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ON SECOND ORDER SURFACES ESTIMATION AND ROTATABILITY

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ABSTRACT

The design of an experiment is an important component when collecting data to gain a deeper understanding of a problem. It is from the data collected that inferential statements concerning some phenomenon have to be made; therefore, we wish to extract as much relevant information as possible from the data collected. Depending on the nature of the problem, good designs may be very different. The special type of problem studied here is the estimation of second order response surfaces. This type of response surfaces are often used to locally approximate the response in a neighborhood of its maximum.

The first of the three papers included in the present study provides a brief overview of one of the most common designs of handling this problem. This design is a fractional two-level factorial design augmented with a star. An alternative design, called the complemented simplex design, is developed and compared with the augmented fractional factorial design. It is shown that the simplex design (up to six dimensions) is at least as good as the fractional factorial design with respect to a defined design criterion. The comparison is made within the class of rotatable designs. Unfortunately, it shows that the complemented simplex design cannot be made rotatable in more than six dimensions.

The second paper shows how saturated designs can be constructed from the complemented simplex design. These designs are compared with improved Koshal designs (up to six dimensions). Neither design was found to be superior to the other in all dimensions. Also, which design is superior depends on the design criterion.

The third paper illustrates the complexity of rotatability and the difficulties in measuring rotatability. A graphical method of presenting degree of/lack of rotatability is presented.

Key Words: Factorial Designs, Variance Function, D-optimality, Rotatability, Simplex Designs, Saturated Designs, Koshal Designs.

CONTENTS

Introduction

This thesis consists of three separate papers, all dealing with problems in the field of experimental designs. The problems have their origin in an industrial process, where an assumed relationship (of second order nature and with a known maximum) between a response variable and several explanatory variables exists. It is of interest to establish this relationship using as few observations as possible, due to the high cost connected to each observation.

The construction of experimental designs is one component in Response Surface Methodology (RSM), which comprises a group of statistical tools for model building and model exploitation. The type of problems in RSM have been discussed in numerous papers and textbooks over the years. One of the most important developers of RSM is George Box, who, with co-authors, wrote some classical papers in the early 1950s and is still going strong.

The designed experiment, when the assumed underlying model is of second order, is by tradition on one of the two forms: (i) a fraction of a two level factorial design, augmented with a star (composite design) or (ii) a fraction of a three level factorial design. A factorial design is a design where the factors (explanatory variables) only takes a few different values, two respectively three in the above mentioned designs. The star portion in the composite design consists of $2k$ points (k =# of factors) symmetrically placed out on the k axes in the factor space. Of these two designs, the composite design is the most often used and best understood design. The composite design have several desirable features. In general, it is not possible to construct a fractional three level factorial design, with the same nice properties as a composite design, using approximately the same number of design points.

One might now ask how we can construct a design, not necessarily a factorial design, for estimating a second order surface with a known maximum, using fewer observations than the smallest possible fractional composite design? Further, the accuracy of the estimated model must be about as good as that of the composite design.

If the underlying model had been of first order, the problem should be to find an alternative design to a fractional factorial two-level design. One such possible design is the simplex design. A regular simplex is defined by $k + 1$ points in k dimensions, with some fixed distance between all pairs of points. So, in the two dimensional case, take one observation in each corner of a triangle, and in the three dimensional case, take one observation in each corner of a tetrahedron. By adding a center point, we have

constructed a design consisting of $k + 2$ design points to estimate a model with $k + 1$ parameters.

In the first paper, the idea of using a simplex as a part of a design is further developed to also include second order surfaces. In order to estimate all parameters in the model, the simplex design must be complemented with additional design points. Even if it is possible to use this "complemented simplex design" for a full second order model, the paper deals with the problem in the situation when the maximum is known.

When the number of observations in a design is reduced to a minimum, i.e., to the number of parameters to estimate, we have what is called a saturated design. The second paper shows how saturated designs for different types of second order models can be constructed by removing points from the complemented simplex design. A saturated design for estimating a second order model was given by Koshal in 1933. This design is slightly improved, and thereafter compared with the design constructed from the complemented simplex design.

The third, and last, paper discusses some issues of rotatability. Under the conditions that the postulated model is correct, and an appropriate metric is chosen, a design is said to be rotatable if the distribution of information of the surface is spherically distributed about the design origin. The question whether a design is rotatable or not has been discussed since the 1950s, but the first papers to discuss how to measure the degree of/lack of rotatability were not published until 1988 (Draper & Guttman and Khuri). In this paper we concentrate on a graphical method, by Giovanitti-Jensen & Myers, for presenting the degree of/lack of rotatability.

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A Comparison of Two Designs for Estimating a Second Order Surface With a Known Maximum

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Abstract

Two level fractional factorial designs with a star are often used when working with lower polynomial models. In this paper an alternative design is discussed and compared with the fractional factorial design. We are working under the assumption that the true underlying model is of second order with a known maximum point.

Keywords: Fractional factorial design, Simplex, Variance function, Rotatability.

Contents

1 Background And Introduction

Quadratic Response Surface Methodology focuses on finding the optimum levels of some control variables $\xi = (\xi_1, \ldots, \xi_k)$, to optimize the value of y. Y is assumed to depend on the control variables through a polynomial function of second order. The two level fractional factorial design is well known, well described and well used in practice when working with lower polynomial models. The reasons for this are many. The design is easy to construct by hand and easy to understand. Also it allows you, in a first order model, to mix both qualitative and quantitative variables. In this paper we concentrate on second order models with only quantitative variables.

The construction of a design, i.e. the determination of design points, is today easily done with a computer. Say, for example, you wish to estimate a plane using a design with one observation in each corner of a tetrahedron. The coordinates of the design points is then derived with advantage by a computer. To choose one design before an other, because of its constructional benefits is no longer a valid argument.

The fractional factorial design is a good design in many situations, but should not be used blindly. When facing a new problem, it is of great importance to identify the most important goals. Say for example the model $Y = \alpha + \beta x + \gamma x^2 + \varepsilon$ is to be estimated. How can we choose the best design for doing this? Depending on if the primary goal is to minimize the joint confidence ellipsoid for all three model parameters (D-optimum design) or to minimize the confidence interval for γ (D_s-optimum design), different designs is to be considered as the best design. What is said with this is that designs that works well in some situations, should not be used without being checked in a new close related situation.

Another important aspect to look at, when comparing designs, is the number of experimental points used by the designs. Since each observation is connected with a cost, it is of interest to keep down the number of experimental points.

The problem discussed in this paper assumes that the optimum point is known, but it is of interest to estimate a whole region of the surface around this point. The problem can appear in an industrial process where the optimum point is known. Now the process

has to move, the reason can be environmental restrictions on the process or a possibility to produce to a lower cost. It is therefore of interest to explore the response surface around the optimum point.

Assume that the optimal point is $\xi_{opt} = (\xi_{1,opt}, \ldots, \xi_{k,opt})$ and that the expected response in this point is

$$\eta_{\xi_{opt}} = E[Y_{\xi_{opt}}],$$

where

$$Y_\xi = \beta'_0 + \sum_{i=1}^{k} \beta'_i \xi_i + \sum_{i=1}^{k} \beta'_{i,i} \xi_i^2 + \sum_{i=1}^{k} \sum_{j=1}^{i-1} \beta'_{i,j} \xi_i \xi_j + \varepsilon,$$

ε distributed as a $N(0,\sigma^2)$ random variable. Further we assume that the second order approximation of the surface is adequate over the region of interest.

Since the optimum point is known, it is possible to simplify the model by doing an origin shift. Let $\psi_i = \xi_i - \xi_{i,opt}$. A direct consequence of this transformation is that the new system will take its optimum value in the origin. Since the optimum point is known, the system satisfies

$$\left.\frac{\partial \eta_\psi}{\partial \psi_i}\right|_{\psi=\psi_{opt}=0} = 0, \; i = 1, \ldots, k.$$

Under these restrictions it is easily verified that the model can be written as

$$\eta_\psi = \beta''_0 + \sum_{i=1}^{k} \beta''_{i,i} \psi_i^2 + \sum_{i=1}^{k} \sum_{j=1}^{i-1} \beta''_{i,j} \psi_i \psi_j.$$

In next section is a design criterion defined and discussed. Thereafter follows two sections in which the two designs under investigation in this paper are defined, namely the fractional factorial design with a star and the simplex design with complement points. After that are the two designs compared and the last section puts the light on some final remarks.

2 One Way To Compare Designs

A designed experiment is defined by its design matrix **D**,

$$\mathbf{D} = \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1k} \\ x_{21} & x_{22} & \cdots & x_{2k} \\ \vdots & \vdots & & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{nk} \end{pmatrix}$$

where k is the number of explanatory variables and n is the number of experimental points in the design. Each row describes the setup for one experimental point, which is called a run.

