Further Aspects on an Example of D-optimal Designs in the Case of Correlated Errors

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Further Aspects on an Example of D-optimal Designs in the Case of Correlated Errors*

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Abstract

The aim of this paper is discussion on particular aspects of the extension of a classic example in the design of experiments under the presence of correlated errors. Such extension allows us to study the effect of the correlation range on the design. We discuss the dependence of the information gained by the D-optimum design on the covariance bandwidth and also we concentrate to some technical aspects that occurs in such settings.

Keywords: Design of experiment, D-optimality, optimum design, correlation, information matrix

1 Introduction

At present designing methods for linear models with uncorrelated observations have reached a high level in theory and application. But there are many problems where

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models with correlated observations are more adequate, e.g. in environmental science, mining or meteorology. This directly leads to the consideration of random fields. In this paper we discuss mainly theoretical aspects of a design of experiments under the presence of correlated errors, which main ideas was given in [Müller and Stehlík 04]. There we consider a modification of the Example 6.4 studied in [Näther 85] and have the real random field

$$X(x) = \vartheta_1 + \vartheta_2 x + e(x) \tag{1}$$

(simple linear regression), with design space $V = [-1, 1]$ and a covariance function

$$\text{cov}(x, z) = \begin{cases} 1 - \frac{d_{xz}}{\delta}, & \text{for } d_{xz} < \delta, \\ 0, & \text{for } d_{xz} \geq \delta. \end{cases} \tag{2}$$

with $\delta = 1$, where $d_{xz} = |z - x|$ denotes the distance between the design points. In this paper we will let the parameter δ vary to allow correlation with differing range and study the effects of such varying on the D-optimal design and gained information.

One of the fundamental assumptions, the knowledge of the covariance function, is in most cases almost unrealistic. It seems to be artificial, that the first moment $E(X(x))$ is assumed to be unknown whereas the more complicated second one is assumed to be known. In literature we can find some continuity considerations, that means, that small changes in the covariance structure often entail only small changes in the results obtained. For "good" covariance functions a small change of covariance function leads to only a small change of the results, but, continuity tell us nothing about the magnitude of variation of an optimal design and single design can perform extremely good or extremely bad for varying covariance function. To avoid such problems, in many practical situations the minimax and Bayes-approach is successful (see [Näther 85] for details).

In present paper we follow two ways on looking at the correlation parameter. On the one hand, covariance parameter can be considered as a nuisance one, on the other hand, covariance parameter is considered as known, at least it has to be estimated. The paper is organized as follows. In sections *Two-point designs* and *Three-point designs* we discuss the results for both treatments of the covariance parameter. We hope, that the number of subsections will be helpful for better orientation through the paper. To maintain the continuity of the explanation some formulas are included into the *Appendix*.

2 Two-point designs

In this section we consider exact designs having only two design points $\{x, z\}$, $-1 \leq x < z \leq 1$. For $\delta \geq 0$ we introduce a function

$$J_\delta(x) = \begin{cases} 1, & \text{for } x \in [0, \delta), \\ 0, & \text{otherwise.} \end{cases}$$

In the case $\delta = 0$ we have $J_0(x) = 0$, which will represent the uncorrelated case. Here and further we use notation d for the distance when it is clear, which points are assumed. In [Müller and Stehlík 04] we maximize the log-likelihood function $L = \log f(\vartheta, u)$, where $f(\vartheta, .)$ is the normal density of the vector $u = (X - \vartheta_1 - \vartheta_2 x, Z - \vartheta_1 - \vartheta_2 z)^T$ with zero mean and the covariances given by (2). Notice, that when $\delta < 2$, function $\mathrm{cov}(x, z)$ is not differentiable with respect to the covariance parameter for $\delta = d$, despite both one-sided derivations exist. The classic Fisher's information $E\left(\frac{d \log f}{d\vartheta}\right)^2$ assumes the differentiability with respect to the parameter (see e.g. [Rao 65]). This opens a problem of interpretation of the formally defined (e.g. by one-sided limits) information matrix for such values. Still, the classic Fisher's information can be well defined over some open set.

Proposition 1 *The elements $M_{i,j}$ of the Fisher information matrix M according to models (1) and (2) given above have the form:*

$$M_{1,1} = E\left(-\frac{\partial^2 L}{\partial \vartheta_1^2}\right) = 2\frac{1 + (-1 + \frac{d}{\delta})J_\delta(d)}{1 - (1 - \frac{d}{\delta})^2 J_\delta(d)}$$

$$M_{1,2} = E\left(-\frac{\partial^2 L}{\partial \vartheta_1 \partial \vartheta_2}\right) = \frac{(x + z)\left(1 + (-1 + \frac{d}{\delta})J_\delta(d)\right)}{1 - (1 - \frac{d}{\delta})^2 J_\delta(d)}$$

$$M_{2,2} = E\left(-\frac{\partial^2 L}{\partial \vartheta_2^2}\right) = \frac{x^2 + z^2 + 2xz(-1 + \frac{d}{\delta})J_\delta(d)}{1 - (1 - \frac{d}{\delta})^2 J_\delta(d)}$$

The elements $M_{1,3}$, $M_{2,3}$ and $M_{3,3}$ are well defined for $2 < \delta$, otherwise ($\delta \leq 2$) for $\delta \in (0, d) \cup (d, +\infty)$. Then the elements $M_{1,3}$ and $M_{2,3}$ can be continuously prolonged on $(0, +\infty)$, despite the element $M_{3,3}$, where jump $(\lim_{\delta \to d+} - \lim_{\delta \to d-}) M_{3,3} = \frac{1}{d^2}$ occurs. For appropriate values we have

$$M_{3,3} = E\left(-\frac{\partial^2 L}{\partial \delta^2}\right) = J_\delta(d)\frac{d^2 - 2\delta d + 2\delta^2}{\delta^2 (2\delta - d)^2}$$

and

$$M_{1,3} = E\left(-\frac{\partial^2 L}{\partial \vartheta_1 \partial \delta}\right) = M_{2,3} = E\left(-\frac{\partial^2 L}{\partial \vartheta_2 \partial \delta}\right) = 0.$$

To illustrate the behavior of the elements have a look on Figure 1 which displays the $M_{1,1}$ and $M_{3,3}$ for various values of d and $\delta = 1.5$ and also on Figure 2, which plots the $M_{1,2}$ and $M_{2,2}$ for various values of z, where $x = -1$ and $\delta = 1.5$.

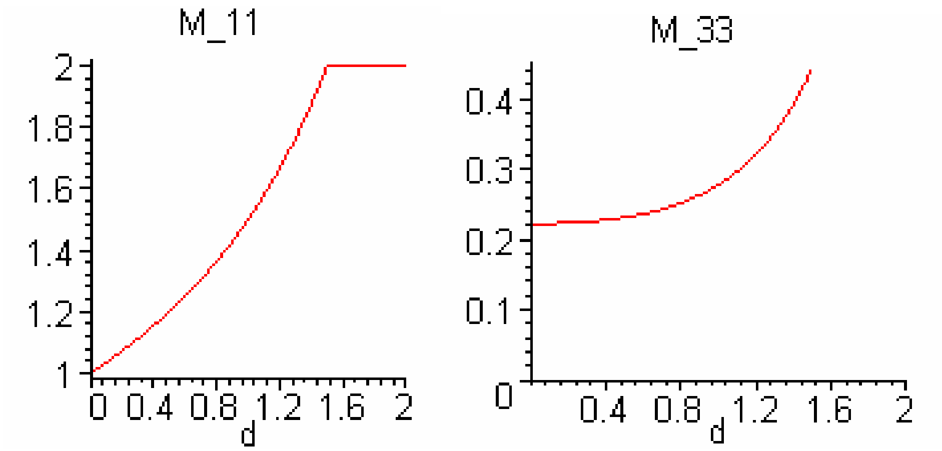

Figure 1: The elements of information matrix.

