag{6.4}$$

For $n = 2$ equation (6.4) holds trivially. Assume also that (6.4) is true for some n and we are going to show it for $n+1$. Let $\mathbf{0}_{k,\ell}$ be the $k \times \ell$ matrix of zeros and let

$$\Delta(n) := \big(-(d_1+d_2+\ldots+d_n)q_1q_2\ldots q_n, -(d_2+d_3\ldots+d_n)q_2q_3\ldots q_n, \ldots, -d_nq_n\big)^\top.$$

With the help of representation (6.1) one can easily see that

$$\frac{\partial C(n+1,r)}{\partial\alpha} = \left[\begin{array}{c:c} \frac{\partial C(n,r)}{\partial\alpha} & \Delta(n) \\ \hdashline \Delta^\top(n) & 0 \end{array}\right],$$

whereas (6.2) implies

$$C^{-1}(n+1,r) = \left[\begin{array}{c:c} C^{-1}(n,r) & \mathbf{0}_{n,1} \\ \hdashline \mathbf{0}_{1,n} & 0 \end{array}\right] + \left[\begin{array}{c:c} \Lambda_{1,1}(n) & \Lambda_{1,2}(n) \\ \hdashline \Lambda_{1,2}^\top(n) & (1-q_n^2)^{-1} \end{array}\right],$$

where

$$\Lambda_{1,1}(n) := \left[\begin{array}{c:c} \mathbf{0}_{n-1,n-1} & \mathbf{0}_{n-1,1} \\ \hdashline \mathbf{0}_{1,n-1} & \frac{q_n^2}{1-q_n^2} \end{array}\right] \qquad \text{and} \qquad \Lambda_{1,2}(n) := \left[\begin{array}{c} \mathbf{0}_{n-1,1} \\ \hdashline -\frac{q_n}{1-q_n^2} \end{array}\right].$$

In this way

$$C^{-1}(n+1,r)\frac{\partial C(n+1,r)}{\partial\alpha} = \left[\begin{array}{c:c} C^{-1}(n,r)\frac{\partial C(n,r)}{\partial\alpha} & C^{-1}(n,r)\Delta(n) \\ \hdashline \mathbf{0}_{1,n} & 0 \end{array}\right] + \left[\begin{array}{c:c} \mathcal{K}_{1,1}(n) & \mathcal{K}_{1,2}(n) \\ \hdashline \mathcal{K}_{2,1}(n) & \mathcal{K}_{2,2}(n) \end{array}\right],$$

with

$$\mathcal{K}_{1,1}(n) := \left[\begin{array}{c} \mathbf{0}_{n-1,n} \\ \hdashline -\dfrac{q_n}{1-q_n^2}\big(\Delta^\top(n) - (q_n\Delta^\top(n-1),0)\big) \end{array}\right], \qquad \mathcal{K}_{1,2}(n) := \left[\begin{array}{c} \mathbf{0}_{n-1,1} \\ \hdashline -\dfrac{d_n q_n^3}{1-q_n^2} \end{array}\right],$$

$$\mathcal{K}_{2,1}(n) := \frac{1}{1-q_n^2}\big(\Delta^\top(n) - (q_n\Delta^\top(n-1),0)\big), \qquad \mathcal{K}_{2,2}(n) := \frac{d_n q_n^2}{1-q_n^2}.$$

Hence,

$$\begin{aligned} M_\alpha(n+1) =& M_\alpha(n) + \operatorname{tr}\left\{C^{-1}(n,r)\frac{\partial C(n,r)}{\partial\alpha}\mathcal{K}_{1,1}(n)\right\} \\ &+ \operatorname{tr}\left\{C^{-1}(n,r)\Delta(n)\mathcal{K}_{2,1}(n)\right\} + \frac{1}{2}\operatorname{tr}\left\{\mathcal{K}_{1,1}^2(n)\right\} + \mathcal{K}_{2,1}(n)\mathcal{K}_{1,2}(n) + \frac{1}{2}\mathcal{K}_{2,2}^2(n). \end{aligned} \tag{6.5}$$