A matrix of more importance is the designs **X**-matrix. This matrix depends both on the design matrix **D** and on the model chosen. For the special model in this paper the **X**-matrix looks like

$$\mathbf{X} = \begin{pmatrix} 1 & x_{11}^2 & x_{12}^2 & \cdots & x_{1k}^2 & x_{11}x_{12} & x_{11}x_{13} & \cdots & x_{1,k-1}x_{1k} \\ 1 & x_{21}^2 & x_{22}^2 & \cdots & x_{2k}^2 & x_{21}x_{22} & x_{21}x_{23} & \cdots & x_{2,k-1}x_{2k} \\ \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots & & \vdots \\ 1 & x_{n1}^2 & x_{n2}^2 & \cdots & x_{nk}^2 & x_{n1}x_{n2} & x_{n1}x_{n3} & \cdots & x_{n,k-1}x_{nk} \end{pmatrix} = \begin{pmatrix} \mathbf{x}_1 & \mathbf{x}_2 & \cdots & \mathbf{x}_n \end{pmatrix}^t.$$

On what grounds would we choose one design over the other when performing a designed experiment? Obviously there is a need for design criteria that helps us to choose the most appropriate design for solving a particular problem. One such criterion is based on the variance function V_x. The variance of a predicted response at a point $\mathbf{x}$ is given by $\mathrm{Var}(\hat{y}(\mathbf{x})) = \mathbf{x}^t(\mathbf{X}^t\mathbf{X})^{-1}\mathbf{x}\,\sigma^2$. The variance function is defined to be the standardized variance $V_x = (n/\sigma^2)\mathrm{Var}(\hat{y}(\mathbf{x}))$. When comparing designs it is helpful to use V_x rather than $\mathrm{Var}(\hat{y}(\mathbf{x}))$, since $\mathrm{Var}(\hat{y}(\mathbf{x}))$ always will be smaller if an extra design point is added to the design. It is of interest to hold down the number of experimental points, therefore should the designs be compared on a standardized basis. The following example shows the idea.

Ex. 1.

Consider the model $Y = \beta_0 + \beta_1 x + \varepsilon$.

Assume that the design with design matrix $\mathbf{D}_1$ is chosen,

$$\mathbf{D}_1 = \begin{pmatrix} 0 \\ 1 \\ 2 \\ 3 \end{pmatrix}, \quad \mathbf{X}_1 = \begin{pmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{pmatrix}.$$

Then is $\mathrm{Var}(\hat{y}(\mathbf{x})) = (\sigma^2/10)(2x^2 - 6x + 7)$ and $V_x = (4/10)(2x^2 - 6x + 7)$.

If we instead chose to use the design $\mathbf{D}_2$,

$$\mathbf{D}_2 = \begin{pmatrix} \mathbf{D}_1 \\ \mathbf{D}_1 \end{pmatrix}, \quad \mathbf{X}_2 = \begin{pmatrix} \mathbf{X}_1 \\ \mathbf{X}_1 \end{pmatrix}$$

then is $\mathrm{Var}(\hat{y}(\mathbf{x})) = (\sigma^2/20)(2x^2 - 6x + 7)$ and $V_x = (8/20)(2x^2 - 6x + 7)$.

If $\mathrm{Var}(\hat{y}(\mathbf{x}))$ is used as a design criterion, $\mathbf{D}_2$ is to prefer before $\mathbf{D}_1$, since the variance of a predicted value is lower in each point. A better design can always be found by replicating $\mathbf{D}_1$ several times. However, when using V_x as the design criterion the two designs are on equal footing, which of course makes sense in this case.

The use of V_x can also be motivated by arguing in the following manner. Assume we have two designs $\mathbf{D}_1$ and $\mathbf{D}_2$, consisting of n_1 and n_2 design points respectively. Each design gives us the possibility to estimate the predicted response $\hat{y}(\mathbf{x})$ in a point $\mathbf{x}$. Let $\mathrm{Var}_1(\hat{y}(\mathbf{x}))$ and $\mathrm{Var}_2(\hat{y}(\mathbf{x}))$ represent the variances of the predicted responses for the two designs. With respect to the variances of the estimated responses, is it better to replicate $\mathbf{D}_1$ n_2 times or is it better to replicate $\mathbf{D}_2$ n_1 times? In both situations are $n_1 \times n_2$ runs performed. By replicating the designs in the described way, the variance of the predicted response can be shown to be $\mathrm{Var}_1(\hat{y}(\mathbf{x})) / n_2$ and $\mathrm{Var}_2(\hat{y}(\mathbf{x})) / n_1$. We prefer $\mathbf{D}_1$ before $\mathbf{D}_2$ if

$$\mathrm{Var}_1(\hat{y}(\mathbf{x})) / n_2 \leq \mathrm{Var}_2(\hat{y}(\mathbf{x})) / n_1$$

or equivalently if

$$n_1 \mathrm{Var}_1(\hat{y}(\mathbf{x})) \leq n_2 \mathrm{Var}_2(\hat{y}(\mathbf{x})).$$

3 The Fractional Factorial Design With A Star

A widely used technique when estimating a second order surface, with k control variables, is to use a two level 2^{k-p} fractional factorial design, complemented with a star and a center point. The star portion of this design consists of the 2k points $(\pm\alpha,0,\ldots,0)$, $(0,\pm\alpha,0,\ldots,0)$, ... , $(0,\ldots,0,\pm\alpha)$ for some choice of α. A full two level factorial design consists of all possible combinations of $\xi_i = \xi_{i,opt} \pm S_i$, $i = 1,\ldots,k$. It is more convenient to work with a scaled version of the explanatory variables, namely $x_i = \psi_i / S_i = (\xi_i - \xi_{i,opt}) / S_i$. Then, the full two level factorial designs consist of all possible combinations of $x_i = \pm 1$, $i = 1,\ldots,k$, and the model is written as

$$\eta_x = \beta_0 + \sum_{i=1}^{k} \beta_{i,i} x_i^2 + \sum_{i=1}^{k} \sum_{j=1}^{i-1} \beta_{i,j} x_i x_j .$$

A fractional factorial design means that not all 2^k, but 2^{k-p} for some p, combinations of $x_i = \pm 1$, i=1,...,k are used in the design . An example illustrates the idea, for a more detailed description see Box & Draper [1987].

Ex. 2.

Consider the model $E[Y] = \beta_0 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{33} x_3^2 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3$.

The problem is to find the smallest fractional factorial design with a star (i.e. the design with the fewest number of experimental points) that can estimate all the parameters in the model. The design matrix $\mathbf{D}_{full}$, and its relating $\mathbf{X}_{full}$-matrix, for the full design are shown on next page.

The interaction terms in the model must be estimated from the factorial part of the design. There are 3 interaction terms in the model, so it is enough to have a 2^{3-1} design to estimate the interaction terms. The fraction used in the design can be chosen in different ways, some more attractive than others. By choosing the fraction where for all observations $x_{i1} \times x_{i2} \times x_{i3} = 1$, we ensure that no estimates of interaction terms are alias with other estimates of interaction terms. The final design matrix $\mathbf{D}_{frac}$ and its relating $\mathbf{X}_{frac}$-matrix are shown on next page.

$$\mathbf{D}_{\text{full}} = \begin{pmatrix} 1 & -1 & -1 \\ -1 & -1 & -1 \\ 1 & 1 & -1 \\ -1 & 1 & -1 \\ 1 & -1 & 1 \\ -1 & -1 & 1 \\ 1 & 1 & 1 \\ -1 & 1 & 1 \\ 0 & 0 & 0 \\ \alpha & 0 & 0 \\ -\alpha & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & -\alpha & 0 \\ 0 & 0 & \alpha \\ 0 & 0 & -\alpha \end{pmatrix}, \quad \mathbf{X}_{\text{full}} = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & 1 & -1 & 1 & -1 \\ 1 & 1 & 1 & 1 & 1 & -1 & -1 \\ 1 & 1 & 1 & 1 & 1 & 1 & -1 \\ 1 & 1 & 1 & 1 & -1 & -1 & -1 \\ 1 & 1 & 1 & 1 & -1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & -1 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & \alpha^2 & 0 & 0 & 0 & 0 & 0 \\ 1 & \alpha^2 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & \alpha^2 & 0 & 0 & 0 & 0 \\ 1 & 0 & \alpha^2 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & \alpha^2 & 0 & 0 & 0 \\ 1 & 0 & 0 & \alpha^2 & 0 & 0 & 0 \end{pmatrix}$$

$$\mathbf{D}_{\text{frac}} = \begin{pmatrix} 1 & -1 & -1 \\ -1 & 1 & -1 \\ -1 & -1 & 1 \\ 1 & 1 & 1 \\ 0 & 0 & 0 \\ \alpha & 0 & 0 \\ -\alpha & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & -\alpha & 0 \\ 0 & 0 & \alpha \\ 0 & 0 & -\alpha \end{pmatrix}, \quad \mathbf{X}_{\text{frac}} = \begin{pmatrix} 1 & 1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & 1 & -1 & 1 & -1 \\ 1 & 1 & 1 & 1 & 1 & -1 & -1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & \alpha^2 & 0 & 0 & 0 & 0 & 0 \\ 1 & \alpha^2 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & \alpha^2 & 0 & 0 & 0 & 0 \\ 1 & 0 & \alpha^2 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & \alpha^2 & 0 & 0 & 0 \\ 1 & 0 & 0 & \alpha^2 & 0 & 0 & 0 \end{pmatrix}$$

In general, the models discussed in this paper have

$$1+k+\binom{k}{2}=1+\frac{k}{2}+\frac{k^2}{2}$$

parameters, one intercept term, k quadratic terms and $\binom{k}{2}$ interaction terms. The smallest possible fraction that can be used to estimate the interaction terms consists of 2^{k-p} factorial points, where p is the largest integer such that $2^{k-p} \geq \binom{k}{2}$.

4 The Complemented Simplex Design

An alternative design to use is a simplex design complemented with some points. A simplex is defined by k+1 points in the k-dimensional space. I.e., in the plane a simplex is defined by a triangle and in 3 dimensions it is defined by a tetrahedron.