Proof *The negative log-likelihood has form*

$$-L = constant + \frac{m(x)^2 + m(z)^2 - 2cov(x,z)m(x)m(z)}{2\det\Sigma} + \frac{1}{2}\log\det\Sigma,$$

where we use $m(x) = X(x) - \vartheta_1 - \vartheta_2 x$ *and* $\det\Sigma = 1 - cov^2(x,z)$. *After application of the appropriate derivatives we obtain:*

$$-\frac{\partial^2 L}{\partial\vartheta_1^2} = 2\frac{1 - cov(x,z)}{\det\Sigma}$$

$$-\frac{\partial^2 L}{\partial\vartheta_2^2} = \frac{x^2 + z^2 - 2xz\,cov(x,z)}{\det\Sigma}$$

$$-\frac{\partial^2 L}{\partial\vartheta_1\partial\vartheta_2} = \frac{(x+z)\,(1 - cov(x,z))}{\det\Sigma}$$

For appropriate values we have derivatives

$$-\frac{\partial^2 L}{\partial\vartheta_1\partial\delta} = (m(x) + m(z))\,\frac{d}{d\delta}\frac{cov(x,z)}{\det\Sigma}$$

$$-\frac{\partial^2 L}{\partial\vartheta_2\partial\delta} = (zm(x) + xm(z))\,\frac{d}{d\delta}\frac{cov(x,z)}{\det\Sigma}$$

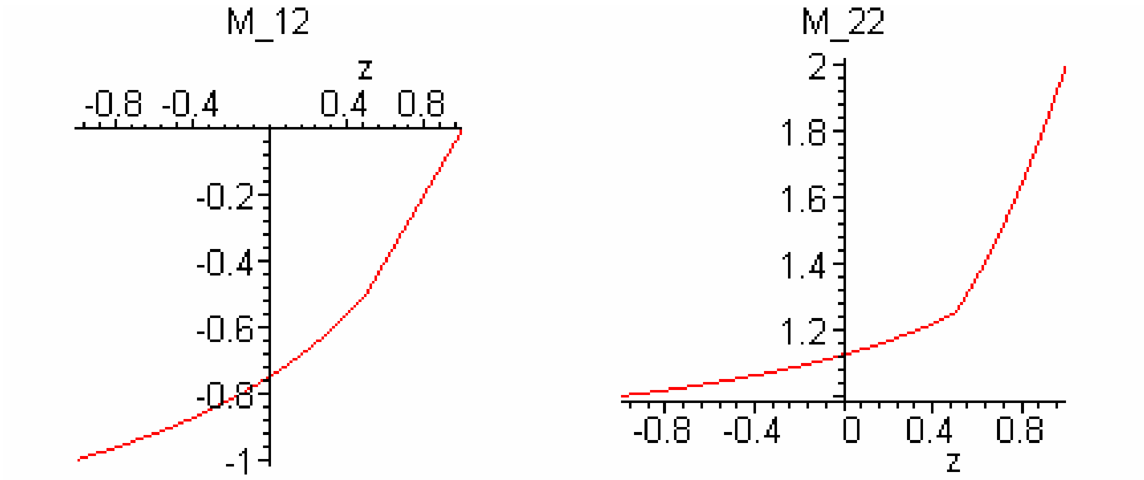

Figure 2: The elements of information matrix.

$$-\frac{\partial^2 L}{\partial \delta^2} = J_\delta(d)\frac{10\delta^2 d - m(x)^2\delta^2 d - m(z)^2\delta^2 d - 2m(x)m(z)\delta^2 d - 6\delta d^2 - 4\delta^3 + d^3}{\delta^2(d-2\delta)^3}$$

Note, that

$$\frac{d}{d\delta}\frac{cov(x,z)}{\det\Sigma} = \begin{cases} \frac{d^2-2\delta d+2\delta^2}{d(2\delta-d)^2}, & \textit{for } 0<d<\min\{\delta,2\}, \\ 0, & \textit{for } \min\{\delta,2\}<d<2. \end{cases}$$

Finally, we have $cov(x,z) = (1-\frac{d}{\delta})J_\delta(d)$, $E(m(x)) = E(m(z)) = 0$, $E(m^2(x)) = E(m^2(z)) = 1$ *and* $E(m(x)m(z)) = cov(x,z)$. □

2.1 Covariance parameter is fixed value

In this subsection we suppose that δ is fixed. The D-optimality criterion function has thus the form $\Phi(M) = -\log\det M$ and it can be written as function of the distance d, i.e.

$$\Phi(d) = \begin{cases} -\log\frac{\delta^2 d}{2\delta-d}, & \text{for } 0<d<\min\{\delta,2\}, \\ -\log d^2, & \text{for } \min\{\delta,2\}\le d\le 2. \end{cases}$$

The minimum of $\Phi(d)$ is attained for $d=2$, which corresponds to the design $\{-1,1\}$. Finally, we have (see [Müller and Stehlík 04], Proposition 1):

Proposition 2 *The design* $\{-1,1\}$ *is D-optimal for all* $\delta \geq 0$.

Here we can see that the optimal design under correlation coincides with the uncorrelated case and does not depend upon the parameter δ. Figure 3, illustrating the result stated by Proposition 1, plots the value of the design criterion for various values of x, $-1 < x < 1$ and δ, $0 < \delta < 2.5$, when $z = 1$ is fixed. As we can see, the minimal value is still attained for $x = -1$.

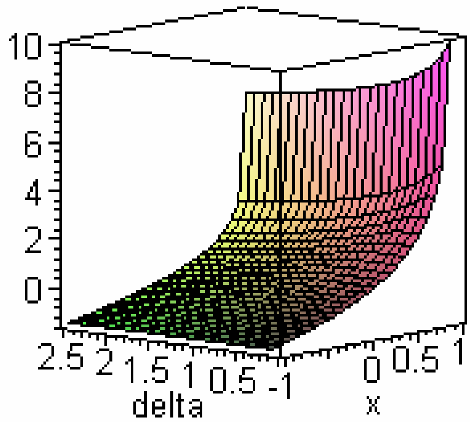

Figure 3: The criterion function.

Now let us little speak about the minimum of the criteria function, function $\min \Phi(\delta)$, $0 \leq \delta$ where δ is fixed parameter. This has a form

$$\min \Phi(\delta) = \begin{cases} -\log 4 & \text{if } 0 \leq \delta < 2; \\ -\log \frac{\delta^2}{\delta - 1} & \text{if } 2 \leq \delta. \end{cases}$$

Function $\min \Phi$ is continuous, constant for $0 \leq \delta < 2$, has zero derivation for $\delta = 2$ and is strictly decreasing for $2 < \delta$ and

$$\lim_{\delta \to +\infty} \min \Phi(\delta) = -\infty.$$

Figure 4 shows this behavior for $0 \leq \delta < 10$.

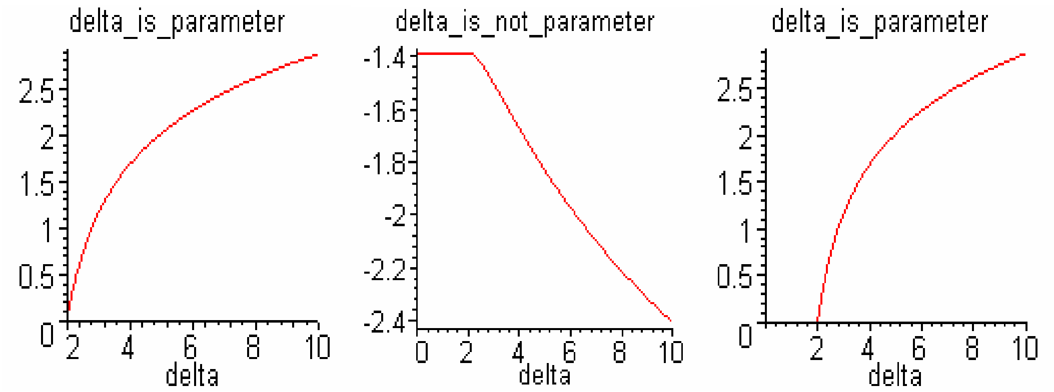

Figure 4: The minimum and infimum of criterion function.

