# UNIFORMLY OPTIMAL DESIGNS: A SPATIAL EXAMPLE*

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**ABSTRACT**
In this paper we consider optimal design of experiments in the case of correlated observations, for which the regression function is approximately linearly related to the covariance function. This situation may arise when observing a random field with a given covariance structure. Müller & Pàzman (2002) have further developed the concept of design measures for approximate information matrices for the construction of a design algorithm. We will utilize this algorithm for an example on spatial design.

**Key words**: regression experiment, correlated errors, random field, gradient algorithm, approximate information matrix.

**RESUMEN**
En este trabajo consideramos el diseño óptimo de experimentos en el caso de variables correlacionadas, para las cuales la función de regresión está relacionada aproximadamente en forma lineal con la función de covarianza. Esta situación puede aparecer cuando se observa un campo aleatorio con una estructura de covarianza determinada. Muller & Pàzman (2002) han desarrollado aún más el concepto de medidas de diseño para matrices de información aproximadas para la construcción de un algoritmo de diseño. Utilizamos este algoritmo en un ejemplo de diseño espacial.

MSC: 62K05

## 1. INTRODUCTION

Spatial data collection schemes usually exhibit two decisive features that distinguish them from classical regression designs (cf. the review paper by Fedorov, 1996). First, spatial observations are often determined by local correlations, which are unaccounted for by standard optimum design of experiments techniques. Second, at least in the framework of random field models, there is implicitly no possibility for instantaneously replicated measurements, so that the classical concept of design measures is not applicable. Müller & Pàzman (2002) have developed an extension of information matrices with a different definition of design measures, that allowed them to construct a design optimisation algorithms.

Still, however some heuristics are used in the definition of these algorithms: the problem is smoothed and designs are computed iteratively and without restrictions on the number of design points. In a simple direct approach, when the regression function is generated linearly by the covariance function (see Näther, 1985), the exact optimal designs can be readily derived from the resulting design measures. Thus this set-up will be considered in this note.

## 2. UNIFORMLY OPTIMAL DESIGNS

Let $\Xi$ denote the design space (a finite set of potential trials). At each $x \in \Xi$ one can observe a random field

$$y(x) = f^T(x)\theta + \varepsilon(x).$$

Here $f^T(x)\theta$ is the response function at x containing m unknown parameters $\theta = (\theta_1,\ldots, \theta_m)^T \in \Re^m$. The noise $\varepsilon(x)$ is supposed to have zero mean and a covariance function

$$Cov[\varepsilon(x), \varepsilon(z)] = \sigma^2 C(x,z),$$

with C(x,z) known, and $\sigma^2$ unknown.

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In some experiments the regression function f(x) is related to the covariance function C(x,z) by a linear relation

$$f(x) = \Sigma_{z \in D} C(x,z)\, r(z), \quad \forall\, x \in \Xi$$

where $D = \{x_1,\ldots,x_N\}$ is some finite set without replications (i.e. $x_i \neq x_j$ if $i \neq j$) and $r(z) \in \Re^m$ are given vectors. This set D is uniformly optimum among all exact designs with respect to any given convex design criterion $\Phi[.]$ (see Näther, 1985 or Müller & Pàzman, 2002 for a proof).

## 3. THE ALGORITHM

Perturbing the original random field by a design dependent virtual white noise allowed Müller & Pàzman (2002) to derive a standard iterative algorithm for the construction of design measures in the given context. Such an algorithm consists of a stepwise one-point correction of the design. That means at the n-th step we take

$$\xi_{n+1} = n\xi_n /(n+1) + \delta(.,x^*) /(n+1),$$

where $\xi_n$ is the design measure in the n-th step and $\delta(.,x^*)$ is the design measure concentrated at one point $x^*$. This point is chosen such as to minimize the directional derivative of the design criterion in the direction of $\delta(.,x^*)$. In the current situation this algorithm boils down to a very simple and elegant structure, namely to add measure according to the allocation rule:

$$x^* = \arg\min_{x \in \Xi} \xi_n^{-1}(x) \{d(x) - [\Sigma_{z \in \Xi} d(z)]\, \Im_{B\xi n}(x) / N_{B\xi n}\},$$

where

$$d(x) = a^T(x) \nabla\Phi[J] a(x),$$

with $a(x) = \Sigma_{z \in \Xi} [C^{-1}(\Xi)]_{x,z} f(z)$, and $J = \Sigma_{x,z \in \Xi} f(x)[C^{-1}(\Xi)]_{x,z} f(z)$, being the information matrix.