Now, construct a simplex in k dimensions, $\mathbf{x} = (x_1,\ldots,x_k)$, such that (i) each and one of the k+1 points are at the same distance from the origin and (ii) the distance between each pair of points is the same. Such simplex is called a regular simplex. The complemented simplex design is now defined by having one observation at the origin, one observation in each corner of the simplex (simplex points), and finally, one observation on each ray going from the origin and between each pair of corners (complement points). Altogether this is

$$1+(k+1)+\binom{k+1}{2}=2+\frac{3k}{2}+\frac{k^2}{2}$$

experimental points. Notice that the number of experimental points in this design exceeds the number of parameters in the model with k+1.

The construction of a regular simplex is straightforward. For example consider the case when k=3.

j	x_{1j}	x_{2j}	x_{3j}
1	1	1	1
2	-1	1	1
3	0	-2	1
4	0	0	-3
Scale factor	$\sqrt{2}$	$\sqrt{6}$	$\sqrt{12}$

Let p_i denote the i:th simplex point in the design and let p_{ij} denote the complement point on the ray between the i:th and j:th simplex point. The design matrix **D** is then defined by the design points

$$p_0 = \{0,0,0\}$$

$$p_1 = \{\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{6}}, \frac{1}{\sqrt{12}}\} \times d_s$$

$$p_2 = \{\frac{-1}{\sqrt{2}}, \frac{1}{\sqrt{6}}, \frac{1}{\sqrt{12}}\} \times d_s$$

$$p_3 = \{0, \frac{-2}{\sqrt{6}}, \frac{1}{\sqrt{12}}\} \times d_s$$

$$p_4 = \{0,0, \frac{-3}{\sqrt{12}}\} \times d_s$$

$$p_{12} = (p_1 + p_2) \times d_c$$

$$p_{13} = (p_1 + p_3) \times d_c$$

$$p_{14} = (p_1 + p_4) \times d_c$$

$$p_{23} = (p_2 + p_3) \times d_c$$

$$p_{24} = (p_2 + p_4) \times d_c$$

$$p_{34} = (p_3 + p_4) \times d_c$$

where d_s and d_c are constants that determines the simplex points and the complement points distances from the origin.

5 Comparing The Two Designs

It is of interest to find a good design that makes it possible to estimate the unknown parameters in the above described model. With a good design we mean a design that satisfies some properties like a high level of information and rotatability without using to many experimental points. A high level of information means that the variance of a predicted response is low. Rotatability means that the variance of a predicted response at a point **x** depends only on the distance between the origin and **x**. This means that we can write $V_x = V_\rho$, where $\rho = (x_1^2+...+x_k^2)^{1/2}$.

The two discussed designs will now be compared with respect to the variance function. The fractional factorial design with a star can always be made rotatable by putting the star points at the distance $(2^{k-p})^{1/4}$ from the origin, given that the factorial points are described in terms of 1 and -1 (and therefore are at the distance $\sqrt{k}$ from the origin). The Simplex design with complement points can be made rotatable by putting the complement points at a certain distance from the origin. Unfortunately is this only possible for k up to 6. Therefore will the two cases when $k \leq 6$ and when $k > 6$ be treated separately.

From now a fractional factorial design with a star and a center point will be called a factorial design, and a simplex design with complement points and a center point will be called a simplex design.

5.1 Comparison Up To 6 Dimensions

Assume in the simplex design that the simplex points are at distance one from the origin. The following table shows at which distances, d(k), the complement points should be to make the design rotatable. For k=2 is the design rotatable for any choice of d(k).

k	3	4	5	6
d(k)	$(4/9)^{1/4}$	$(12/16)^{1/4}$	$(32/25)^{1/4}$	$(100/36)^{1/4}$

The two rotatable designs will now be compared with respect to their variance functions. It is of interest to compare the volumes under the variance functions over a

defined region in the x-space. Assume we want to compare the designs over the region $A = \{\mathbf{x} ; \|\mathbf{x}\| \leq 1\}$ and that the model used is valid over the region $B = \{\mathbf{x} ; \|\mathbf{x}\| \leq b, b \geq 1\}$ (all the following results holds also if we define $A = \{\mathbf{x} ; -1 \leq x_i \leq 1, i = 1,\ldots,k\}$). For all rotatable designs discussed in this paper we have that Vol is of the form

$$\text{Vol} = \int_A V_x dx = c_1 + \frac{c_2}{d^4} + \frac{c_3}{d^2}.$$

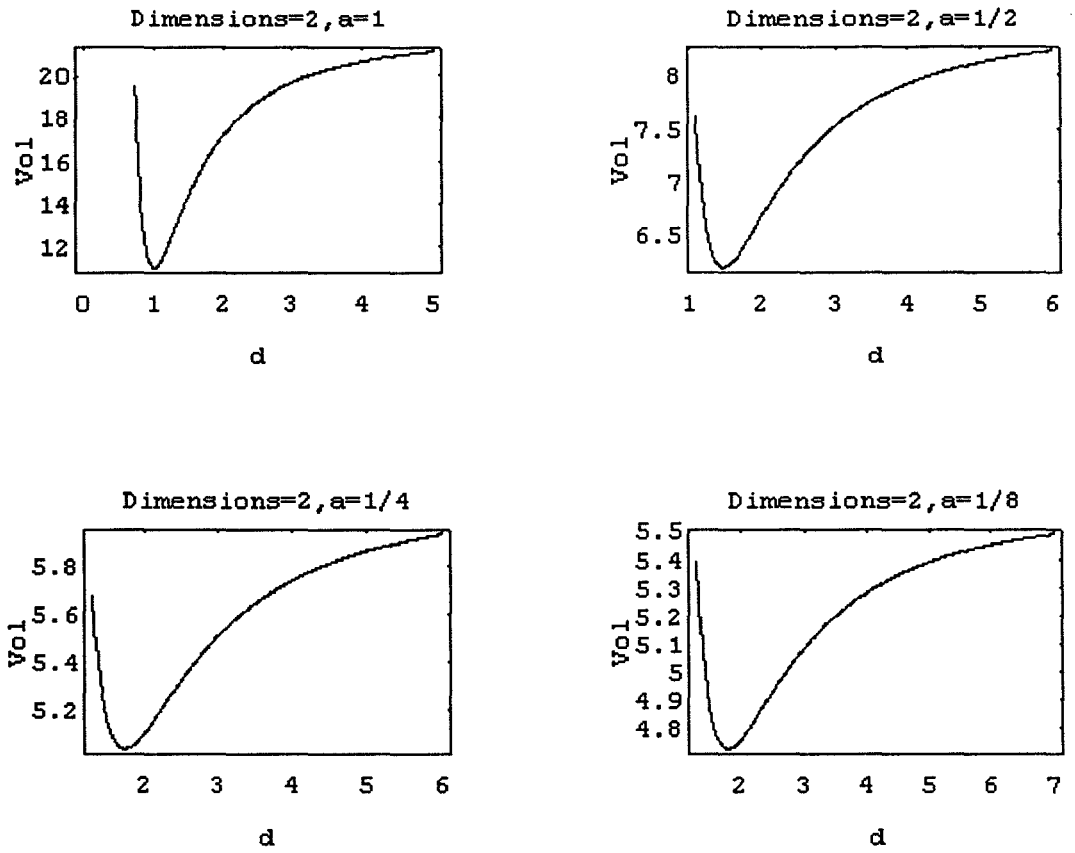
Now, for each k construct the rotatable factorial design that minimizes $\text{Vol} = \int_A V_x dx$ under the restriction that all design points belong to B, and do the same for the simplex design. The number of experimental points used in the two design are

k	2	3	4	5	6
Factorial	7	11	17	27	29
Simplex	7	11	16	22	29

The designs can now be compared with respect to Vol. In the following graphs the y-axis represents Vol, i.e. the volume under the variance function over the region A. The x-axis represents the distance from the origin to the outermost points in the rotatable design. For the factorial design this is always the distance from the origin to the factorial points. For the simplex design it is for $k \leq 4$ the distance from the origin to the simplex points and for $k \geq 5$ the distance from the origin to the complement points.

The case $k = 2$ needs some extra consideration. Let the simplex points in the simplex design be at distance d from the origin and the complement points at distance $a \times d$ from the origin with $a \leq 1$. It does not matter whether a is chosen to be smaller than 1 or greater than 1, since for $a = 1$ the simplex part of the design and the complementary part of the design are mirror images of each other. The simplex design is rotatable for any choice of a and d. The problem is to chose a and d in the best way, i.e., in a way that minimizes the volume under the variance function.

For a equals $1, \frac{1}{2}, \frac{1}{4}$ and $\frac{1}{8}$ respectively, we get the following graphs.

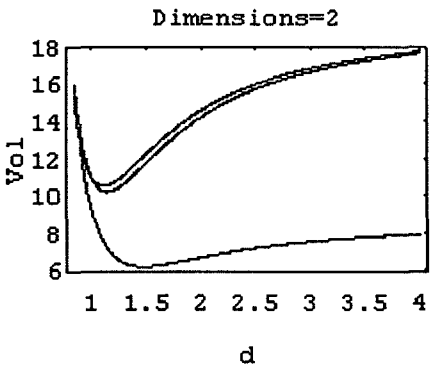


The graphs shows how the volume under the variance function changes with d. In each of the four cases there is a unique d that minimizes the volume. Note the different scales on the y-axis in the four graphs.