2.2 Covariance parameter is value of interest

Now let us δ treat as parameter. The D-optimality criterion function Φ is the only distance function again,

$$\Phi(d) = \begin{cases} -\log d\frac{d^2-2\delta d+2\delta^2}{(2\delta-d)^3}, & \text{for } 0 < d < \min\{\delta, 2\}, \\ +\infty, & \text{for } \min\{\delta, 2\} \leq d \leq 2, \end{cases}$$

which is decreasing for $0 < d < \min\{\delta, 2\}$. Finally, we obtain (see [Müller and Stehlík 04], Proposition 2):

Proposition 3 *There exists an exact D-optimal design $\{-1, 1\}$ when $2 < \delta$ and there exists no exact D-optimal design for $\delta \leq 2$.*

If we are also interested in the "approximate" optimal design, such that the value of criteria function for it is closed to infimum of criteria function, then

Proposition 4 *For $0 < \delta \leq 2$ we have η-approximate ($0 < \eta << \delta$) optimal design $\{x, x + \delta - \eta\}$ where $-1 \leq x \leq 1 - \delta$. Here $\eta << \delta$ means, that the ratio $\frac{\delta}{\eta}$ is large number.*

The minimal value of the criteria function for given parameter $\delta > 2$

$$\min \Phi(\delta) = -\log \frac{2 - 2\delta + \delta^2}{2(\delta - 1)^3},$$

(note, that function is defined only for $\delta > 2$!) is, despite the fixed-δ case, strictly increasing for $\delta > 2$ and

$$\lim_{\delta \to +\infty} \min \Phi(\delta) = +\infty.$$

Have a look on Figure 4, which plots the $\min \Phi(\delta)$ for $2 < \delta < 10$. As we can see, the minimum attained for $2 < \delta$ (the only correlated observations) is increasing function of the covariance parameter. We are interested also on comparison of correlated and uncorrelated case, and we compute, in correspondence with finite grids practice, the infimum of the criteria function

$$\inf \Phi(\delta) = \begin{cases} 0 & \text{if } 0 \leq \delta \leq 2; \\ \min \Phi(\delta) & \text{if } 2 < \delta. \end{cases}$$

Function (have a look on Figure 4) $\inf \Phi(\delta)$ is continuous, constant for $0 \leq \delta \leq 2$ and strictly increasing for every $\delta > 2$ and we have

$$\lim_{\delta \to +\infty} \inf \Phi(\delta) = +\infty.$$

We can conclude that when both the slope and intercept are parameters of our interest (δ is fixed), then larger covariance is, the more information about the parameters D-optimal design gains, (note, that for every $\delta \leq 2$ we gain the same information, because here independent observations are possible). When δ is treated as parameter of interest, then for $\delta > 2$ information decrease with increasing of δ, and for every $\delta \leq 2$ approximate D-optimal design gains the same information. The Figure 4 makes the behavior of information very clear.

2.3 Particular cases

Let us little discuss some particular cases of the two-point design.

Symmetrical design

If we assume that optimal design have a symmetrical form $\{-x, x\}, 0 < x \leq 1$ with $0 < \delta \leq 2$ (**both the correlated and uncorrelated measurements are possible**), then the criteria function has form

$$f(x) = \begin{cases} -\log x \frac{2x^2 - 2\delta x + \delta^2}{2(\delta - x)^3}, & \text{for } 0 < 2x < \delta, \\ +\infty, & \text{for } \delta \leq 2x, \end{cases}$$

and is strictly decreasing on $(0, \frac{\delta}{2})$ but we have no exact optimal design. If we consider the "approximate" optimal design, then for $0 < \delta \leq 2$ we have η-approximate ($0 < \eta << \delta$) optimal design $\{-0.5\delta + \eta, 0.5\delta - \eta\}$. When **the only correlated measurements are possible**, i.e. $2 < \delta$, the criteria function $f(x) = -\log x \frac{2x^2 - 2\delta x + \delta^2}{2(\delta - x)^3}, 0 < x \leq 1$, is strictly decreasing and the optimal symmetrical design is $\{-1, 1\}$.

Only independent observations

When we suppose, that we have **only uncorrelated** observations and design $\{x, z\}$, we obtain $M_{1,1} = 2$, $M_{1,2} = x + z$ and $M_{2,2} = x^2 + z^2$ and criteria function has the form $\Phi(M) = -\log\det M = -\log d^2$. Then we also have the optimal design $\{-1, 1\}$. Figure 5 plots the value of the design criterion for various values of x and z for the uncorrelated case.

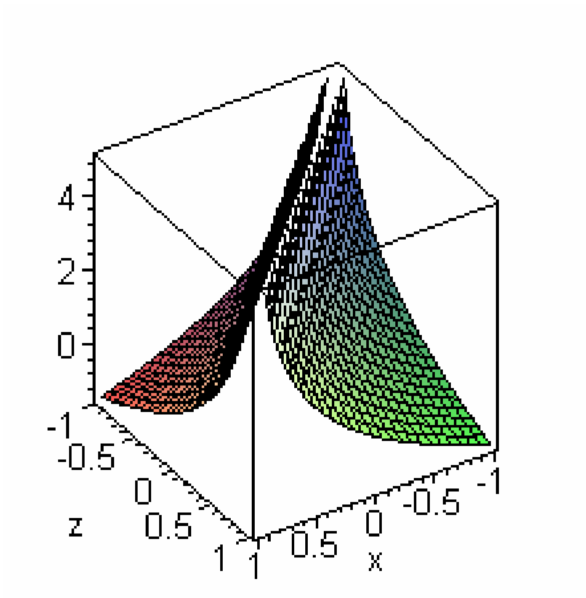

Figure 5: The criterion function for uncorrelated case.

Design for intercept

Now let us study the case, when there is **only one parameter, intercept,** ϑ_1, (δ is not the parameter of interest). Then criteria function has form

$$\Phi(d) = -\log 2\frac{1 + (-1 + \frac{d}{\delta})J_\delta(d)}{1 - (1 - \frac{d}{\delta})^2 J_\delta(d)}$$

(see also Figure 6, which plots the $\Phi(d)$ for various values of $0 \le \delta \le 2.5$ and $0 < d \le 2$).

Proposition 5 *The following designs $\{x, z\}$, $-1 \le x < z \le 1$ are D-optimal:*

- *For the uncorrelated case ($\delta = 0$) is every design $\{x, z\}$, $-1 \le x < z \le 1$ D-optimal.*
- *When both correlated and uncorrelated observations are possible ($0 < \delta \le 2$), the every design $\{x, x + \Delta\}$, $-1 \le x \le 1 - \delta$ and $\delta \le \Delta \le 1 - x$ is D-optimal.*

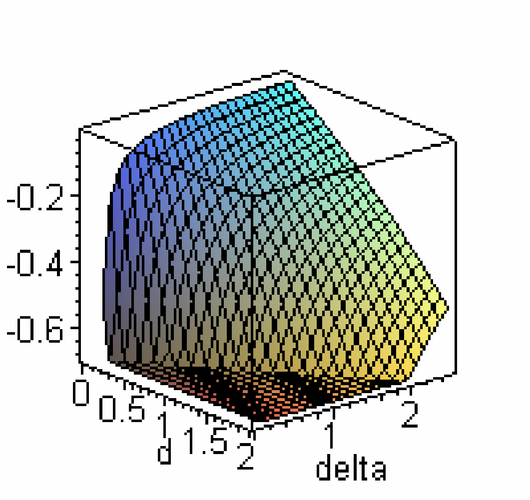

Figure 6: The criterion function for intercept, delta is fixed parameter.

- *When only correlated observations are possible ($\delta > 2$), the minimum of the criterion function is attained for $\{-1, 1\}$.*

Proof *The criteria function can be written in form*

$$\Phi(d) = \begin{cases} -\log \frac{2\delta}{2\delta - d}, & \text{for } 0 < d < \min\{\delta, 2\}, \\ -\log 2, & \text{for } \min\{\delta, 2\} \le d \le 2, \end{cases}$$

and is continuous, decreasing for $0 < d < \min\{\delta, 2\}$ *and constant for* $\min\{\delta, 2\} \le d \le 2$.$\square$

The minimum of the criteria function

$$\min \Phi(\delta) = \begin{cases} -\log 2 & \text{if } 0 \le \delta \le 2, \\ -\log \frac{\delta}{\delta - 1} & \text{if } 2 < \delta \end{cases}$$

is continuous, constant for $0 \le \delta < 2$, strictly increasing for $2 < \delta$ and

$$\lim_{\delta \to +\infty} \min \Phi(\delta) = 0.$$

Now let δ be the **parameter of interest**. Then we obtain the criterion function

$$\Phi(d) = \begin{cases} -\log 2 \frac{d^2 - 2\delta d + 2\delta^2}{\delta(2\delta - d)^3}, & \text{for } 0 < d < \min\{\delta, 2\}, \\ +\infty, & \text{for } \min\{\delta, 2\} \le d \le 2, \end{cases}$$

which is decreasing for $0 < d < \min\{\delta, 2\}$. Finally, we obtain:

Proposition 6 *There exists an exact D-optimal design* $\{-1, 1\}$ *when* $2 < \delta$ *and there exists no exact D-optimal design for* $\delta \leq 2$*. If we consider the "approximate" optimal design, then for* $0 < \delta \leq 2$ *we have* η*-approximate* $(0 < \eta << \delta)$ *optimal design* $\{x, x + \delta - \eta\}$ *where* $-1 \leq x \leq 1 - \delta$*.*

The minimal value of the criteria function for given parameter $\delta > 2$

$$\min \Phi(\delta) = -\log \frac{2 - 2\delta + \delta^2}{2\delta(\delta - 1)^3},$$

(note, that function is defined only for $\delta > 2$!) is strictly increasing and

$$\lim_{\delta \to +\infty} \min \Phi(\delta) = +\infty.$$

The infimum of the criteria function has the form

$$\inf \Phi(\delta) = \begin{cases} -\log \frac{2}{\delta^2} & \text{if } 0 \leq \delta \leq 2; \\ \min \Phi(\delta) & \text{if } 2 < \delta. \end{cases}$$

Function $\inf \Phi(\delta)$ is continuous, strictly increasing for every δ and we have

$$\lim_{\delta \to 0+} \inf \Phi(\delta) = -\infty.$$

and

$$\lim_{\delta \to +\infty} \inf \Phi(\delta) = +\infty.$$

The figure 7 makes the behavior of infimum of the criteria clear. *We can conclude,*

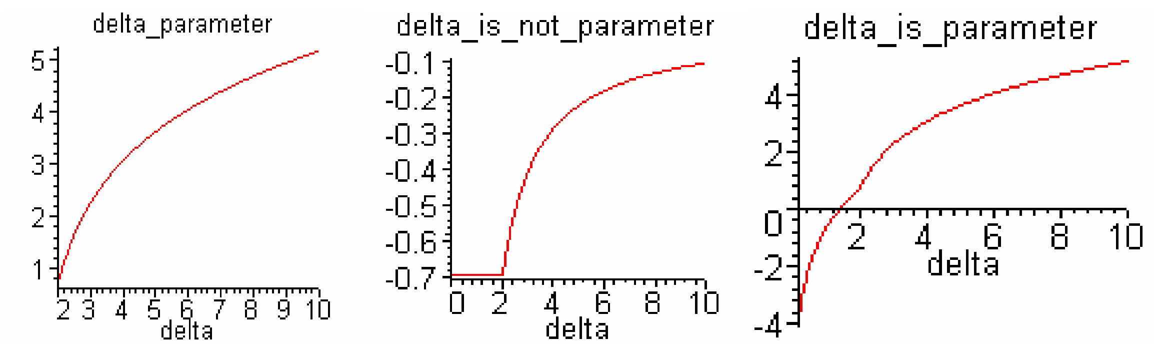

Figure 7: The minimum and infimum of criterion function for intercept.

that for case the intercept (mean) is parameter of interest (and δ *is only fixed value),* *the uncorrelated measurements gains more information about the mean as the correlated ones (note, that uncorrelated observations can be measured only for $\delta \leq 2$ and for these values of covariance parameter the D-optimal design gains the same amount of information). When the δ is treated as parameter of interest, the situation is more simple: the information strictly decreases with increasing of covariance parameter δ. The conclusion is also clear from the Figure 7.*

Design for slope

Now let us study the case, where the **only parameter** of interest **is the slope**, ϑ_2, (δ is fixed). Then we obtain the criteria function

$$\Phi(x,z) = -\log \frac{x^2 + z^2 + 2xz(-1 + \frac{d}{\delta})J_\delta(d)}{1 - (1 - \frac{d}{\delta})^2 J_\delta(d)}$$

(see also Figure 8 that displays $\Phi(x,z)$ for various z and δ, $x = -1$ is fixed).

Proposition 7 *The design $\{-1, 1\}$ is D-optimal for all $\delta \geq 0$.*

Proof *The continuous criteria function can be written in form*

$$\Phi(x,z) = \begin{cases} -\log \frac{\delta(\delta d + 2xz)}{2\delta - d}, & \text{for } 0 < d < \min\{\delta, 2\}, \\ -\log(x^2 + z^2) & \text{for } \min\{\delta, 2\} \leq d \leq 2. \end{cases}$$

Function $\Phi(x,z)$ has no zero derivative for $0 < d < \min\{\delta, 2\}$ and $\Phi(-1,z)$ is decreasing for $-1 < z < \min\{-1+\delta, 2\}$ and $\Phi(x,1)$ is increasing for $\min\{1-\delta, 2\} < x < 1$. Function $-\log(x^2 + z^2)$ has global minimum for $(-1, 1)$. This shows that $\Phi(x,z)$ attains its global minimum for design $\{-1, 1\}$. $\square$

The minimum of the criteria function

$$\min \Phi(\delta) = \begin{cases} -\log 2 & \text{if } 0 \leq \delta \leq 2, \\ -\log \delta & \text{if } 2 < \delta \end{cases}$$

is continuous, constant for $0 \leq \delta \leq 2$, strictly decreasing for $2 < \delta$ and

$$\lim_{\delta \to +\infty} \min \Phi(\delta) = -\infty.$$

Now let δ be **parameter of interest**. Then the criterion function

$$\Phi(d) = \begin{cases} -\log \frac{(\delta d + 1)(d^2 - 2\delta d + 2\delta^2)}{\delta(2\delta - d)^3}, & \text{for } 0 < d < \min\{\delta, 2\}, \\ +\infty, & \text{for } \min\{\delta, 2\} \leq d \leq 2 \end{cases}$$

is decreasing for $0 < d < \min\{\delta, 2\}$. Finally, we have proved:

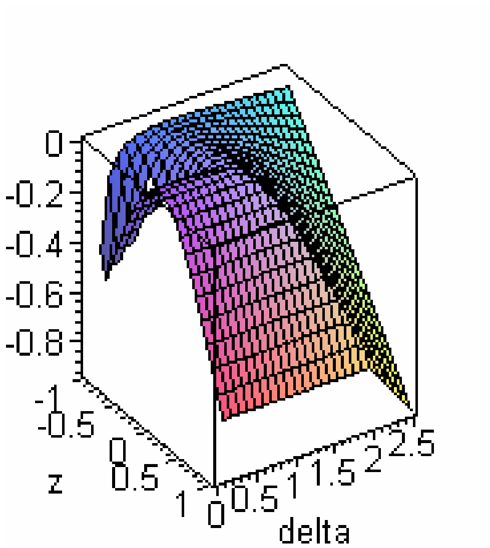

Figure 8: The criterion function for slope, delta is fixed parameter.

Proposition 8 *There exists an exact D-optimal design* $\{-1, 1\}$ *when* $2 < \delta$ *and there exists no exact D-optimal design for* $\delta \leq 2$. *If we also consider the "approximate" optimal design, then for* $0 < \delta \leq 2$ *we have* η*-approximate* $(0 < \eta << \delta)$ *optimal design* $\{x, x + \delta - \eta\}$ *where* $-1 \leq x \leq 1 - \delta$.