After long but straightforward calculations one can obtain

$$\begin{aligned} &\operatorname{tr}\left\{C^{-1}(n,r)\frac{\partial C(n,r)}{\partial\alpha}\mathcal{K}_{1,1}(n)\right\} = 0, \qquad \operatorname{tr}\left\{C^{-1}(n,r)\Delta(n)\mathcal{K}_{2,1}(n)\right\} = \frac{d_n^2 q_n^2}{1-q_n^2}, \\ &\operatorname{tr}\left\{\mathcal{K}_{1,1}^2(n)\right\} = \mathcal{K}_{2,1}(n)\mathcal{K}_{1,2}(n) = \mathcal{K}_{2,2}^2(n) = \frac{d_n^2 q_n^4}{(1-q_n^2)^2}, \end{aligned}$$

so (6.5) implies

$$M_\alpha(n+1) = M_\alpha(n) + \frac{d_n^2 q_n^2(1+q_n^2)}{(1-q_n^2)^2},$$

which completes the proof. □

6.3. Proof of Theorem 3

Consider first the case when we are interested in the estimation of one of the parameters α or β and other parameters are considered as nuisance. If α is the parameter of interest then according to (3.2) the Fisher information on α equals $M_\alpha(n) = \sum_{i=1}^{n-1} F(d_i,\delta_i)$, where

$$F(d,\delta) := \frac{d^2q^2(1+q^2)}{(1-q^2)^2} \geq 0, \qquad \text{with} \quad q := \exp\big(-\alpha d - \beta\delta\big).$$

Due to the separation of the different data points in the expression of $M_\alpha(n)$ it suffices to consider the properties of the function $F(d,\delta)$ for $d,\delta \geq 0,\ d\delta \neq 0$. Obviously,

$$\frac{\partial F(d,\delta)}{\partial d} = \frac{2dq^2\big((1-q^4) - \alpha d(1+3q^2)\big)}{(1-q^2)^3} \quad \text{and} \quad \frac{\partial F(d,\delta)}{\partial \delta} = \frac{-2\beta d^2q^2(1+3q^2)}{(1-q^2)^3}, \tag{6.6}$$

so the critical points of $F(d,\delta)$ are $(0,\delta),\ \delta>0$. However, at these points the determinant of the Hessian is zero and for $\delta>0$ we have $F(0,\delta)=0$. Moreover, short calculation shows that if $d\delta \neq 0$ then $F(d,\delta) < 1/(2\alpha^2)$ and $\lim_{d,\delta\to 0} F(d,\delta) = 1/(2\alpha^2)$. Hence, the supremum of F is reached at $d=\delta=0$, but in our context, $d_i \neq 0,\ \delta_i \neq 0$ for $i=1,2,\ldots,n-1$.

A similar result can be obtained in the case when β is the parameter of interest.

Now, consider the case when both α and β are unknown. According to (3.1) and (3.2) the corresponding objective function to be maximized is

$$\Phi(d_1,\ldots,d_{n-1},\delta_1,\ldots,\delta_{n-1}) = \det\big(M_r(n)\big) = \sum_{i=1}^{n-1}\sum_{j=1}^{n-1}(d_i^2\delta_j^2 - d_i\delta_i d_j\delta_j)\frac{q_i^2(1+q_i^2)}{(1-q_i^2)^2}\frac{q_j^2(1+q_j^2)}{(1-q_j^2)^2}$$

$$= \sum_{i=2}^{n-1}\sum_{j=1}^{i-1}(d_i\delta_j - d_j\delta_i)^2\frac{q_i^2(1+q_i^2)}{(1-q_i^2)^2}\frac{q_j^2(1+q_j^2)}{(1-q_j^2)^2} \geq 0. \tag{6.7}$$

Obviously, for an equidistant design, where $d_1 = \ldots = d_{n-1}$ and $\delta_1 = \ldots = \delta_{n-1}$, the above function equals 0, that is this design cannot be optimal. Further,

$$\frac{\partial\Phi}{\partial d_1} = \frac{2q_1^2(1+q_1^2)}{(1-q_1^2)^2}\big(d_1\widetilde{M}_\beta(1) - \delta_1\widetilde{M}_{\alpha,\beta}(1)\big) - \frac{2\alpha q_1^2(1+3q_1^2)}{(1-q_1^2)^3}\big(d_1^2M_\beta(1) + \delta_1^2\widetilde{M}_\alpha(1) - 2d_1\delta_1\widetilde{M}_{\alpha,\beta}(1)\big), \tag{6.8}$$

$$\frac{\partial\Phi}{\partial \delta_1} = \frac{2q_1^2(1+q_1^2)}{(1-q_1^2)^2}\big(\delta_1\widetilde{M}_\alpha(1) - d_1\widetilde{M}_{\alpha,\beta}(1)\big) - \frac{2\beta q_1^2(1+3q_1^2)}{(1-q_1^2)^3}\big(d_1^2\widetilde{M}_\beta(1) + \delta_1^2\widetilde{M}_\alpha(1) - 2d_1\delta_1\widetilde{M}_{\alpha,\beta}(1)\big),$$

where $\widetilde{M}_\alpha(k)$, $\widetilde{M}_\beta(k)$ and $\widetilde{M}_{\alpha,\beta}(k)$, $k = 1,2,\ldots,n-2$, are the elements of the Fisher information matrix on $r = (\alpha,\beta)^\top$ corresponding to observations $\big\{Y(s_i,t_i),\ i = k,k+1,\ldots,n\big\}$ (see (3.1)), that is