In practice a and d cannot be chosen arbitrarily. Say for example that the control variables can be controlled up to two decimals. That is, if a variable is set to be 0.50, it could be any value between 0.495 and 0.505. This gives an error of approximately 1 percent. If instead the variable was set to 0.05 (could happen for small a), the true value could be any value between 0.045 and 0.055. This gives an error of approximate 10 percent. So the smaller a is, the greater is the relative error in the controlled variable. How close to the origin the complement points can be is therefore determined by the accuracy of the controlled variables. A reasonable choice of a is $a = \frac{1}{2}$, meaning that the distance from the origin to the simplex points is twice as big as the distance between the origin and the complement points. This is what is used when comparing the simplex design with the factorial design in two dimensions.

There is also a limit on how far away from the origin the experimental points can be located. Experimental points cannot be located outside the region over which the model is valid. This means we must have $d \leq b$.

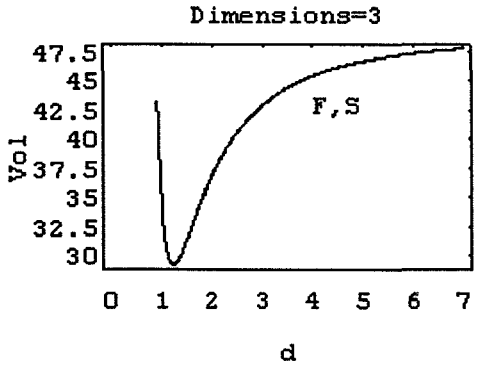
In the following graph are the two designs compared.

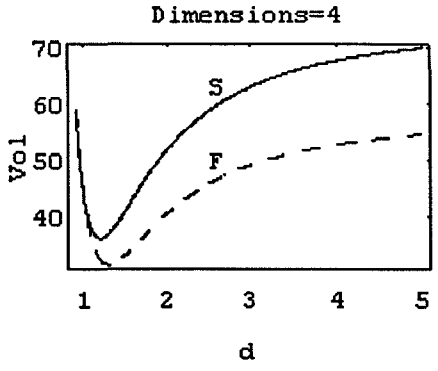


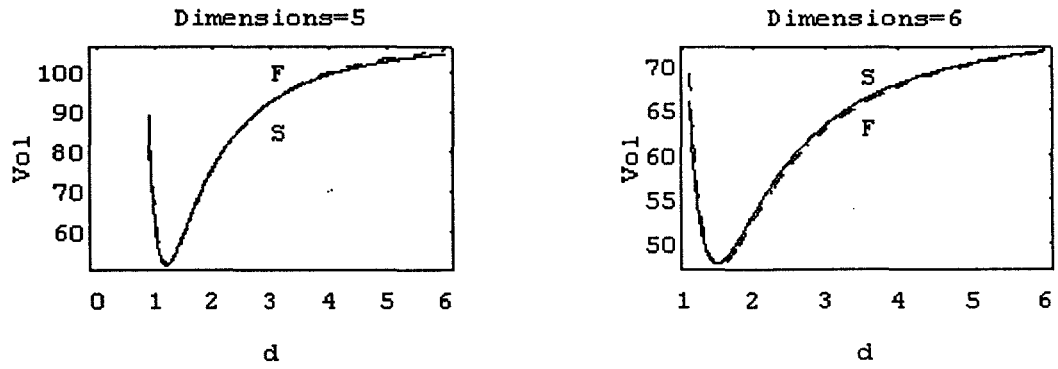
The two curves that are close together, are the curve for the factorial design and the curve for the simplex design when $a = 2^{-\frac{1}{4}}$. The reason for this choice of a is that this makes the distance between the simplex points and complement points in the simplex design the same as the distance between the factorial points and the star points in the factorial design. The lower curve in the graph is the curve when $a = \frac{1}{2}$.

With respect to the volume under the variance function, the two designs are almost identical when $a = 2^{-\frac{1}{4}}$. The smaller a can be chosen, the more superior is the simplex design. Also note that the simplex design with $a = \frac{1}{2}$ is superior the factorial design in the point where the factorial design is minimized.

Comparisons of the designs when $k = 3,\ldots,6$ are presented in the following graphs. The factorial design is abbreviated with F, and the simplex design with S.







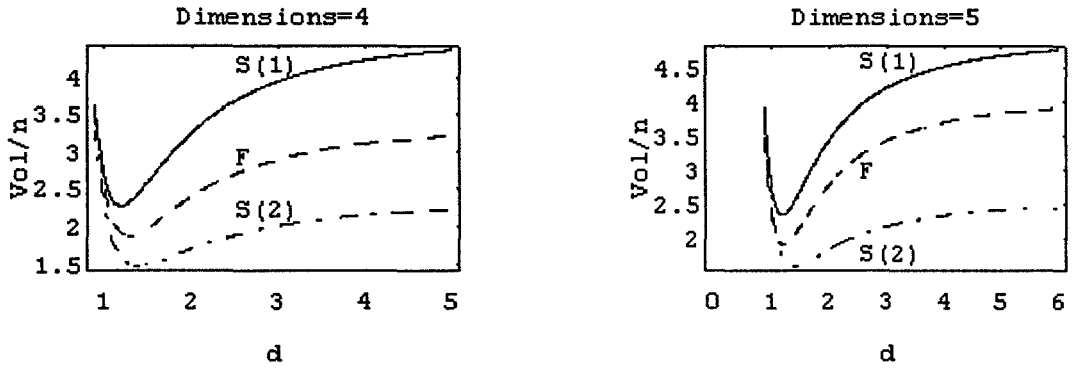
When k equals 3, the two designs are rotations of each other, and will therefore of course have the same variance function. When k equals 4 is the factorial design superior the simplex design. For k equals 5 and 6 are the two designs almost identical with respect to Vol.

In a practical situation, there is a cost tied up to each observation and it is not normally possible to replicate the design several times. Therefore, when one of two designs with unequal number of design points is to be chosen, and the smaller design produces less accurate estimates than the larger design, a decision has to be made whether more accurate predictions to the cost of more observations is to prefer before fewer observations to the cost of less accurate predictions. In this situation we are more interested to compare the volumes under $\mathrm{Var}(\hat{y}(\mathbf{x}))$ rather than the volumes under V_x, and keeping the number of observations used in mind. That is, we will study the graph Vol/n vs. d to detect the designs different ability to predict the response, and hereby, given the number of design points used by each design, decide which design is to prefer.

Designs with equal number of design points are easy to compare. In this situation we chose the design that produces the most accurate predictions. Also, if the design with the fewest number of design points produces more accurate predictions than its competitor, the choice of design is clear.

Let us see what happens when the simplex designs in 4 and 5 dimensions are extended with an extra center point. First we note that in 4 dimensions the simplex design and the factorial design have equally many design points and in 5 dimensions the simplex design has 4 design points less than the factorial design.

Now study the graphs of Vol/n vs. d.



In 4 dimensions we see that the simplex design with two center points works better than the factorial design. The result in 5 dimensions is more surprisingly. Despite the fact that the simplex design with two center points has 4 design points less than the factorial design, the variances of the predicted responses are smaller from this design.

To sum up, in 3 dimensions are the two discussed designs rotations of each other. In 6 dimensions the two designs have equally many design points. From a practical point of view it is irrelevant, with respect to Vol, which design to use. In 2, 4 and 5 dimensions the simplex design works better than the factorial design, after adding one extra center point to the simplex design in 4 and 5 dimensions. Still the number of design points will not exceed the number of design points in the factorial design.

5.2 More Than 6 Dimensions

As mentioned earlier, it is not possible to make the simplex design rotatable in dimensions higher than 6. To see why, we will first see when a design is rotatable.

For simplicity assume k=2. We have a design **D** and the relating **X**-matrix. When the true underlying model is of the kind discussed in this paper, it can be shown that the design is rotatable if the information matrix is of the form

$$\mathbf{X}'\mathbf{X} = \{\omega\}_{i,j} = \begin{pmatrix} \gamma & \delta & \delta & 0 \\ \delta & 3\lambda & \lambda & 0 \\ \delta & \lambda & 3\lambda & 0 \\ 0 & 0 & 0 & \lambda \end{pmatrix}$$

The extension to higher dimensions is obvious. Let us take a look at some of the elements in the information matrix when k=7. The simplex design is such that the simplex points are at distance 1 from the origin and the complement points are at distance d from the origin. For example, we need for a rotatable design that $\{\omega\}_{2,2} = \{\omega\}_{4,4}$. But in 7 dimensions is $\{\omega\}_{2,2} = \frac{1}{2} + \frac{49}{48}d$ and $\{\omega\}_{4,4} = \frac{7}{12} + \frac{49}{48}d$. Obviously there is no d to make $\{\omega\}_{2,2} = \{\omega\}_{4,4}$. As indicated here the simplex design in 7 dimensions can be made rotatable by letting d go to infinity. This is however a result of no practical value. And in higher dimensions is not possible at all to make the design rotatable. For example in 8 dimensions, we have $\{\omega\}_{2,2} = \frac{1}{2} + \frac{343}{288}d \approx \frac{1}{2} + 1.19\ d$ and $\{\omega\}_{4,4} = \frac{7}{12} + \frac{2107}{1728}d \approx \frac{7}{12} + 1.22\ d$. Of course we can not find any positive d to make the two elements equal.

6 Final Remarks

The classical use of simplex designs arises from problems where we have a restriction of the type $\sum_{i=1}^{k} x_i = 1$. This happens in applications where the proportion of x_i is the only thing that matters.

When thinking of a simplex and its ability to cover a region in the k-dimensional space using only $k+1$ points, and its symmetrical properties, one is tempted to extend the use of simplexes in the theory of experimental designs. In this paper one possible application has been discussed.