The minimal value of the criteria function for given parameter $\delta > 2$

$$\min \Phi(\delta) = -\log \frac{(2\delta + 1)(2 - 2\delta + \delta^2)}{4\delta(\delta - 1)^3},$$

(note, that function is defined only for $\delta > 2$!) is, despite the fixed-δ case, strictly increasing for $\delta > 2$ and

$$\lim_{\delta \to +\infty} \min \Phi(\delta) = +\infty.$$

The infimum of the criteria function

$$\inf \Phi(\delta) = \begin{cases} -\log \frac{1+\delta^2}{\delta^2} & \text{if } 0 \leq \delta \leq 2; \\ -\log \frac{(2\delta+1)(2-2\delta+\delta^2)}{4\delta(\delta-1)^3} & \text{if } 2 < \delta \end{cases}$$

is continuous, strictly increasing for every δ, and we have

$$\lim_{\delta \to 0+} \inf \Phi(\delta) = -\infty,$$

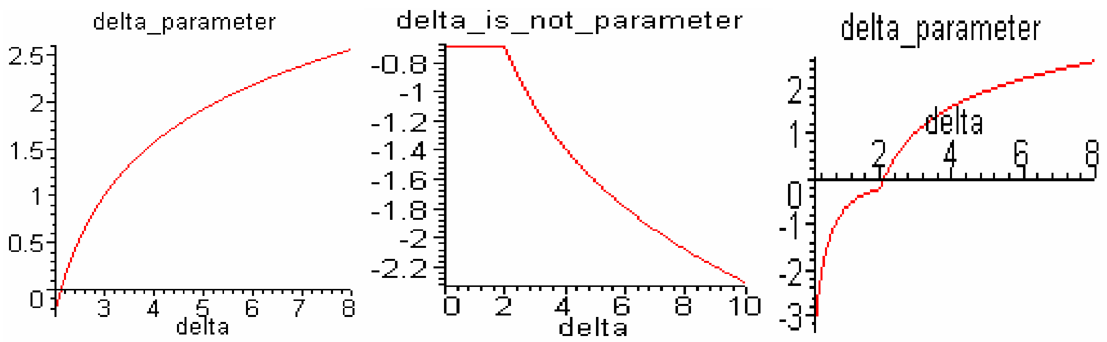

Figure 9: The minimum and infimum of criterion function for slope.

and

$$\lim_{\delta \to +\infty} \inf \Phi(\delta) = +\infty.$$

We can conclude, that if the slope is parameter of interest (δ is fixed), the correlated measurements gains more information about the mean as the uncorrelated ones, the information decrease with increasing of covariance parameter $\delta > 2$ (for $\delta \leq 2$ is the constant information gained, because of possibility to observe without correlation). When δ is treated as parameter of interest, situation is radically changed and the uncorrelated observations gain more information. More exactly, the information gained by exact ($\delta > 2$) or approximate ($\delta \leq 2$) D-optimal design is decreasing with increasing of covariance parameter δ. Figure 9 makes all behavior clear.

3 Three-point designs

In this section we consider more interesting case, the exact design having three points, i.e. let $\{x, y, z\}$, $-1 \leq x < y < z \leq 1$ be a proposed design. The negative log-likelihood has form

$$-L = const + \frac{1}{2}\log\det\Sigma + \frac{1}{2\det\Sigma} \times \{\left(1 - \mathrm{cov}^2(y,z)\right) m(x)^2 +$$
$$+ \left(1 - \mathrm{cov}^2(x,z)\right) m(y)^2 + \left(1 - \mathrm{cov}^2(x,y)\right) m(z)^2 +$$
$$+2\left(\mathrm{cov}(z,y)\mathrm{cov}(x,z) - \mathrm{cov}(x,y)\right) m(x)m(y) +$$
$$+2\left(\mathrm{cov}(x,y)\mathrm{cov}(y,z) - \mathrm{cov}(x,z)\right) m(x)m(z) +$$
$$+2\left(\mathrm{cov}(x,y)\mathrm{cov}(x,z) - \mathrm{cov}(y,z)\right) m(y)m(z)\},$$

where $\det\Sigma = 1 - \mathrm{cov}^2(x,y) - \mathrm{cov}^2(y,z) - \mathrm{cov}^2(x,z) + 2\mathrm{cov}(x,y)\mathrm{cov}(y,z)\mathrm{cov}(x,z)$.

3.1 Covariance parameter is fixed

In this subsection we discuss the case when $\delta \geq 0$ is fixed parameter. The determinant of the information matrix can be written in the form

$$\det M = \frac{2ad_{yz}d_{xy} - 2bd_{xz}d_{xy} - 2cd_{xz}d_{yz} + 3(x^2+y^2+z^2) - (x+y+z)^2}{1 - a^2 - b^2 - c^2 + 2abc},$$

where $a = (1 - \frac{d_{xz}}{\delta})J_\delta(d_{xz})$, $b = (1 - \frac{d_{yz}}{\delta})J_\delta(d_{yz})$ and $c = (1 - \frac{d_{xy}}{\delta})J_\delta(d_{xy})$.

When $\delta = 0$, **(all observations are uncorrelated)** the maximum of the $\det M(x,y,z) = 3(x^2+y^2+z^2) - (x+y+z)^2$ is attained for designs $\{-1,-1,1\}$ and $\{-1,1,1\}$. When $\delta > 2$, **(all observations are correlated)** the maximum of the

$$\det M(d_{xz}) = \frac{\delta^2 d_{xz}}{2\delta - d_{xz}}$$

is attained for $\{-1,y,1\}$ where y is arbitrary.

The most complex situation is for $0 < \delta \leq 2$ **(observations can be correlated).** If $d_{xz} < \delta$ then we have the correlated case (because $d_{xy} + d_{yz} = d_{xz}$) and for $d_{xz} \to \delta$ the supremum δ^2 of $\det M$ for the correlated case is reached. Now let $d_{xz} = \delta + \Delta$ for $0 \leq \Delta \leq 2 - \delta$. The maximum of the function $d_{xy} \to \det M$ under the constraint $d_{xz} = \delta + \Delta$ is attained for the two points δ and Δ with a common value m_Δ. We have $\lim_{\Delta \to 0+} m_\Delta = \delta^2$ and the function $\Delta \to m_\Delta$ is strictly increasing

So, we made a (more detailed) proof of

Theorem 1 *([Müller and Stehlík 04]) The following designs are D-optimal:*

- *For the uncorrelated case ($\delta = 0$) the D-optimal design exhibits repetitions, the criterion function attains its global minimum $-\log 8$ for the designs $\{-1,-1,1\}$ and $\{-1,1,1\}$.*
- *When both correlated and uncorrelated observations are possible ($0 < \delta \leq 2$), we obtain two D-optimal designs $\{-1,-1+\delta,1\}$ and $\{-1,1-\delta,1\}$ with a common minimum value of the criterion function.*
- *When only correlated observations are possible ($\delta > 2$), the minimum of the criterion function is attained for $\{-1,y,1\}$ where y is arbitrary.*

In [Näther 85] is shown (Theorem 6.6) that since the covariance function can be expressed as a linear function of the responses, a uniformly optimal design is $\{-1,0,1\}$. A simplified proof of it is given in [Müller and Pázman 03].

3.2 Covariance parameter is value of interest

Now let us treat the covariance parameter $0 < \delta$ as the variable of the objective function. When $\delta < 2$, then the function $\mathrm{cov}(x, y)$ is not differentiable with respect to the covariance parameter for the $\delta = d_{xy}$, and similarly $\mathrm{cov}(x, z)$ for $\delta = d_{xz}$ and $\mathrm{cov}(y, z)$ for $\delta = d_{yz}$, despite both one-sided derivations exists. Here occurs the problem of interpretation of formally defined information matrix again. Still, it can be well (classically) defined over some open set. The determinant of the information matrix can be written in the form $g(d_{xy}, d_{xz}, d_{yz})$, where g is a quite complex function (can be found in Appendix). When $2 < \delta$, **(only correlated measurements are possible)** the maximum of the

$$\det M = d_{xz} \frac{3d_{xz}^2 - 8\delta d_{xz} + 8\delta^2}{2(2\delta - d_{xz})^3}$$

is attained for $\{-1, y, 1\}$ where y is arbitrary, $x < y < z$.

Now let us suppose the most complex situation $0 < \delta \leq 2$ **(some observations can be also uncorrelated).** First let us have $1 < \delta < 2$. If $d_{xz} < \delta$ then we have correlated case (because of $d_{xy} + d_{yz} = d_{xz}$) and for $d_{xz} \to \delta$ the supremum $\frac{3}{2}$ of $\det M$ for the correlated case is reached. Now let $d_{xz} = \delta + \Delta$ for $0 \leq \Delta \leq 2 - \delta$. The element $M_{3,3} = E\left(-\frac{\partial^2 L}{\partial \delta^2}\right)$ of the information matrix has the form $\frac{2\delta^2 - 2\delta d_{xy} + d_{xy}^2}{\delta^2(-2\delta + d_{xy})^2}$, for $0 < d_{xy} \leq \Delta$,

$$\frac{2\Delta^3\delta + \Delta^4 + 12d_{xy}^2\Delta\delta - 2\Delta\delta^2 d_{xy} + 2\delta^3 d_{xy} + 2d_{xy}^2\delta^2 - 8\Delta d_{xy}^3 +}{\delta^2(-2\delta d_{xy} + 2d_{xy}^2 + \Delta^2 - 2\Delta d_{xy})^2} +$$

$$\frac{+\Delta^2\delta^2 - 8\delta d_{xy}^3 + 8d_{xy}^2\Delta^2 - 4\Delta^3 d_{xy} + 4d_{xy}^4 - 8\delta d_{xy}\Delta^2}{\delta^2(-2\delta d_{xy} + 2d_{xy}^2 + \Delta^2 - 2\Delta d_{xy})^2},$$

for $\Delta < d_{xy} < \delta$ and $\frac{d_{xy}^2 - 2\Delta d_{xy} + \delta^2 + \Delta^2}{\delta^2(d_{xy} - \Delta + \delta)^2}$ for $\delta \leq d_{xy} < \delta + \Delta$. Function $d_{xy} \to M_{3,3}$ is strictly increasing for $0 < d_{xy} \leq \Delta$ and for $\frac{\delta+\Delta}{2} < d_{xy} < \delta$, and decreasing for $\Delta < d_{xy} < \frac{\delta+\Delta}{2}$ and for $\delta \leq d_{xy} < \delta + \Delta$. The general expression for the $M_{3,3}$ can be found in Appendix.

