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# SATURATED DESIGNS FOR SECOND ORDER MODELS

by

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# Saturated Designs
# For
# Second Order Models

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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], have 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 the alphabetic optimality criteria's. 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. 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 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 consist 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 consist 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 exist saturated designs called Koshal designs, see Koshal[1933]. The idea behind the construction of such design 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.

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

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

$$A_0 = \left\{ a_{ij} \middle| \{\omega\}_{ij} = 0, \forall \text{ i and } j \geq i \right\}$$
$$A_\delta = \left\{ a_{ij} \middle| \{\omega\}_{ij} = \delta, \forall \text{ i and } j \geq i \right\}$$
$$A_\xi = \left\{ a_{ij} \middle| \{\omega\}_{ij} = \xi, \forall \text{ i and } j \geq i \right\}$$
$$A_\lambda = \left\{ \frac{a_{ij}}{k} \middle| \{\omega\}_{ij} = k\lambda, k \in \{1,3\}, \forall \text{ i and } j \geq i \right\}$$

Let the number of elements in $A_\ell$ be $n_\ell$, $\ell \in \{\delta, \xi, \lambda\}$. Now form

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

The measure of rotatability is now defined as

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

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

## 5 The Improved Koshal Design Vs. The Complemented Simplex Design

The complemented simplex design is naturally divided in two sets of experimental points, the simplex points and the complement points. Also the Koshal design 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 so the determinants of their respectively information matrices is maximized. Thereafter are the measures of deviation from a rotatable design found.

The results up to 6 dimensions are summarized in the following tables. Det stands for the determinant of the information matrix, Rot stands for the measure of deviation from a rotatable design. In the simplex design, 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 design, 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 design is superior the complemented simplex design with respect to Det. However, in 2,3 and 4 dimensions the complemented simplex design has a smaller value on Rot, and will therefore provide a more uniform information of the response surface. In 5 and 6 dimensions is the improved Koshal design better than the complemented simplex design with respect to Rot.

The complemented simplex design 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 is the complemented simplex design superior the improved Koshal design with respect to Det. With respect to Rot is the complemented simplex better than the improved Koshal in 2,3 and 4 dimensions. Specially, in 2 dimension is the complemented simplex design rotatable. In 5 and 6 dimensions is the improved Koshal design still better than the complemented simplex design 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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