One extension of the model discussed in this paper is to let at least one factor affect the response variable independently of the other factors. For example we can have three factors interacting with each other and a fourth factor that does not interact with the three other factors. This model looks like

$$E[Y] = \beta_0 + \beta_{1,1}x_1^2 + \beta_{2,2}x_2^2 + \beta_{3,3}x_3^2 + \beta_{4,4}x_4^2 + \beta_{1,2}x_1x_2 + \beta_{1,3}x_1x_3 + \beta_{2,3}x_2x_3.$$

One could use any of the two designs presented in this paper, with a small modification, to estimate the parameters. For the example mentioned here, take the design for the three dimensional case. Each point in this design is of the type $p = \{v_1, v_2, v_3\}$. The design in four dimensions is now defined by all points of the type $p = \{v_1, v_2, v_3, 0\}$ and one additional point $\{0,0,0,\kappa\}$. This design is rotatable in $R^3 = \{\mathbf{x}\ ;\ x_4 = 0\}$. The choice of κ can be discussed. One may choose κ so that Vol is minimized, or one may prefer to choose κ in a way that makes the precision of predictions in the x_4 direction as equal as possible the precision of predictions in the x_1, x_2 and x_3 directions.

A related topic under examination is how saturated designs, i.e. designs that have equally many design points as parameters to estimate, can be constructed when the true underlying surface is of second order. The maximum point may or may not be known. One or several factors may or may not interact with the other factors.

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Saturated Designs for Second Order Models

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1994

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Abstract

Construction of saturated designs for different types of second order models are discussed. Also a comparison between two types of saturated designs for the full second order model is presented.

Keywords: D-optimal, Koshal design, Rotatability, Simplex Design.

CONTENTS

1 Introduction

The complemented simplex design, see Claes Ekman [1994], has good properties when estimating a second order surface with a known maximum up to 6 dimensions. It can be made rotatable and it is at least as good as a fractional factorial design with a star with respect to some alphabetic optimality criteria. In this paper we discuss how saturated designs, i.e. designs having equally many design points as parameters to estimate, can be constructed when estimating a second order surface.

We assume that the underlying surface has a maximum. The maximum point may or may not be known. We may also let any predictor interact or not interact with any other predictor.

A simplex is defined by $k+1$ points in k dimensions. A regular simplex is a simplex where all points are at the same distance from the center of the simplex, and the distance between each pair of points is the same. The complemented simplex design is defined by having one design point in each corner of the simplex, called simplex points, and one design point on each ray that goes from the center of the simplex and between each pair of simplex points, called complement points, and eventually, one or several center points. The simplex points are denoted p_i, $i = 1,\ldots,k+1$, and the complement points are denoted p_{ij}, $i = 1,\ldots,k$, $j = i+1,\ldots,k+1$. The design point p_{ij} is the complement point on the ray that goes between the simplex points p_i and p_j.

2 The Models And The Designs

In the following subsections are saturated designs for some different types of second order models described.

2.1 Second Order Model With Unknown Maximum Point

The second order model looks like

$$E[Y] = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum_{i=1}^{k} \sum_{j=1}^{k-1} \beta_{ij} x_i x_j$$

where Y is the response variable and $x_1, \ldots, x_k$ are the predictors. This model has

$$1 + k + k + \binom{k}{2} = 1 + \frac{3k}{2} + \frac{k^2}{2}$$

parameters. The complemented simplex design, without centerpoints, has

$$k + 1 + \binom{k+1}{2} = 1 + \frac{3k}{2} + \frac{k^2}{2}$$

design points and is therefore a saturated design.

2.2 Second Order Model With Known Maximum Point

When the maximum point is known, the model can be simplified by doing an origin shift. The model can now be written as

$$E[Y] = \beta_0 + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \sum_{i=1}^{k} \sum_{j=1}^{k-1} \beta_{ij} x_i x_j .$$

This model has

$$1 + k + \binom{k}{2} = 1 + \frac{k}{2} + \frac{k^2}{2}$$

parameters. Consider the design consisting of one center point and the complement points in a complemented simplex design. This design has

$$1+\binom{k+1}{2}=1+\frac{k}{2}+\frac{k^2}{2}$$

design points and is therefore saturated.

2.3 When Some Predictors Do Not Interact With The Other

The first case to consider is when one predictor does not interact with any of the other predictors. We will now find a saturated design for this type of model. Start with the saturated design for the model with the $k-1$ interacting factors. Each design point in this design is of the type $p=\{v_1,\ldots,v_{k-1}\}$, say. The design for the model where one predictor does not interact with the other predictors consists of the design points of the type $p=\{v_1,\ldots,v_{k-1},0\}$, and one or two additional points. Two additional points are required if we do not know the maximum point, and therefore need both the linear and quadratic term in the model. If the maximum point is known, it is enough to have the quadratic term in the model. If two additional points are needed, take them as $\{0,\ldots,0,\pm\alpha\}$, if only one is needed, any of the two will do.

If we have two predictors not interacting with the others, the design consists of the points of the type $p=\{v_1,\ldots,v_{k-2},0,0\}$ and also the points $\{0,\ldots,0,\pm\alpha,0\}$ and $\{0,\ldots,0,0,\pm\alpha\}$. Further extension is obvious.

We could also think about a more messy situation when we allow all predictors to interact or not interact with any other predictor. If the simplex is constructed as described in Claes Ekman [1994] the design may be reduced in the following way.

The design point p_{ij} is the complement point that contains most information about the interaction between x_{i-1} and x_{j-1}. Therefore, if there is no interaction between x_{i-1} and x_{j-1}, p_{ij} is removed from the design. This means that the complement points that are left in the design, are those that contains most information about the interaction terms in the model.

3 Another Saturated Design

It is not easy to find examples of saturated designs in the literature for models in general. However, for polynomial models there exists saturated designs called Koshal designs, see Koshal[1933]. The idea behind the construction of such designs is very intuitively. How to proceed is best shown through an example.

Assume we are working in three dimensions. The model looks like

$$E[Y] = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{33} x_3^2 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3 .$$

There are 10 parameters to estimate, so we are looking for a design with 10 design points. Take one observation in the origin, (0,0,0), to estimate the intercept term. Next, to estimate the linear terms, take observations in (1,0,0), (0,1,0) and (0,0,1). To estimate the quadratic terms, take observations in (2,0,0), (0,2,0) and (0,0,2). Finally, the interaction terms are estimated by observations in (1,1,0), (1,0,1) and (0,1,1). The design matrix **D** looks like

$$\begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{pmatrix}$$

This design is very asymmetrical around the origin, but can be substantially improved. First, the design points used for estimating the quadratic terms can be exchanged with the points (−1,0,0), (0,−1,0) and (0,0,−1). Second, the design points used for estimating the interaction terms can be more spread out by exchange them with the points (1,1,0), (−1,0,1) and (0,−1,−1). The **D** matrix for this new design looks like

$$\begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \\ 1 & 1 & 0 \\ -1 & 0 & 1 \\ 0 & -1 & -1 \end{pmatrix}$$

The design points for estimating the interaction terms in the improved design, are constructed by following rules.

- If the number of explanatory variables is odd, then change the "interaction points" in the original Koshal design so that each coordinate is represented with equally many 1 as −1.
- If the number of explanatory variables is even, then change the "interaction points" in the original Koshal design so that the coordinates for half of the explanatory variables is represented with one more 1 than −1. The other half is represented with one more −1 than 1.

The already described example illustrates the idea when k is odd. When k is even, say $k = 4$, the following "interaction parts" of the original Koshal design and the improved design are obtained

$$\begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 1 \end{pmatrix}, \quad \begin{pmatrix} 1 & 1 & 0 & 0 \\ -1 & 0 & -1 & 0 \\ 1 & 0 & 0 & -1 \\ 0 & -1 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & -1 & -1 \end{pmatrix}.$$

4 A Measure On Rotatability

One aspect of interest when looking at designs is whether the design is rotatable or not. When comparing two non-rotatable designs, one might ask which one is most rotatable?

Designs for the special model we wish to compare here, that is the full second order model, are rotatable just when the information matrices are of a special form. What this form looks like is exemplified for the special case when $k = 2$, extension to higher dimensions is straightforward. The matrix is symmetric, therefore is only the upper triangle shown.

$$\{\omega\}_{ij} = \begin{pmatrix} \gamma & 0 & 0 & \delta & \delta & 0 \\ . & \delta & 0 & 0 & 0 & 0 \\ . & . & \delta & 0 & 0 & 0 \\ . & . & . & 3\lambda & \lambda & 0 \\ . & . & . & . & 3\lambda & 0 \\ . & . & . & . & . & \lambda \end{pmatrix}$$

Assume now we have a design **D** and its relating **X**-matrix. Further assume that the information matrix, $\mathbf{X}^t\mathbf{X}$, for this design looks like

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} & a_{15} & a_{16} \\ . & a_{22} & a_{23} & a_{24} & a_{25} & a_{26} \\ . & . & a_{33} & a_{34} & a_{35} & a_{36} \\ . & . & . & a_{44} & a_{45} & a_{46} \\ . & . & . & . & a_{55} & a_{56} \\ . & . & . & . & . & a_{66} \end{pmatrix}$$

The question we asks us is how much does this information matrix deviate from a rotatable design's information matrix? Let

$$A_0 = \left\{ a_{ij} \middle| \{\omega\}_{ij} = 0, \forall \text{ i and } j \geq i \right\}$$

$$A_\delta = \left\{ a_{ij} \middle| \{\omega\}_{ij} = \delta, \forall \text{ i and } j \geq i \right\}$$

$$A_\lambda = \left\{ \frac{a_{ij}}{k} \middle| \{\omega\}_{ij} = k\lambda, k \in \{1,3\}, \forall \text{ i and } j \geq i \right\}$$

Let the number of elements in A_ℓ be n_ℓ, $\ell \in \{\delta, \lambda\}$. Now form

$$\bar{a}_\ell = \frac{\sum_{A_\ell} a_{ij}}{n_\ell}, \quad \ell \in \{\delta, \lambda\}.$$

The measure of rotatability is now defined as

$$\text{Rot} = \sum_{A_0} (a_{ij} - 0)^2 + \sum_{\ell \in \{\delta,\lambda\}} \sum_{A_\ell} \left(a_{ij} - \bar{a}_\ell\right)^2$$

The design is rotatable whenever $\text{Rot} = 0$.