We have

$$\lim_{d_{xy} \to \Delta^-} M_{3,3} = \frac{2\delta^2 - 2\Delta\delta + \Delta^2}{\delta^2(2\delta - \Delta)^2} < \frac{-2\Delta^2\delta + \Delta^3 + 2\delta^3 + \Delta\delta^2}{\Delta\delta^2(2\delta - \Delta)^2} = \lim_{d_{xy} \to \Delta^+} M_{3,3}$$

and

$$\lim_{d_{xy} \to \delta^-} M_{3,3} = \frac{-2\Delta^2\delta + \Delta^3 + 2\delta^3 + \Delta\delta^2}{\Delta\delta^2(2\delta - \Delta)^2} > \frac{2\delta^2 - 2\Delta\delta + \Delta^2}{\delta^2(2\delta - \Delta)^2} = \lim_{d_{xy} \to \delta^+} M_{3,3}.$$

We have positive jump $j(\delta) = \lim_{d_{xy}\to\Delta^+} M_{3,3} - \lim_{d_{xy}\to\Delta^-} M_{3,3} = \lim_{d_{xy}\to\delta^-} M_{3,3} - \lim_{d_{xy}\to\delta^+} M_{3,3}$,

$$j(\delta) = \frac{1}{\Delta(2\delta - \Delta)}.$$

There is no global maximum of $\det M$ for any Δ.

Now let us have $\delta = 2$. Then the function $d_{xy} \to \det M$ is strictly decreasing for $0 < d_{xy} < 1$ and strictly increasing for $1 < d_{xy} < 2$ and defined on the open set $(0, 2)$ (repetitions are not allowed!). So there exist no global maximum of $\det M$.

Now let $0 < \delta \leq 1$. If $d_{xz} < \delta$ then we have correlated case ($d_{xy} + d_{yz} = d_{xz}$) and for $d_{xz} \to \delta$ the supremum $\frac{3}{2}$ of $\det M$ for the correlated case is reached. Now let $d_{xz} = \delta + \Delta$ for $0 \leq \Delta < \delta$. Then we obtain behavior as in the previous case ($1 < \delta \leq 2$) and have no optimal design. For $\Delta \geq \delta$ has the element $M_{3,3} = E\left(-\frac{\partial^2 L}{\partial \delta^2}\right)$ form $\frac{2\delta^2 - 2\delta d_{xy} + d_{xy}^2}{\delta^2(-2\delta + d_{xy})^2}$, for $0 < d_{xy} < \delta$, 0, for $\delta \leq d_{xy} \leq \Delta$ and $\frac{d_{xy}^2 - 2\Delta d_{xy} + \delta^2 + \Delta^2}{\delta^2(d_{xy} - \Delta + \delta)^2}$ for $\Delta < d_{xy} < \delta + \Delta$. We clearly have no global maximum of $\det M$. Finally, we obtain:

Theorem 2 *([Müller and Stehlík 04]) Let $\{x, y, z\}$, $-1 \leq x < y < z \leq 1$ is proposed design, with variance parameter $\delta, 0 < \delta$. Then when both correlated and uncorrelated observations are possible ($0 < \delta \leq 2$), we have no exact optimal design (but still we find the best one on finite grid). When the only correlated observations are possible ($2 < \delta$), as in the fixed case, the minimum of the criteria function is attained for $\{-1, y, 1\}$ where y is arbitrary, $x < y < z$, which constitutes the set of D-optimum designs.*

3.3 Particular cases

Design for intercept

Now let us study the case, when there is **only one parameter, intercept,** ϑ_1, (δ is not the parameter of interest). Then criteria function has form

Proposition 9 *The following designs $\{x, y, z\}$, $-1 \leq x < y < z \leq 1$ are D-optimal:*

- *For the uncorrelated case ($\delta = 0$) is every design $\{x, y, z\}$ D-optimal.*
- *When both correlated and uncorrelated observations are possible ($0 < \delta \leq 2$), then for ($0 < \delta \leq 1$) every design $\{x, y, z\}$, where all $d_{ij} \geq \delta$ (only uncorrelated observations) is D-optimal. For ($1 < \delta \leq 2$) the designs $\{-1, -1 + \delta, 1\}$ and $\{-1, 1 - \delta, 1\}$ are D-optimal.*

- *When only correlated observations are possible ($\delta > 2$), the minimum of the criterion function is attained for $\{-1, y, 1\}$ where y is arbitrary.*

Proof *For* ***the uncorrelated*** *case ($\delta = 0$) we have $M_{1,1} = E\left(-\frac{\partial^2 L}{\partial \vartheta_1^2}\right) = 3$. When $2 < \delta$,* ***(only correlated measurements are possible)*** *the maximum of the information*

$$\det M = M_{1,1} = \frac{2\delta}{2\delta - d_{xz}}$$

is attained for $\{-1, y, 1\}$ where y is arbitrary, $x < y < z$.

Now let us suppose the most complex situation $0 < \delta \leq 2$ ***(some observations can be also uncorrelated).*** *If $d_{xz} < \delta$ then we have correlated case (because of $d_{xy} + d_{yz} = d_{xz}$) and for $d_{xz} \to \delta$ the supremum 2 of the information for the correlated case is reached. Now let $d_{xz} = \delta + \Delta$. The element $M_{1,1}$ has form $I(d_{xy})$ when only cov(x, y) is non-zero and $I(d_{yz})$ when only cov(y, z) is non-zero, where*

$$I(d) = \frac{d - 4\delta}{d - 2\delta}$$

is an increasing function and $\lim_{d \to \delta} I(d) = 3$. Further the element $M_{1,1}$ has form

$$J(x, y, z) = \frac{\delta^2 + 2\delta x - 2\delta z + 4y^2 - 4zy + z^2 - 4xy + 2zx + x^2}{\delta^2 + 2\delta x + 2y^2 - 2xy + x^2 - 2\delta z - 2zy + z^2}$$

when cov(x, y) and cov(y, z) are non-zero. Function $J(x, y, x + \delta + \Delta)$ is increasing for $d_{xy} > \frac{\delta+\Delta}{2}$ and decreasing for $d_{xy} < \frac{\delta+\Delta}{2}$ and

$$\lim_{y \to x+\delta-} J(x, y, x + \delta + \Delta) = \lim_{y \to x+\Delta+} J(x, y, x + \delta + \Delta) = I(\Delta).$$

□

Now let us discuss the particular case of **three-point design having the form** $\{-1, y, 1\}$, $-1 < y < 1$ with fixed δ, $0 < \delta \leq 1$. Then the information matrix and criteria function f have form $M_{1,1} = \frac{y+1-4\delta}{y+1-2\delta}$, $M_{1,2} = \frac{(1-\delta)(1+y)}{y+1-2\delta}$, $M_{2,2} = \frac{2\delta y + y - y\delta^2 - 2\delta + 1 - \delta^2}{y+1-2\delta}$ and $f(y) = -\log 2\delta \frac{2y - \delta y - \delta - 2}{y+1-2\delta}$ for $-1 < y \leq -1+\delta$, $M_{1,1} = 3$, $M_{1,2} = y$, $M_{2,2} = 2+y^2$ and $f(y) = -\log(2y^2+6)$ for $-1+\delta < y < 1-\delta$ and $M_{1,1} = \frac{y-1+4\delta}{y-1+2\delta}$, $M_{1,2} = \frac{(1-\delta)(1-y)}{y-1+2\delta}$, $M_{2,2} = \frac{2\delta y + y - y\delta^2 + 2\delta - 1 + \delta^2}{y-1+2\delta}$ and $f(y) = -\log 2\delta \frac{2y - \delta y + \delta + 2}{y-1+2\delta}$ for $1 - \delta \leq y < 1$. Function f is strictly decreasing on $(-1, -1 + \delta)$, increasing on $(1 - \delta, 1)$ and is even for $-1 + \delta < y < 1 - \delta$. The criteria function is continuous and for $0 < \delta < 1$ attains its minimum for points $-1 + \delta$ and $1 - \delta$ with the common value

$$-\log(8 + 2\delta^2 - 4\delta).$$

For $\delta = 1$ has optimal design the form $\{-1, 0, 1\}$, which coincidences with the result given by [Näther 85]. In the limit uncorrelated case ($\delta = 0$) there is no optimal design without repetitions, the criteria function attains its global minimum $-\log 8$ for designs $\{-1, -1, 1\}$ and $\{-1, 1, 1\}$. The Figure 10 illustrates overall behavior of criteria function for various y and $0 < \delta \leq 1$ ($x = -1$ and $z = 1$ are fixed).