The gradient matrix $\nabla\Phi[J]$ of $\Phi[J]$ has entries $\partial\Phi[J]/\partial J_{ij}$; i,j = 1,…,m. The set of support points with maximal measure is denoted by $B_{\xi n}$ and its number by $N_{B\xi n}$. $\Im_{B\xi n}(x)$ stands for the indicator function corresponding to set B. As starting design the uniform design $\underline{\xi}$ on $\Xi$ is routinely chosen. Note that this algorithm, other than such attempting to directly calculate exact optimal designs, is very simple in structure and performs very quickly. The time consuming inversion of the covariance matrix needs only to be performed in the first step and the remaining computational operations at every iteration are of much lower complexity.

This algorithm yields a design measure, but since no a priori restrictions on the number of support points are imposed, the measure should always be uniform and supported on the whole $\Xi$. However, computations show that the measures resulting from the algorithm above are not uniform. The reason for this, we believe, is the use of the approximations for smoothing the problem. At this step some experimentation on the computer and some heuristics are unavoidable, especially because we still cannot exclude the possibility that there is some non-uniform $\xi_N^*$, which solves the optimisation problem. This non-uniform solution $\xi_N^*$ for $N = N_\Xi$ has an interesting feature: a larger value of $\xi_N^*(x)$ indicates that observations at x contain more information about the parameter $\theta$ (just as in the classical uncorrelated case). Since for uniformly optimal designs – and only for such – the amount of information is the same for $\underline{\xi}$ and the non-uniform solution D, we conjecture that our algorithm converges to a corresponding design measure $\xi_N^*$ in all such cases. This is corroborated by an interpretation in terms of norms given in Müller & Pàzman (2002).

## 4. A SPATIAL EXAMPLE

In set-ups from spatial contexts it is of utmost importance that we have quick and efficient algorithm for screening designs. It is obvious that the one given in Section 3 can be readily used for identifying uniformly optimal designs.

Let us, for example, consider the simple linear (spatial) regression

$$y(x) = (1, x_{[1]}, x_{[2]})\theta + \varepsilon(x); \quad x = (x_{[1]}, x_{[2]})^T \in [-1,1]^2$$

with the covariance function

$$C(x,z) = \begin{cases} (1-|x_{[1]}-z_{[1]}|)\cdot(1-|x_{[2]}-z_{[2]}|); & \max(|x_{[1]}-z_{[1]}|, |x_{[2]}-z_{[2]}|) < 1 \\ 0; & \max(|x_{[1]}-z_{[1]}|, |x_{[2]}-z_{[2]}|) \geq 1 \end{cases},$$

We applied the algorithm given in the previous section (for D-optimality, i.e. $\Phi[J] = -\log|J|$) to this example. Our gradient method (after just a few steps) yielded a design measure that practically collapses at the 9-point design D = {(-1,-1), (-1,0), (-1,1), (0,-1), (0,0), (0,1), (1,-1), (1,0), (1,1)}, as can be seen from Figure 1.