5 The Improved Koshal Design Vs. The Complemented Simplex Design

The complemented simplex designs are naturally divided in two sets of experimental points, the simplex points and the complement points. Also the Koshal designs can be divided in a similar way, by the interaction points, the star points and the center point. In the following when the two designs are compared, we allow the different sets of experimental points to be at any distance from the origin. Of course, we cannot have design points outside the region over which the model is valid. For simplicity, assume the model is valid only over the unit sphere.

The primary criteria used when comparing the two designs is the D-criteria. A design is said to be D-optimal if it maximizes the determinant of the information matrix. This means that the joint confidence ellipsoid for the parameter estimates is minimized. The two designs are constructed in a way that maximizes the determinants of their respectively information matrices. Thereafter are the measures of deviation from a rotatable design calculated.

The results up to 6 dimensions are summarized in the following table. Det stands for the determinant of the information matrix, Rot stands for the measure of deviation from a rotatable design. In the simplex designs, d(0;s) is the distance from the origin to the simplex points in the D-optimal design and d(0,c) is the distance from the origin to the complement points. In the Koshal designs, d(0,s) is the distance from the origin to the star points and d(0,i) is the distance from the origin to the interaction points.

	SIMPLEX				**KOSHAL**			
Dim	**d(0,s)**	**d(0,c)**	**Det**	**Rot**	**d(0,s)**	**d(0,i)**	**Det**	**Rot**
2	0.77	1	1.63	0.50	1	1	4	2.63
3	0.87	1	0.25	1.73	1	1	1	4.06
4	0.91	1	0.012	6.47	1	1	0.062	10.6
5	0.93	1	$1.7\ 10^{-4}$	15.1	1	1	$9.8\ 10^{-4}$	13.5
6	0.95	1	$7.6\ 10^{-7}$	28.7	1	1	$3.8\ 10^{-6}$	24.1

We can see from the table that the improved Koshal designs are superior the complemented simplex designs with respect to Det. However, in 2,3 and 4 dimensions the complemented simplex designs have a smaller value on Rot, and will therefore provide a more uniform information of the response surface. In 5 and 6 dimensions are the improved Koshal designs better than the complemented simplex designs also with respect to Rot.

The complemented simplex designs suffer from the lack of a center point. Let us see what happens if an extra center point is added to each design.

	SIMPLEX				KOSHAL			
Dim	**d(0,s)**	**d(0,c)**	**Det**	**Rot**	**d(0,s)**	**d(0,i)**	**Det**	**Rot**
2	1	1	30.4	0	1	1	8	2.63
3	1	1	9.36	3.06	1	1	2	4.06
4	1	1	0.72	8.97	1	1	0.12	10.6
5	1	1	0.015	18.6	1	1	$2.0\ 10^{-3}$	13.5
6	1	1	$9.2\ 10^{-5}$	32.6	1	1	$7.6\ 10^{-6}$	24.1

Now are the complemented simplex designs superior the improved Koshal designs with respect to Det. With respect to Rot are the complemented simplex designs better than the improved Koshal designs in 2,3 and 4 dimensions. Specially, in 2 dimension is the complemented simplex design rotatable. In 5 and 6 dimensions are the improved Koshal designs still better than the complemented simplex designs with respect to Rot. From this one can conclude that a center point is valuable for a design.

Saturated designs do not allow estimation of the error, and should therefore be handled with care. By adding one or several center points, this drawback is eliminated.

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A NOTE ON ROTATABILITY

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1994

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Abstract

The need of a measure of rotatability is discussed and exemplified through some examples. The examples also shows the difficulties with measuring rotatability. A graphical technique for exploring the variance function is discussed.

Keywords: Measure of Rotatability, Graphical Approach.

CONTENTS

1 Introduction

When constructing designs, rotatability is one property that has to be considered. A design is said to be rotatable if there exists a point $\mathbf{x}_0$ (the designs center point) such that the variance of a predicted value in a point $\mathbf{x}$, $\mathrm{Var}(\hat{y}(\mathbf{x}))$, only depends on the distance between $\mathbf{x}_0$ and $\mathbf{x}$, and of course on the experimental error. See Box and Draper [1987].

For some classes of models, rotatable designs can always be constructed. Specially, this is true for polynomial models (Box and Draper [1987]). For other types of models, or when blocked designs are used, it may not be possible to find an exact rotatable design. Another situation when a rotatable design not can be found, is when the number of experiments that are required not can be performed.

This leads us to the problem of measuring rotatability. This is a fairly new topic in the theory of construction of designs and has its origin in two articles from 1988, Khuri [1988] and Draper and Guttman [1988]. These two articles deals with single number measures of rotatability. A design's departure from a rotatable design can take many forms. Also is the departure different at different distances from the design center. This complexity makes it impossible, which is also mentioned by Draper and Guttman[1988], to describe the degree of/lack of rotatability with a single number. Giovanitti-Jensen and Myers [1989] suggest a graphical method of assessing the degree of/lack of rotatability, using what they call a variance dispersion graph.

In next section we will study an example to emphasize the complexity of rotatability. Thereafter is the graphical method presented together with an alternative method for constructing such graphs. The last section includes a brief discussion of the problem with measuring rotatability, and some words about a related property to rotatability, but not so well understood or examined.

2 An Example of a Non-Rotatable Design

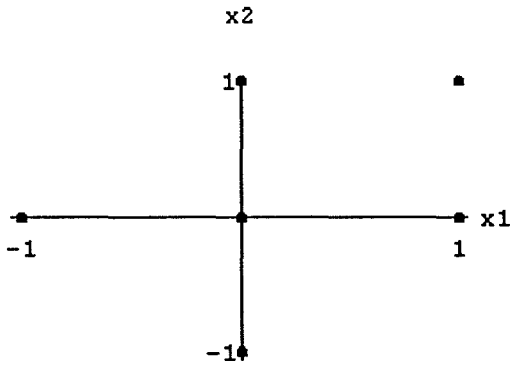
Consider following situation. We have a response variable Y and two explanatory variables x_1 and x_2. Over a well defined region we want to determine the functional relationship between the response variable and the explanatory variables. The usual assumptions of i.i.d. normally distributed measurement errors are assumed. We know that the relationship is on one of the two forms;

$$\text{(i)} \quad E[Y] = \beta_0 + \beta_1 x_1 + \beta_2 x_2$$
$$\text{(ii)} \quad E[Y] = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{12} x_1 x_2$$

Now assume that the collection of data is of such nature that changing the levels of the explanatory variables and the preparations for a set of runs are connected with great costs. Because of this we like to perform only one set of runs, minimum of six observations to be able to estimate model (ii), and to use as few levels as possible. One possible design meeting these restrictions is the design with design matrix

$$\mathbf{D} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \\ 0 & -1 \\ 1 & 0 \\ -1 & 0 \\ 1 & 1 \end{pmatrix}$$

What this design looks like is shown in next figure. As seen, the design has an



asymmetrical pattern, and we would not expect it to be rotatable. Intuitively one would guess that the variance of the predictions are lower when both x_1 and x_2 are greater

than zero, compared with other points at the same distance from the origin. The variance of a predicted value in any point $\mathbf{x}$, can be shown to be

$$\mathrm{Var}(\hat{y}(\mathbf{x})) = \mathbf{x}^t (\mathbf{X}^t\mathbf{X})^{-1} \mathbf{x}\, \sigma^2$$

where $\mathbf{X}$ is the designs $\mathbf{X}$-matrix and σ^2 is the variance of the experimental error and $\hat{y}(\cdot)$ is the fitted model.

We are now interested in studying $\mathrm{Var}(\hat{y}(\cdot))$ at fixed distances from the origin. To do this, introduce polar coordinates

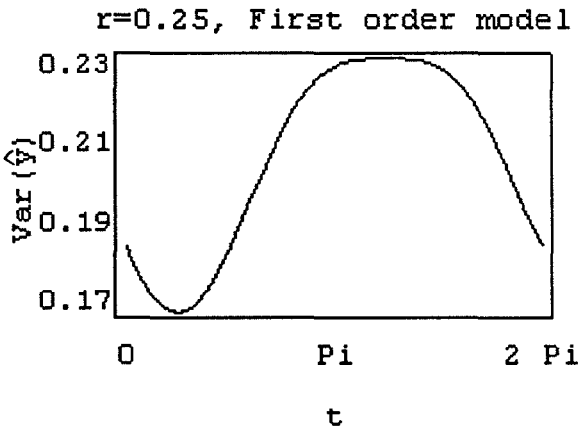
$$\begin{cases} x_1 = r\cos(t) \\ x_2 = r\sin(t) \end{cases}$$

where $r \in (0,\infty)$ and $t \in (0,2\pi)$. Now, hold r fixed and let t go from 0 to 2π. By constructing graphs for some different values of r, we will get a good picture of how $\mathrm{Var}(\hat{y}(\cdot))$ behaves in different directions and how this behavior depends on r.