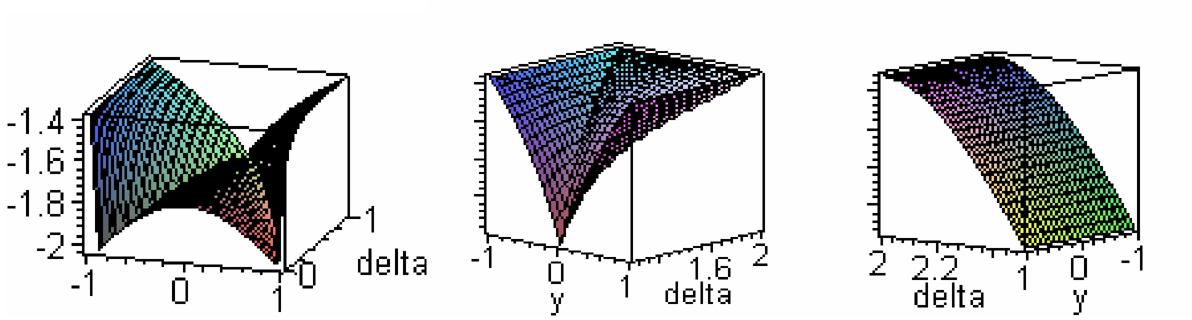

Figure 10: The criterion function.

Now let us have fixed δ, $1 < \delta \leq 2$. Then the information matrix and criteria function f have the forms $M_{1,1} = \frac{y+1-4\delta}{y+1-2\delta}$, $M_{1,2} = \frac{(1-\delta)(1+y)}{y+1-2\delta}$, $M_{2,2} = \frac{2\delta y+y-y\delta^2-2\delta+1-\delta^2}{y+1-2\delta}$ and $f(y) = -\log 2\delta\frac{2y-\delta y-\delta-2}{y+1-2\delta}$ for $-1 < y \leq 1-\delta$, $M_{1,1} = \frac{\delta^2-4\delta+4y^2}{\delta^2-4\delta+2y^2+2}$, $M_{1,2} = \frac{y\delta^2-4\delta y+4y}{\delta^2-4\delta+2y^2+2}$, $M_{2,2} = -\frac{y^2\delta^2-4\delta y^2-4+8\delta-2\delta^2}{\delta^2-4\delta+2y^2+2}$ and $f(y) = -\log 2\delta\frac{(4-\delta)(y^2-1)}{\delta^2-4\delta+2y^2+2}$ for $1-\delta < y < -1+\delta$ and $M_{1,1} = \frac{y-1+4\delta}{y-1+2\delta}$, $M_{1,2} = \frac{(1-\delta)(1-y)}{y-1+2\delta}$, $M_{2,2} = \frac{2\delta y+y-y\delta^2+2\delta-1+\delta^2}{y-1+2\delta}$ and $f(y) = -\log 2\delta\frac{2y-\delta y+\delta+2}{y-1+2\delta}$ for $-1+\delta \leq y < 1$. Continuous criteria function is strictly decreasing on $(-1, 1-\delta)$, increasing on $(-1+\delta, 1)$, is even for $1-\delta < y < -1+\delta$ and for $1 < \delta < 2$ attains its minimum in points $-1+\delta$ and $1-\delta$ with the common value

$$-\log 2\delta^2\frac{4-\delta}{3\delta-2}.$$

The Figure 10 pretty illustrates overall behavior of criteria function for various y and $1 < \delta \leq 2$ ($x = -1$ and $z = 1$ are fixed) again.

Now let us suppose $\delta > 2$. Then we obtain the constant (independent on y) criteria function. We have $M_{1,1} = \frac{\delta}{\delta-1}$, $M_{1,2} = 0$, $M_{2,2} = \delta$ and

$$f = -\log\frac{\delta^2}{\delta-1}.$$

The Figure 10 pretty illustrates overall behavior of criteria function for various y and $2 \leq \delta \leq 2.5$ ($x = -1$ and $z = 1$ are fixed). Note, that criteria function is decreasing function of covariance parameter δ and $\lim_{\delta\to+\infty} f(\delta) = -\infty$ holds. Have

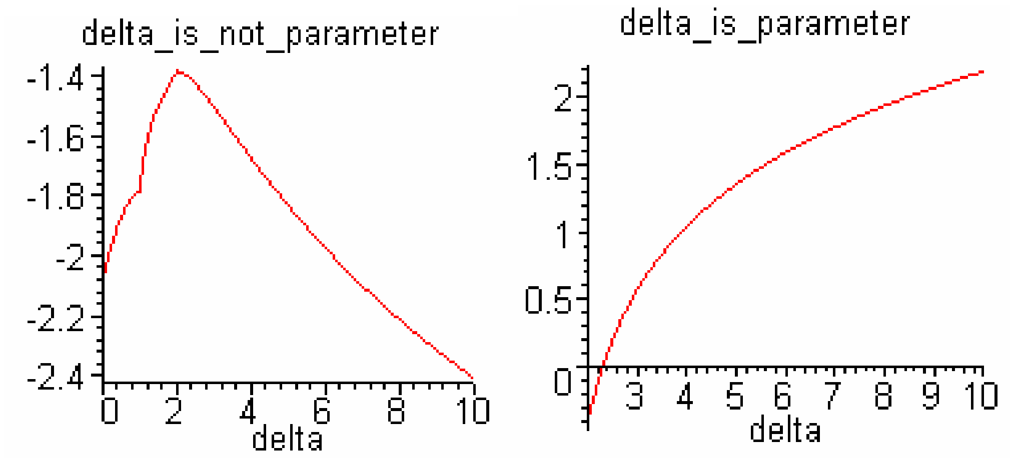

Figure 11: The minimum of criterion function.

a look on Figure 12, which plots this for various y and $0 \leq \delta \leq 8$ ($x = -1$ and $z = 1$ are fixed).

Now let us little speak about the minimum of the criteria function, function $\min \Phi(\delta)$, $0 \leq \delta$. This has a form

$$\min \Phi(\delta) = \begin{cases} -\log(8 + 2\delta^2 - 4\delta) & \text{if } 0 \leq \delta \leq 1; \\ -\log 2\delta^2 \frac{4-\delta}{3\delta-2} & \text{if } 1 < \delta < 2; \\ -\log \frac{\delta^2}{\delta-1} & \text{if } 2 \leq \delta. \end{cases}$$

Function $\min \Phi$ is continuous, strictly increasing for $0 \leq \delta < 1$, has zero left-handed derivation for $\delta = 1$ (notice on Figure 11!), strictly increasing for $1 < \delta < 2$, has zero right-handed derivation for $\delta = 2$ (notice on Figure 11!) and is strictly decreasing for $2 < \delta$. As we have already mentioned,

$$\lim_{\delta \to +\infty} \min \Phi(\delta) = -\infty.$$

The Figure 13 (see Figure 1 in [Müller and Stehlík 04]), which plots the value of the design criterion for various values of y and $0 < \delta \leq 2.5$, when $x = -1$ and $z = 1$ are fixed, makes the behavior of the optimal design very transparent. It is easy to see that minimal points lie along the main axes and that the design (at least the central point) gets irrelevant when the correlation is large enough.