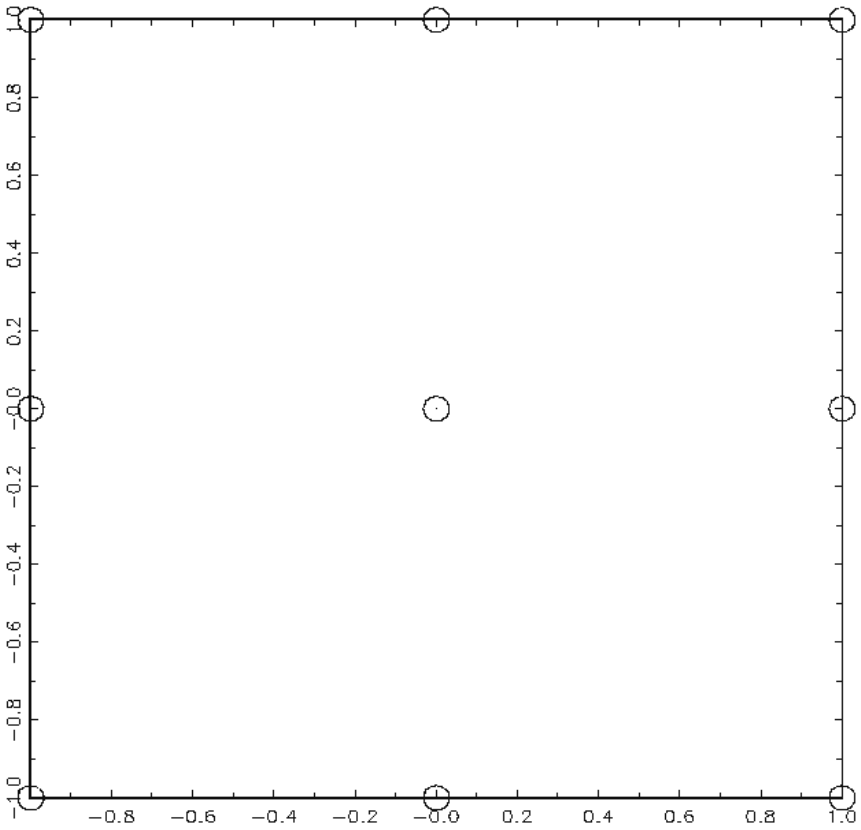


**Figure 1**. The calculated design measure for a spatial example; area of circles correspond to weights.

Indeed, for this design D = $\{z_1,\ldots z_9\}$ the condition for uniformly optimal designs in Section 2 holds obviously for all $x \in [-1,1]^2$, as can be further derived from

$$\begin{pmatrix} 1 \\ x_{[1]} \\ x_{[2]} \end{pmatrix} = C(x,z_1)\begin{pmatrix} 1 \\ -1 \\ -1 \end{pmatrix} + C(x,z_2)\begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix} + C(x,z_3)\begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix}$$

$$+ C(x,z_4)\begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} + C(x,z_5)\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + C(x,z_6)\begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} .$$

$$+ C(x,z_7)\begin{pmatrix} 1 \\ 1 \\ -1 \end{pmatrix} + C(x,z_8)\begin{pmatrix} 1 \\ 1 \\ -0 \end{pmatrix} + C(x,z_9)\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

This design is thus the optimum design giving the full information about $\theta$, which is contained in the random field $\{y(x): x \in [-1,1]^2\}$.

## 5. CONCLUSIONS

The example presented here demonstrates that the given gradient algorithm is of potential use in applications, especially in complex – e.g. spatial - settings, where enumerative methods are unfeasible.

Such applications can be found in various fields, especially in the design of computer simulation experiments (see Sacks *et al.*, 1989 for various set-ups). There, the covariance matrix is usually assumed to be known up to scalar parameter, which is certainly one of many possible directions of extending our technique. For a comparison of the method to alternative ones refer to Chapter 5 in Müller (2001).

## REFERENCES


FEDOROV, V.V. (1996): "Design of spatial experiments: model fitting and prediction", in Gosh, S. & Rao, C.R., eds., **Handbook of Statistics**, 13, Elsevier, Amsterdam 515-553.

MÜLLER, W.G. (2001): **Collecting Spatial Data. Optimum design of experiments for random fields**, 2nd edition, Physica Verlag, Heidelberg.

MÜLLER, W.G. & A. PAZMAN (2002): **Measures for designs in experiments with correlated errors**, submitted.

NÄTHER, W. (1985): **Effective Observation of Random Fields**, Teubner Texte zur Mathematik - Band 72, Teubner Verlag, Leipzig.

SACKS, J.; W.J. WELCH; T.J. MITCHELL and H.P. WYNN (1989): "Design and analysis of computer experiments", **Statistical Science**, 4(4): 409-435.