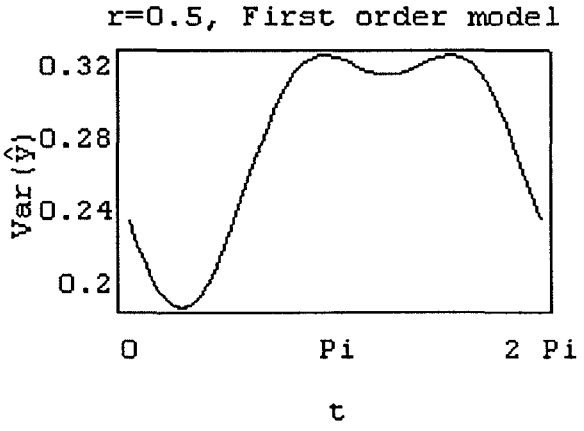
Let us now examine model (i) and model (ii) one by one.

2.1 Examination of the first order model

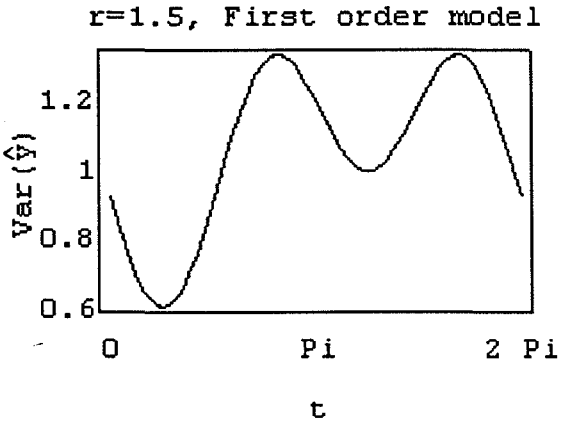
For $r = 0.25$ we obtain the following graph. Not surprisingly, the best predictions are

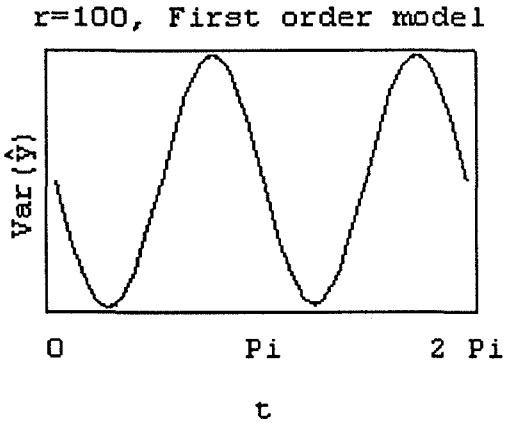


made in the direction $t = \pi/4$, i.e. in the direction towards the design point (1,1). The worst prediction are made in the opposite direction, $t = 5\pi/4$. When $r = 0.5$, next graph, $\mathrm{Var}(\hat{y}(\cdot))$ looks somewhat different. The best predictions are still made in the direction of $t = \pi/4$. However, the worst predictions are now made in two new directions, $t = 5\pi/4 \pm t_r, r = 0.5$. When r gets large, t_r tends to $\pi/2$.



From a practical point of view it is of interest to study $\mathrm{Var}(\hat{y}(\cdot))$ for moderate values of r (r not much larger than the distance from the design center to the outermost design point), but from a theoretical viewpoint, also large values of r are of interest. The two following graphs shows the behavior of $\mathrm{Var}(\hat{y}(\cdot))$ when $r = 1.5$ and $r = 100$.



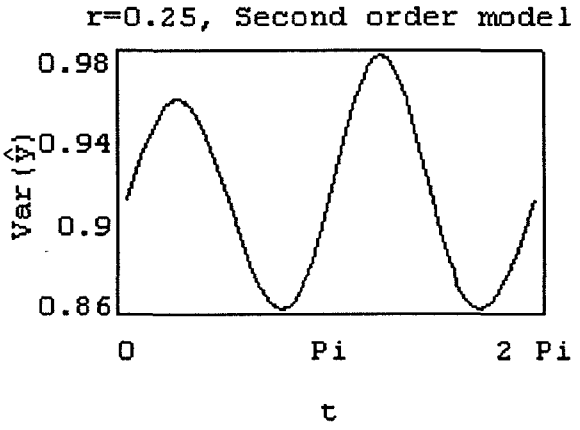


The last graph, $r = 100$, does not show the values of $\mathrm{Var}(\hat{y}(\cdot))$. What is interesting is the shape of $\mathrm{Var}(\hat{y}(\cdot))$. The best predictions are made in the two directions $t = \pi/4$ and $t = 5\pi/4$, for large r, and the worst predictions are made in the two directions $t = 3\pi/4$ and $t = 7\pi/4$. Notice that for small values of r, $t = 5\pi/4$ is the worst direction for predictions, but as r gets larger the predictions are better and better (relative other directions) and asymptotically it is the best direction together with $t = \pi/4$.

We have seen that even for the simplest of models, the degree of/lack of rotatability will not be easily described. Let us now examine the second order model.

2.2 Examination of the second order model

This model is somewhat more complicated than the first order model. Still, intuitively, it is reasonable to believe that predictions are made with greater accuracy in the direction $t = \pi/4$. By studying the graph of $\mathrm{Var}(\hat{y}(\cdot))$ when $r = 0.25$ we see that this is not true for small values of r.

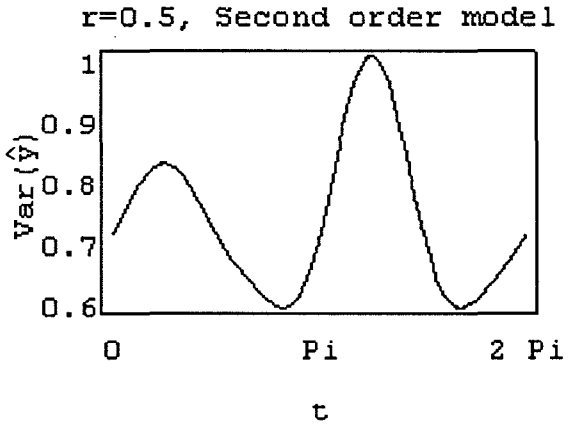


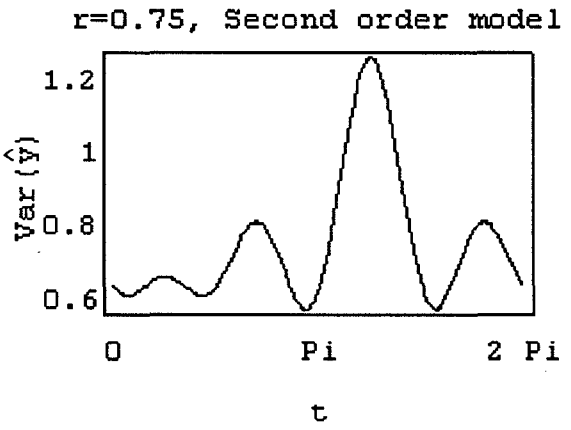
In fact, the best predictions are made in the directions $t = 5\pi/4 \pm t_r, r = 0.25$. When r tends to zero, it can be shown that t_r tends to $\pi/2$. Further, when r is small, $\mathrm{Var}(\hat{y}(t = \pi/4)) \approx \mathrm{Var}(\hat{y}(t = 5\pi/4))$, and $t = \pi/4$ and $t = 5\pi/4$ are the worst directions of predictions. So compared with the first order model is the situation very different.

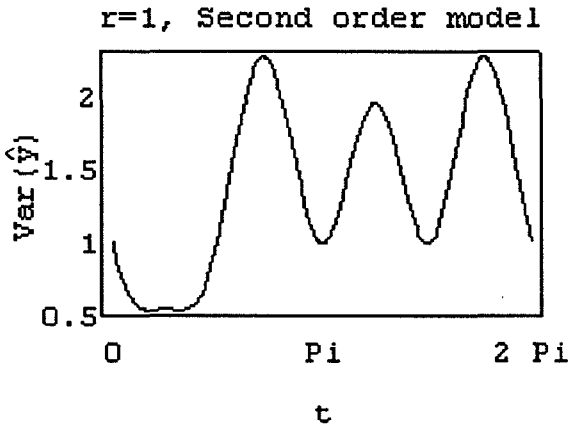
By introducing polar coordinates, and then study $\mathrm{Var}(\hat{y}(\mathbf{x})) = \mathbf{x}^t(\mathbf{X}^t\mathbf{X})^{-1}\mathbf{x}\,\sigma^2$, for small values of r, one will gain a mathematical understanding of the behavior of $\mathrm{Var}(\hat{y}(\cdot))$ close to the origin. However, it is not easy to see intuitively why $\mathrm{Var}(\hat{y}(\cdot))$ behaves as it does in the graph above. So even in this trivial example with a simple

design and a well understood model, the behavior of $\mathrm{Var}(\hat{y}(\cdot))$ at fixed distances from the design center is not easy to grasp.