Now δ is treated as **parameter of interest**. As we can see, an interesting global solution can only be found for $\delta > 2$. Then the information matrix and D-optimality criteria function Φ has the following form $M_{1,1} = \frac{2\delta}{2\delta - d_{xz}}$, $M_{1,2} = \frac{\delta(x+z)}{2\delta - d_{xz}}$,

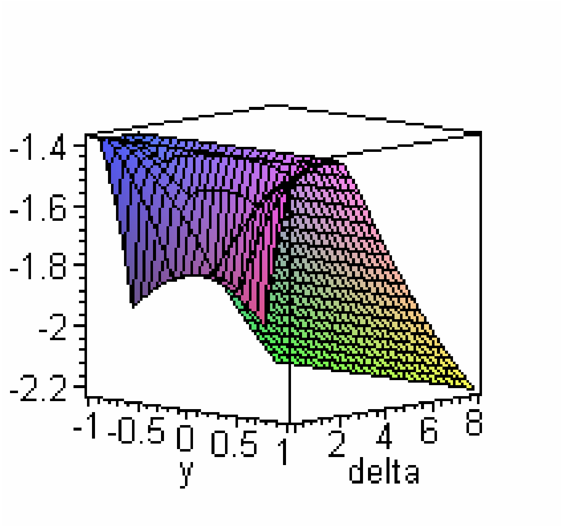

Figure 12: The criterion function.

$M_{2,2} = \delta\frac{2xz+\delta d_{xz}}{2\delta-d_{xz}}$ $M_{3,3} = \frac{3d_{xz}^2-8\delta d_{xz}+8\delta^2}{2\delta^2(2\delta-d_{xz})^2}$ and $M_{1,3} = M_{2,3} = 0$. The D-optimality criteria function Φ does not depend on y and has form

$$\Phi(d_{xz}) = -\log d_{xz}\frac{3d_{xz}^2 - 8\delta d_{xz} + 8\delta^2}{2(2\delta - d_{xz})^3}.$$

When we take an optimal design $\{-1, y, 1\}$, we obtain the minimal value of the criteria function for given parameter $\delta > 2$

$$\min \Phi(\delta) = -\log \frac{3 - 4\delta + 2\delta^2}{2(\delta - 1)^3},$$

(note, that function is defined only for $\delta > 2$!) and, despite the fixed-δ case, $\min \Phi(\delta)$ is strictly increasing for $\delta > 2$ and finally, reaches infinity

$$\lim_{\delta\to+\infty} \min \Phi(\delta) = +\infty.$$

Have a look on Figure 11, which plots the $\min \Phi(\delta)$ for $2 < \delta < 10$.

4 Appendix

Here we provide the expression for $M_{3,3}$ and g function. We have

$$M_{3,3} = \sum_i J_\delta(d_i)G(d_i)+\sum_{i\neq j} J_\delta(d_i)J_\delta(d_j)H(d_i, d_j)+J_\delta(d_{xy})J_\delta(d_{xz})J_\delta(d_{yz})h(d_{xy}, d_{xz}, d_{yz}),$$

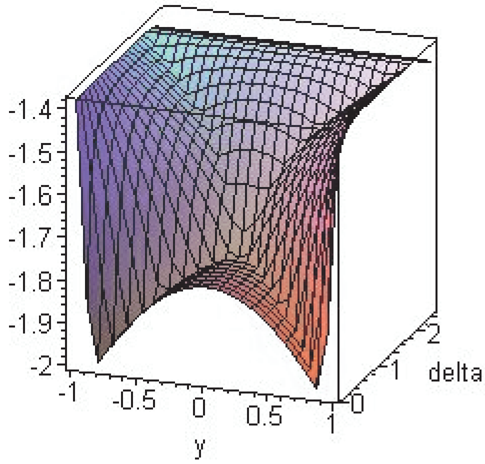

Figure 13: The criterion function.

where $d_i \in \{d_{yz}, d_{xy}, d_{xz}\}$, $G(d) = \frac{2\delta^2-2\delta d+d^2}{\delta^2(2\delta-d)^2}$,

$H(d_1,d_2) = (d_1^6 + d_2^6 + 7d_1^2\delta^4 - 10d_1^3\delta^3 + 8d_1^4\delta^2 - 4d_1^5\delta + 3d_1^4d_2^2 + 3d_1^2d_2^4 - 2d_1\delta^5 - 4d_2^5\delta + 7d_2^2\delta^4 - 10d_2^3\delta^3 + 8d_2^4\delta^2 - 2d_2\delta^5 + 6d_2\delta^3d_3d_1 - 6d_2\delta^2d_3d_1^2 - 2d_2\delta d_3d_1^3 - 2d_2^3\delta d_3d_1 + 12d_2^2\delta d_3d_1^2 - 8d_1^2d_2^3\delta + 14d_1^3\delta^2d_2 - 6d_1^2\delta^3d_2 - 8d_1^3\delta d_2^2 - 4d_1^4d_2\delta + 14d_1\delta^2d_2^3 - 2d_1\delta^4d_2 - 6d_1\delta^3d_2^2 - 4d_1\delta d_2^4 - 2d_2^4\delta d_3 + 2d_2\delta^4d_3 - 6d_2^2\delta^3d_3 + 6d_2^3\delta^2d_3 + 2d_1\delta^4d_3 - 6d_1^2\delta^3d_3 + 6d_1^3\delta^2d_3 - 2d_1^4\delta d_3 - 6d_2^2\delta^2d_3d_1)/\,(\delta^2(\delta^2 - 2d_1\delta + d_1^2 - 2d_2\delta + d_2^2)^3) - G(d_1) - G(d_2)$

and

$h(d_1,d_2,d_3) = (d_3^4\delta^2 + d_2^4\delta^2 + 4d_2\delta^2d_1d_3^2 + 4d_2\delta d_1d_3^3 + 4d_2^3\delta d_1d_3 - 8d_2^2\delta d_1d_3^2 - 4d_3^3\delta^2d_2 + 6d_3^2\delta^2d_2^2 - 4d_3\delta^2d_2^3 - 4d_2^3\delta^2d_1 - 4d_3^3\delta^2d_1 + 4d_2^2\delta^2d_1d_3 + d_1^4\delta^2 + 4d_2d_3\delta^2d_1^2 + 4d_2d_3\delta d_1^3 - 8d_2d_3^2\delta d_1^2 - 4d_1^3\delta^2d_3 + 6d_1^2\delta^2d_3^2 - 4d_2\delta^2d_1^3 + 6d_1^2\delta^2d_2^2 - 8d_3\delta d_1^2d_2^2 + 6d_2^2d_3^2d_1^2)/(\delta^2(d_1^2\delta + d_3^2\delta + d_2^2\delta - 2d_3\delta d_1 - 2d_2\delta d_1 - 2d_2d_3\delta + 2d_2d_3d_1)^2) - H(d_1,d_2) - H(d_2,d_3) - H(d_1,d_3) + G(d_1) + G(d_2) + G(d_3)$.

Function g can be written in the form

$$g(d_{xy}, d_{xz}, d_{yz}) = M_{3,3}\frac{2ad_{yz}d_{xy} - 2bd_{xz}d_{xy} - 2cd_{xz}d_{yz} + 2d_{xy}d_{xz} + 2d_{yz}^2}{1 - a^2 - b^2 - c^2 + 2abc},$$

where $a = (1 - \frac{d_{xz}}{\delta})J_\delta(d_{xz})$, $b = (1 - \frac{d_{yz}}{\delta})J_\delta(d_{yz})$ and $c = (1 - \frac{d_{xy}}{\delta})J_\delta(d_{xy})$.

5 Conclusion

We can conclude, that varying correlation brings more technical and theoretical challenges, still some problems can be overcome by careful choosing of some "benign", twice-differentiable covariance function. The comparison of both correlated and uncorrelated situations will need other criteria, which does not depend on regularity of the information matrix, like the G-criterion, which minimizes the largest expected variance of prediction over the region of interest (see [Fedorov and Hackl 97]). Still we are optimistic and such problem be one topic of our future research.

One of the most important problems, the application of the Fisher's information matrix, need to be justified. The only formal extension from the uncorrelated case bring some problems, e.g. as we have seen, the classical definition of the information matrix depends substantially on the covariance parameter and also the problem of finding the global minimum has occurred.

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