$$\widetilde{M}_\alpha(k) = \sum_{i=k+1}^{n-1}\frac{d_i^2q_i^2(1+q_i^2)}{(1-q_i^2)^2}, \qquad \widetilde{M}_\beta(k) = \sum_{i=k+1}^{n-1}\frac{\delta_i^2q_i^2(1+q_i^2)}{(1-q_i^2)^2}, \qquad \widetilde{M}_{\alpha,\beta}(k) = \sum_{i=k+1}^{n-1}\frac{d_i\delta_iq_i^2(1+q_i^2)}{(1-q_i^2)^2},$$

whereas for $i = 2,3,\ldots,n-1$ we have

$$\frac{\partial\Phi}{\partial d_i} = \frac{2q_i^2(1+q_i^2)}{(1-q_i^2)^2}\big(d_iM_\beta(i) - \delta_iM_{\alpha,\beta}(i)\big) - \frac{2\alpha q_i^2(1+3q_i^2)}{(1-q_i^2)^3}\big(d_i^2M_\beta(i) + \delta_i^2M_\alpha(i) - 2d_i\delta_iM_{\alpha,\beta}(i)\big), \tag{6.9}$$

$$\frac{\partial\Phi}{\partial \delta_i} = \frac{2q_i^2(1+q_i^2)}{(1-q_i^2)^2}\big(\delta_iM_\alpha(i) - d_iM_{\alpha,\beta}(i)\big) - \frac{2\beta q_i^2(1+3q_i^2)}{(1-q_i^2)^3}\big(d_i^2M_\beta(i) + \delta_i^2M_\alpha(i) - 2d_i\delta_iM_{\alpha,\beta}(i)\big).$$

Solving recursively the equations (6.9) under the assumption $d_i\delta_i \neq 0$, $i = 1,2,\ldots,n-1$, for the critical points of Φ we obtain relations

$$\frac{d_i}{d_1} = \frac{\delta_i}{\delta_1} =: c_i > 0, \quad \text{that is} \quad d_i = c_id_1,\ \delta_i = c_i\delta_1, \qquad i = 1,2,\ldots,n-1. \tag{6.10}$$

These solutions also solve (6.8) and short calculations show that for all $d_1,\delta_1,c_1,\ldots,c_{n-1} > 0$ we have $\Phi(d_1,c_1d_1,\ldots,c_{n-1}d_1,\delta_1,c_1\delta_1,\ldots,c_{n-1}\delta_1) = 0$. Hence, critical points determined by (6.10) are minimum points of Φ. In this way, the maximum of the function $\Phi(d_1,\ldots,d_{n-1},\delta_1,\ldots,\delta_{n-1})$ can only be attained at the boundary points, but in our context, $d_i \notin \{0, b_1 - a_1\}$ and $\delta_i \notin \{0, b_2 - a_2\}$. $\square$

6.4. Proof of Theorem 4

As $\det\big(M(n)\big) = M_\theta(n)\det\big(M_r(n)\big) = M_\theta(n)\Phi$, according to (6.3) and (6.7), for unknown parameters α, β and θ the objective function to be maximized is

$$\Psi(d_1,\ldots,d_{n-1},\delta_1,\ldots,\delta_{n-1}) = \left(\frac{2}{1+q_1} + \sum_{i=2}^{n-1}\frac{1-q_i}{1+q_i}\right) \times \left(\sum_{i=2}^{n-1}\sum_{j=1}^{i-1}(d_i\delta_j - d_j\delta_i)^2\frac{q_i^2(1+q_i^2)}{(1-q_i^2)^2}\frac{q_j^2(1+q_j^2)}{(1-q_j^2)^2}\right). \tag{6.11}$$

For $d_1 = \ldots = d_{n-1}$ and $\delta_1 = \ldots = \delta_{n-1}$, we have $\Phi(d_1, \ldots, d_{n-1}, \delta_1, \ldots, \delta_{n-1}) = 0$, thus an equispaced design cannot be optimal.