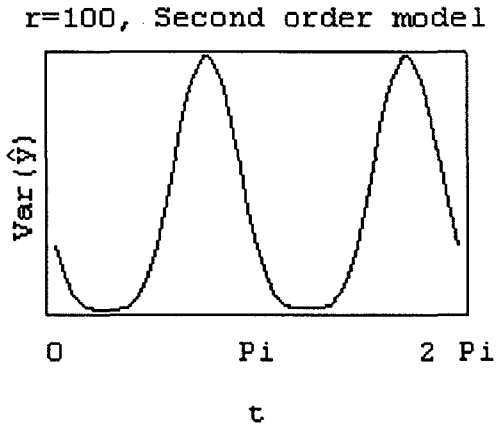
What follows is a sequence of graphs for some different values of r, namely $r = 0.5$, $r = 0.75$ and $r = 1$. The purpose is to show how different $\mathrm{Var}(\hat{y}(\cdot))$ looks at different distances, and also to show the complexity of $\mathrm{Var}(\hat{y}(\cdot))$ at some fixed distances.







The shape of $\mathrm{Var}(\hat{y}(\cdot))$ for the second order model, remains more and more of the shape of the corresponding function for the first order model, when r gets large. This is verified by studying $\mathrm{Var}(\hat{y}(\cdot))$ when $r = 100$. One can see that the curves of $\mathrm{Var}(\hat{y}(\cdot))$, $r = 100$, for the first order model and the second order model have the same characteristics, even if they not are exactly identical.



2.3 Mathematical examination of the variance functions

As seen, the form of $\mathrm{Var}(\hat{y}(\cdot))$ can be very complex at some distances and will not be easily expressed in mathematical terms. When r tends to zero or infinity the expression of $\mathrm{Var}(\hat{y}(\cdot))$ is simplified, and it is worthwhile to study these special cases to learn more about the behavior of the function.

Let V_1 denote $\mathrm{Var}(\hat{y}(\cdot))$ in the first order case, and V_2 the same function in the second order case. The following results are easily verified.

$$
\begin{aligned}
V_1 &\to a_1 + a_1' \sin(t + \pi/4) \quad \text{as} \quad r \to 0, \\
V_1 &\to b_1 + b_1' \sin(2t) \quad \text{as} \quad r \to \infty, \\
V_2 &\to a_2 + a_2' \sin(2t) \quad \text{as} \quad r \to 0, \\
V_2 &\to b_2 + b_2' \sin(2t)\,(1 - \sin(2t)/2) \quad \text{as} \quad r \to \infty
\end{aligned}
$$

This explains why V_2 is so flat when $2t$ is close to $\pi / 4$ and $5\pi / 4$ for large r in the second order model. To see this, let $u = 2t$. A Taylor expansion of $\sin(u)$ around $u = \pi / 4$ (the case $u = 5\pi / 4$ is similar), gives $\sin(u) \approx 1 - (u - \pi / 4)^2 / 2$. Therefore is $\sin(u)\,(1 - \sin(u) / 2) \approx 1 / 2 - (u - \pi / 4)^4 / 8$. That is, in a neighborhood of $u = \pi / 4$ can the function be approximated with a fourth order polynomial function with multiple roots in $\pi / 4$.

3 The Variance Dispersion Graph Approach

A design is said to be rotatable if $\mathrm{Var}(\hat{y}(\cdot))$ is constant on spheres of radius r, centered at the designs center. This means that a non-rotatable design is not constant on spheres, and a natural way of measuring the departure from rotatability is to find $\max\{\mathrm{Var}(\hat{y}(\cdot))\}$ and $\min\{\mathrm{Var}(\hat{y}(\cdot))\}$ on the spheres.

We can now construct a variance dispersion graph by plotting $(\max\{\mathrm{Var}(\hat{y}(\cdot))\}, \min\{\mathrm{Var}(\hat{y}(\cdot))\})$ against r for some appropriate chosen values of r.

The problem is to find $\max\{\mathrm{Var}(\hat{y}(\cdot))\}$ and $\min\{\mathrm{Var}(\hat{y}(\cdot))\}$, for a given r. We have seen in the previous section, that even in a simple situation, $\mathrm{Var}(\hat{y}(\cdot))$ can have a rather complex form.

Giovanitti-Jensen and Myers [1988] suggest two different solutions depending on if the model is of first order or second order. In the first order case it can be shown that $\max\{\mathrm{Var}(\hat{y}(\cdot))\} = (1/N + \lambda_{max} r^2)\sigma^2$ and $\min\{\mathrm{Var}(\hat{y}(\cdot))\} = (1/N + \lambda_{min} r^2)\sigma^2$ where λ_{max} and λ_{min} are the largest and the smallest eigenvalues of $(\mathbf{X}^t\mathbf{X})^{-1}$. In the second order case they use a search algorithm (not described in the paper) to find an optimum. The problem with using such algorithm is commented upon by the authors in their paper and their reflection of this problem is partly reproduced in the following quotation.

> "In many situations, multiple locations exist for the maximum value of the variance on a particular sphere. As in the case of many optimization routines in which one has nonlinear equality constraints and the objective function is this complex, there is no guarantee of finding the global optimum."

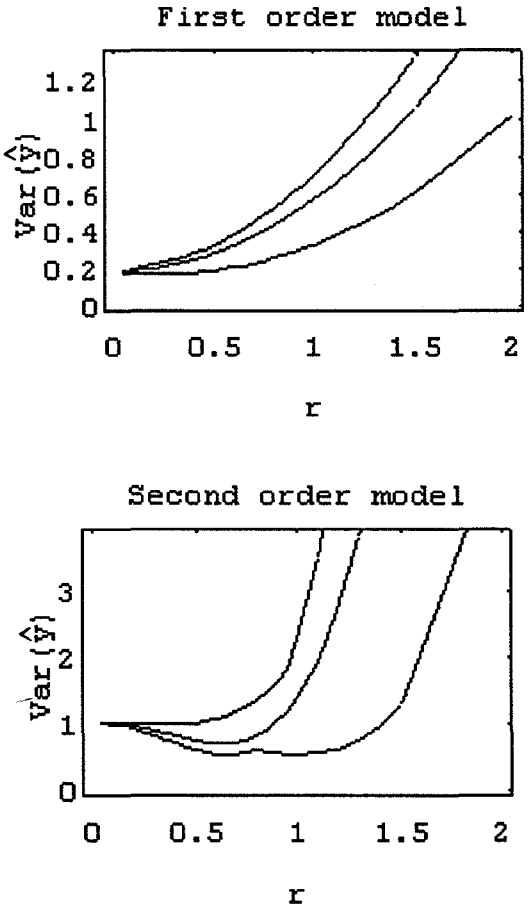
This is a problem that not should be underestimated. Consider the graph of the second order model when $r = 1$. There is local optimum at the point $t = \pi/4$. If the value of $\mathrm{Var}(\hat{y}(\cdot))$ in this point is reported as $\max\{\mathrm{Var}(\hat{y}(\cdot))\}$, this will of course affect the variance dispersion graph negative.

What we need to do is to find all local maxima and minima on the spheres, and then find out which ones are global. This can be done using Lagrange multiplicator. After solving the nonlinear equation system

$$\begin{aligned} \frac{\partial L}{\partial x_1} &= 0 \\ &\vdots \\ \frac{\partial L}{\partial x_k} &= 0 \\ \frac{\partial L}{\partial \lambda} &= 0 \end{aligned}$$

where $L = \mathrm{Var}(\hat{y}(\mathbf{x})) - \lambda(\sum_{i=1}^{k} x_i^2 - r^2)$, it is easily verified which of the optimum values that is global.

It is also useful in the variance dispersion graph, for each r, plot the mean of $\mathrm{Var}(\hat{y}(\cdot))$ on the sphere. If ψ_r is the surface area of the sphere U_r at distance r, the mean is found as $\psi_r^{-1} \int_{U_r} \mathrm{Var}(\hat{y}(\mathbf{x}))\, d\mathbf{x}$. Below is shown what these graphs looks like for the two examples in the previous section.



For studying the characteristics of a design, with respect to rotatability, the variance dispersion graph is useful. When coming to a situation when a visual examination of the graphs not is enough for discriminating between several designs, one need a measure of the degree of/lack of rotatability to be able to pick one of the proposed designs. A measure close related to the variance dispersion graph is the area between the upper and the lower curve. The smaller the better and an area equals zero means that the design is rotatable.

4 Discussion

Rotatability is a property which is important when predictions in all directions are of equal interest. In many situations it is not possible to construct an exact rotatable design, but it shows that in many situations you can often find an almost rotatable design, without suffering (to much) from other nice properties of the design. It is therefore of interest to learn how to compare designs with respect to rotatability, and learn how to construct almost rotatable designs in different situations.

The examples shows the difficulties in understanding the behavior of $\mathrm{Var}(\hat{y}(\cdot))$. Also one can understand the difficulties in measuring the degree of/lack of rotatability with a single value. In a rotatable design is $\mathrm{Var}(\hat{y}(\cdot))$ constant for each fixed value of r, i.e. the graphs in section 2 had been straight lines parallel to the x-axis. It is not hard to imagine that the departure from rotatability can take many forms.

Rotatability implies constant variance on spheres centered at the design center. Taking this one step further, one wishes constant variance over all spheres. That is, constant variance over the whole region of interest. Is it possible to construct such designs? This is a problem that has not been discussed in the literature.

A rotatable design is represented as a single curve in the variance dispersion graph. A design with constant variance over the whole region of interest, would be represented as a line parallel to the x-axis. With this knowledge, one can construct measures of how close a design is to meet the condition of a "constant variance design", and this is a first step in the search of designs with this desired property.

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