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**A COMPARISON OF TWO DESIGNS
FOR ESTIMATING A SECOND ORDER
SURFACE WITH A KNOWN MAXIMUM**

by

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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.

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1 Background And Introduction

Quadratic Response Surface Methodology focuses on finding the optimum levels of some control variables $\xi = (\xi_1, \dots, \xi_k)$, 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 in the three dimensional space by having one observation in each corner of a tetrahedron. The coordinates of the design points can be 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 that has been on for a long time, and by experience 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 $\xi_{\text{opt}} = (\xi_{1,\text{opt}}, \dots, \xi_{k,\text{opt}})$ and that the expected response in this point is

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

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 by doing an origin shift to simplify the model. Let $\psi_i = \xi_i - \xi_{i,\text{opt}}$. 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 has to satisfy that

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

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 a criterion for choosing between designs is defined. 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. 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 \mathbf{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 \mathbf{X} -matrix. This matrix depends both on the design matrix \mathbf{D} and on the model chosen. For the special model in this paper the \mathbf{X} -matrix looks like

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

On what grounds would we choose one design over the other when performing a designed experiment? Obviously there is a need for design criteria's that help us to choose the most appropriate design for solving a particular problem. One such criteria to study is the variance function $V_{\mathbf{x}}$. The variance of a predicted response at a point \mathbf{x} is given by $\text{Var}(\hat{y}(\mathbf{x})) = \mathbf{x}^t (\mathbf{X}^t \mathbf{X})^{-1} \mathbf{x} \sigma^2$. The variance function is defined to be the standardized variance $V_{\mathbf{x}} = (n/\sigma^2) \text{Var}(\hat{y}(\mathbf{x}))$. When comparing designs it is helpful to use $V_{\mathbf{x}}$ rather than $\text{Var}(\hat{y}(\mathbf{x}))$ since $\text{Var}(\hat{y}(\mathbf{x}))$ 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,

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

Now is $\text{Var}(\hat{y}(\mathbf{x})) = (\sigma^2/10)(2x^2 - 6x + 7)$ 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 $\text{Var}(\hat{y}(\mathbf{x}_i)) = (\sigma^2/20)(2x_{i1}^2 - 6x_{i1} + 7)$ and $V_x = (8/20)(2x_{i1}^2 - 6x_{i1} + 7)$.

If $\text{Var}(\hat{y}(\mathbf{x}))$ is used as a design criteria, the design \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 criteria the two designs are on equal footing, which of course makes sense in this case.

The use of V_x can also 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

$\text{Var}_1(\hat{y}(\mathbf{x}))$ and $\text{Var}_2(\hat{y}(\mathbf{x}))$ represent the variance of the predicted response for the two designs. With respect to the variances of the estimated response, 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 $\text{Var}_1(\hat{y}(\mathbf{x}))/n_2$ and $\text{Var}_2(\hat{y}(\mathbf{x}))/n_1$. We prefer \mathbf{D}_1 before \mathbf{D}_2 if

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

or equivalently if

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

3 The Fractional Factorial Design With A Star

A widely used technique when estimating a second order surface, in 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 $(\pm\alpha, 0, \dots, 0)$, $(0, \pm\alpha, 0, \dots, 0)$, \dots , $(0, \dots, 0, \pm\alpha)$ for some choice of α . A full two level factorial design consists of all possible combinations of $\xi_i = \xi_{i, \text{opt}} \pm S_i$, $i = 1, \dots, k$. It is more convenient to work with a scaled version of the explanatory variables, namely $x_i = \psi_i / S_i = (\xi_i - \xi_{i, \text{opt}}) / S_i$. Then, the full two level factorial designs consist of all possible combinations of $x_i = \pm 1$, $i = 1, \dots, k$, and the model is written as

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

A fractional factorial design means that not all 2^k , but 2^{k-p} for some p , combinations of $x_i = \pm 1$, $i=1, \dots, k$ are used in the design. An example will show 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. That is, we need a design with at least 7 experimental points. The design matrix \mathbf{D}_{full} , and the 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.

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

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

In general, the models discussed in this paper has

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

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 consist of

2^{k-p} factorial points, where p is the largest integer so 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 the 3-dimensional space it is defined by a tetrahedron.

Now, construct a simplex in the k -dimensional space $\mathbf{x} = (x_1, \dots, x_k)$ 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 for 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 \mathbf{D} is then defined by the design points

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

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

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

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

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

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

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

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

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

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

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

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

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 too 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 \mathbf{x} depends only on the distance between the origin and \mathbf{x} . That means that we can write $V_{\mathbf{x}} = V_{\rho}$, where $\rho = (x_1^2 + \dots + x_k^2)^{1/2}$.