Further,

$$\frac{\partial \Psi}{\partial d_i} = M_\theta(n)\frac{\partial \Phi}{\partial d_i} - \frac{2\alpha q_i}{(1+q_i)^2}\Phi \qquad \text{and} \qquad \frac{\partial \Psi}{\partial \delta_i} = M_\theta(n)\frac{\partial \Phi}{\partial \delta_i} - \frac{2\beta q_i}{(1+q_i)^2}\Phi,$$

where the expressions for $\partial\Phi/\partial d_i$ and $\partial\Phi/\partial\delta_i$ are given by (6.10). Solving the above equations for the critical points of Ψ we obtain the relations (6.10). However, we have $\Psi(d_1, c_1 d_1, \ldots, c_{n-1}d_1, \delta_1, c_1\delta_1, \ldots, c_{n-1}\delta_1) = 0$, thus the function Ψ attains its minimum at the points determined by (6.10). □

6.5. Proof of Theorem 5

Consider first $M_\theta(n)$ and according to (2.1)

$$M_\theta(n) = M_\theta(n; r_1, r_2) = 1 + \sum_{i=1}^{n-1} f\big(d_i(r_1), \delta_i(r_2)\big), \quad \text{where} \quad f(d,\delta) = \frac{\mathrm{e}^{\alpha d + \beta\delta} - 1}{\mathrm{e}^{\alpha d + \beta\delta} + 1}.$$

Obviously, for $r_1 = 1, \ r_2 = 1$, the geometric progression design corresponds to the equidistant design, which is optimal for the estimation of the trend parameter. For $0 < r_1, r_2 < 1$ one has to prove

$$\frac{\partial M_\theta(n; r_1, r_2)}{\partial r_1} = \sum_{i=1}^{n-1} \frac{\partial f(d_i(r_1), \delta_i(r_2))}{\partial d}\frac{\partial d_i(r_1)}{\partial r_1} > 0, \qquad \frac{\partial M_\theta(n; r_1, r_2)}{\partial r_2} = \sum_{i=1}^{n-1} \frac{\partial f(d_i(r_1), \delta_i(r_2))}{\partial \delta}\frac{\partial \delta_i(r_2)}{\partial r_2} > 0.$$

Now,

$$\frac{\partial f(d,\delta)}{\partial d} = \frac{2\alpha \mathrm{e}^{\alpha d + \beta\delta}}{(\mathrm{e}^{\alpha d + \beta\delta} + 1)^2} > 0,$$

which, as a function of $\alpha d + \beta\delta$, is strictly decreasing. In this way we can use the arguments of Proof of Theorem 5.1 of Zagoraiou and Baldi Antognini (2009), where a one-dimensional OU process is investigated. From $d_i(r) = \delta_i(r) = \frac{(1-r)r^{i-1}}{1-r^{n-1}}, \ i > 1$, we obtain $d_1(r_1) > \ldots > d_{n-1}(r_1)$ and $\delta_1(r_2) > \ldots > \delta_{n-1}(r_2)$ which implies

$$0 < \frac{\partial f\big(d_1(r_1), \delta_1(r_2)\big)}{\partial d} < \ldots < \frac{\partial f\big(d_{n-1}(r_1), \delta_{n-1}(r_2)\big)}{\partial d}.$$

Further,

$$\frac{\partial d_i(r_1)}{\partial r_1} = \frac{r_1^i}{(r_1 - r_1^n)^2}\big((r_1^{n-1}(n-i) - r_1^n(n-i-1) + i - 1 - r_1 i\big), \qquad i = 1, 2, \ldots, n-1,$$

and due to $\sum_{i=1}^{n-1} d_i(r_1) = 1, \ 0 < r_1 \le 1$, we have $\sum_{i=1}^{n-1} \frac{\partial d_i(r_1)}{\partial r_1} = 0$. Now, let j be the smallest integer such that $\frac{\partial d_i(r_1)}{\partial r_1} \ge 0$ for $i = j, \ldots, n-1$, and according to Zagoraiou and Baldi Antognini (2009) such integer exists. Then

$$\sum_{i=1}^{n-1} \frac{\partial f(d_i(r_1), \delta_i(r_2))}{\partial d}\frac{\partial d_i(r_1)}{\partial r_1} = \sum_{i=1}^{j-1} \frac{\partial f(d_i(r_1), \delta_i(r_2))}{\partial d}\frac{\partial d_i(r_1)}{\partial r_1} + \sum_{j=1}^{n-1} \frac{\partial f(d_i(r_1), \delta_i(r_2))}{\partial d}\frac{\partial d_i(r_1)}{\partial r_1} > \frac{\partial f(d_j(r_1), \delta_j(r_2))}{\partial d}\sum_{i=1}^{n-1}\frac{\partial d_i(r_1)}{\partial r_1} = 0.$$

The positivity of the other partial derivative of $M_\theta(n; r_1, r_2)$ can be proved exactly in the same way.

Finally, the second statement of the theorem is a direct consequence of (6.7), since if $r_1 = r_2$ then for all $i = 2, 3, \ldots, n-1$ and $j = 1, 2, \ldots, i-1$ we have $d_i(r_1)\delta_j(r_2) - d_j(r_1)\delta_i(r_2) = 0$. $\square$

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