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 this is 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 volume under the variance function 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 $A = \{\mathbf{x} ; -1 \leq x_i \leq 1, i = 1, \dots, k\}$). For all rotatable designs discussed in this paper we have that Vol is of the form

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

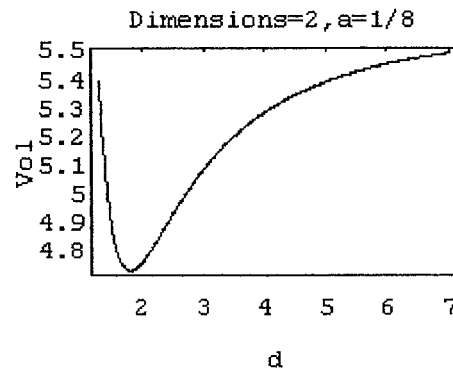
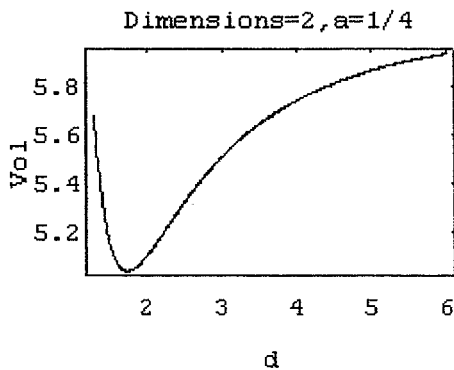
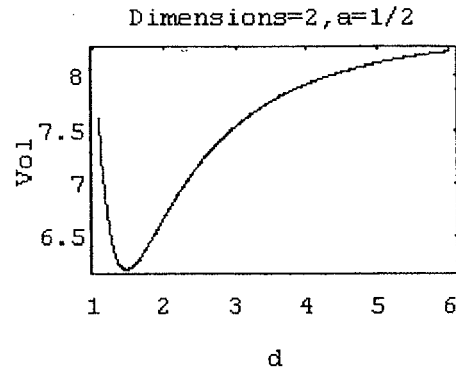
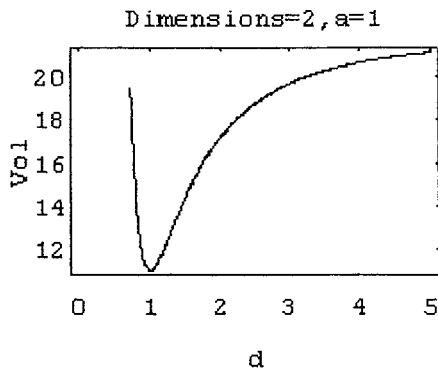
Now, for each k construct the rotatable factorial design that minimizes $\text{Vol} = \int_A V_x d\mathbf{x}$ under the restriction that all design points belong to B , and do the same for the simplex design. The number of experimental points used in the two design are

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 respectively rotatable design. That is for the factorial design 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 for which $k = 2$ need 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 one, 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. so that the volume under the variance function is minimized.

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

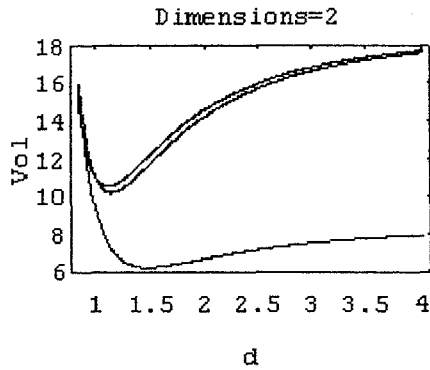


The graphs shows how the volume under the variance function changes with d . In each of the four cases there is unique d that minimizes the volume. Note the different scales on the y-axis in the four graphs.

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, that could be any value between 0.495 and 0.505. This gives an error of approximately 1 percent. If instead the variable were set to be 0.05 (could happens 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 that $d \leq b$.

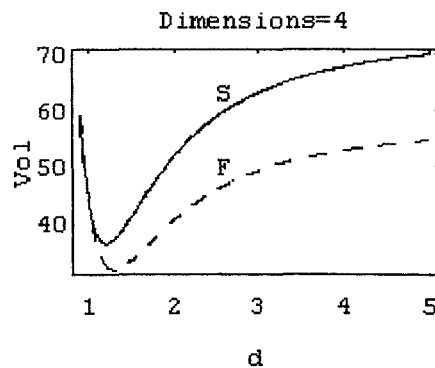
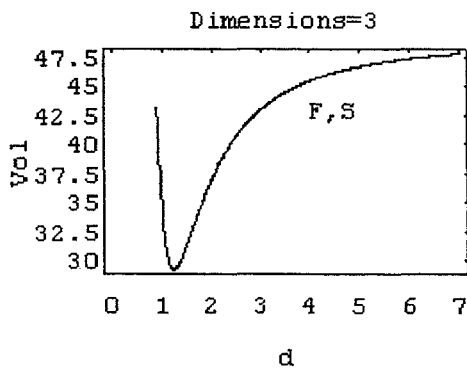
In the following graph are the two designs compared.

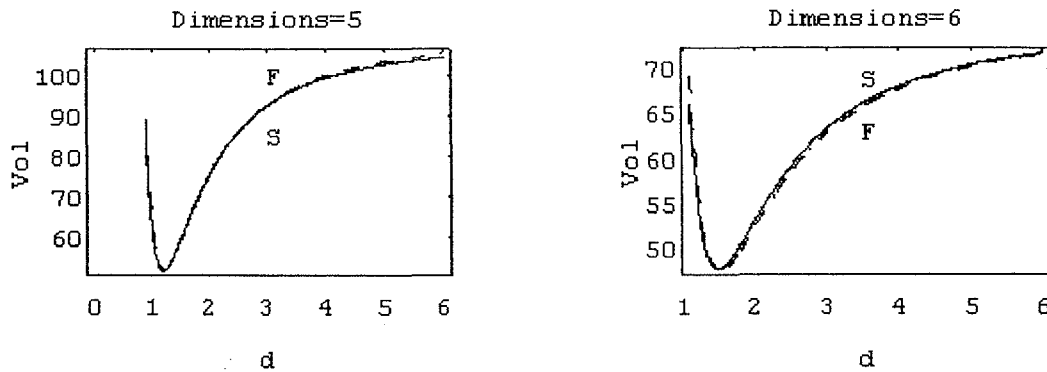


The two curves that are close together are the curve for the factorial design and the curve for the simplex design when $a = 2^{\frac{1}{4}}$. The reason for this choice of a is that this makes the distance between the simplex points and complement points in the simplex design the same as the distance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

With respect to the volume under the variance function, the two designs are almost identical when the distance between the simplex points and the complement points in the simplex design is equal to the distance between the factorial points and the star points in the factorial design. 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.

A comparison of the designs for $k = 3, \dots, 6$ is presented in the following graphs.





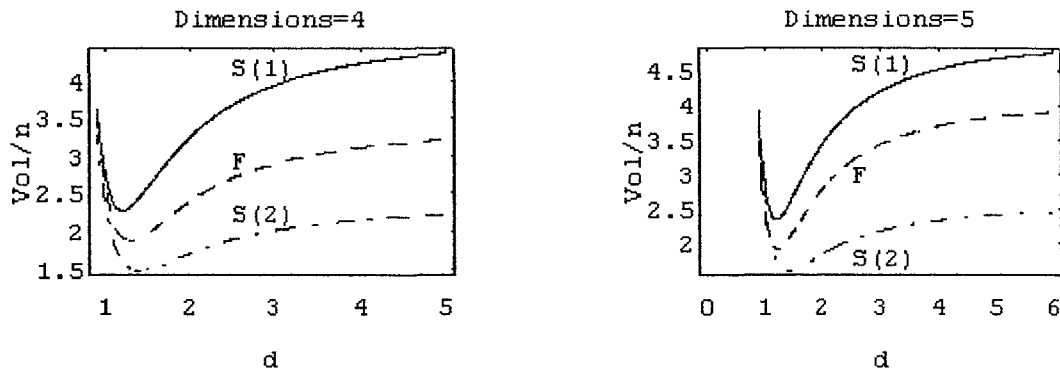
When k equals 3 the two designs are rotations of each other, and will therefore of course have the same variance function. When k equals 4 is the factorial design superior the simplex design. For k equals 5 and 6 are the two designs almost identical with respect to Vol.

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 volume under $\text{Var}(\hat{y}(\mathbf{x}))$ rather than the volume 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 the most accurate predictions than its competitor, the choice of design is clear.

Let us see what happens when the simplex design 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 fewer 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 variance 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 has 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 \mathbf{D} and the relating \mathbf{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 $\{\omega\}_{2,2} = \frac{1}{2} + \frac{343}{288}d \approx \frac{1}{2} + 1.19d$ and $\{\omega\}_{4,4} = \frac{7}{12} + \frac{2107}{1728}d \approx \frac{7}{12} + 1.22d$. Of course we can not find any positive d to make the two elements equal.

6 Final Remarks

The classical use of simplex designs arise 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 $R^3 = \{x ; x_4 = 0\}$. 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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