# THE ANALYSIS OF FIRST AND SECOND ORDER SIMPLEX DESIGNS

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# Introduction

Designed experiments are often used in preparing the mathematical description of a response function characterizing some engineering-technological process. The preliminary designing of experiments and the activation of processes as foreseen by the design permits on the one hand that the estimation of the coefficients of the mathematical model should have the required statistical properties and on the other hand it can provide maximum information with uniform space distribution by the developed model.

In the following designs of experiments closely related to the sequential simplex method will be studied, which is finding growing acceptance in the field of numerical and technical optimation [1].

# 1. On simplex-sum designs

A simplex of dimension n is called a formation in the Euclidean space represented by (n + 1) points which do not lie simultaneously in any single subspace of dimension (n - 1).

Let **D** denote the matrix containing the experimental points of the design matrix. Be the number of experiments in **D**: N = n + 1, i.e. corresponding to the number of the points in a simplex. Then the matrix of the independent variables is:

$$\mathbf{X} = [\mathbf{I}, \mathbf{D}] \tag{1}$$

where I is a column matrix consisting of +1's.

Be X orthogonal in a way that

$$N^{-1}\mathbf{X}^T\mathbf{X} = \mathbf{E} \tag{2}$$

Here E is the unit matrix, furthermore  $\mathbf{X}^T$  is the transposed one of X. We shall admit that in this case the N experimental points are situated in the peaks of a regular simplex of dimension n.

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From Eq. (2) it follows that the rows and columns of the matrix  $N^{-\frac{1}{2}}\mathbf{X}$  form an orthonormed system of vectors. If  $\mathbf{x}_{u}^{T}$  and  $\mathbf{x}_{s}^{T}$  denote the  $u^{th}$  and  $s^{th}$  row, respectively, of matrix  $\mathbf{X}$ , then the scalar product of these is

$$\mathbf{x}_{u}^{T} \mathbf{x}_{s} = \begin{cases} 0 & , & \text{for } u \neq s \\ N = n + 1 & , & \text{for } u = s . \end{cases}$$
(3)

Let  $\mathbf{d}_u^T$  and  $\mathbf{d}_s^T$  denote the  $u^{th}$  and  $s^{th}$  row, respectively, of matrix **D** and  $\Theta_{us}$  the angle of the vectors pointing to the  $u^{th}$  and  $s^{th}$  experimental points. As **X** and **D** are related by (1), the relationships between the corresponding scalar products for each u and s are:

$$\mathbf{x}_{u}^{T} \mathbf{x}_{s} = 1 + \mathbf{d}_{u}^{T} \mathbf{d}_{s}.$$

$$\tag{4}$$

It follows that

$$\mathbf{d}_{u}^{T} \, \mathbf{d}_{s} = \begin{cases} -1 & , & \text{when } u \neq s \\ N = n + 1 & , & \text{when } u = s \end{cases}$$
(5)

with (3) taken into consideration.

The scalar product (5) means in case of u = s the square of the distance measured between the  $u^{th}$  experimental point and the origin; this equals n = N - 1, which is a constant value.

In case of  $u \neq s$  the scalar product is as follows:

$$\mathbf{d}_{u}^{T} \mathbf{d}_{s} = (N-1) \cos \Theta_{uh} = n \cos \Theta_{us} = -1$$

$$\cos\Theta_{us} = \frac{-1}{N-1} = -\frac{1}{n} \tag{6}$$

for every u and s, where  $u \neq s$ , i.e. this is also a constant quantity.

We have in this way that a first order orthogonal design possessing N = n + 1 matrix points corresponds to the points of a regular simplex of dimension n and vice versa. Such designs are at the same time also first order rototable designs [3, 4].

A plan **D** is a *d*-order rototable design if and only if the matrix of momentums  $\mathbf{X}^T \mathbf{X}$  is invariant against the orthogonal transformation of the coordinates, i.e.

$$\mathbf{X}^T \, \mathbf{X} = \mathbf{R}^{T \, [d]} \, \mathbf{X}^T \, \mathbf{X} \mathbf{R}^{[d]}$$

holds identically for any matrix X and orthogonal matrix R. Here the notation  $\mathbf{R}^{[d]}$  means the  $d^{th}$  power of the matrix [3, 4].

From the first order orthogonal or in other terms: linear simplex designs, second order designs may be obtained by the so-called *simplex-sum* [2]. By

the addition of the vectors, — running from the origin to the peaks of a simplex-, adding then by pairs, by threes, ..., by n's, in case of any n, a set of points can be constructed, whose connection to the initial first order design results in a second order rototable design [2, 3]. Such plans are called simplex-sum designs.

The analytical construction of the designs is made in the following way: Let  $\mathbf{D}_1$  denote the matrix containing the experimental points of the first order orthogonal design of the variable *n*. According to what has been said above, the set of vectors formed by the addition of all possible *s* members from *N* rows of the matrix  $\mathbf{D}_1$ , where  $s = 1, 2, \ldots, n$ , will constitute a second order design. To regulate the vector lengths they are multiplied by a constant  $a_s > 0$  called radial multiplier. The newly formed matrix  $\mathbf{D}_{(N'xn)}$  (here the type is denoted by the subscript) is:

$$\mathbf{D} = \begin{bmatrix} a_1 & \mathbf{D}_1 \\ a_2 & \mathbf{D}_2 \\ \vdots \\ a_s & \mathbf{D}_s \\ \vdots \\ a_{n-1} & \mathbf{D}_{n-1} \\ a_n & \mathbf{D}_n \end{bmatrix}$$
(7)

where

$$N' = \sum_{i=0}^{n+1} {n+1 \choose i} - {n+1 \choose 0} = {n+1 \choose n+1} = 2^{n+1} - 2.$$
(8)

The rows of the matrix  $\mathbf{D}_{(C_{n+1}^s \times n)}$  consists of the possible sums of s rows in the matrix  $\mathbf{D}_1$ .

In the following the properties of the simplex-sum design will be studied in case of the radial factors  $\mathbf{a}_1^T = [1,0,0,\ldots,0]$  and  $\mathbf{a}_2^T = [1,a,0,0,\ldots,0]$ , then conclusions will be drawn on the feasibility of economically optimum designs (i.e. with the minimum of experiments).

## 2. Analysis of the linear simplex design

It was seen in the previous section that linear simplex designs are both orthogonal and rototable. By this latter expression is meant that the statistical properties of the design are independent of the orthogonal transformation of the variables. This fact permits to draw wholly general conclusions from the analysis of the design matrix representing a regular simplex of any arbitrary position.

The simplex of dimension n will be constructed in the following way [9]:

$$\mathbf{D}_{1} = \begin{bmatrix} -r_{1} & -r_{2} & -r_{3} & \dots & -r_{n} \\ R_{1} & -r_{2} & -r_{3} & \dots & -r_{n} \\ 0 & R_{2} & -r_{3} & \dots & -r_{n} \\ 0 & 0 & R_{3} & \dots & -r_{n} \\ 0 & 0 & 0 & \dots & R_{n} \end{bmatrix}$$
(9)

where

$$r_i = \sqrt{rac{n+1}{ni(i+1)}} \cdot R \quad ext{and} \quad R_i = \sqrt{rac{i(n+1)}{n(i+1)}} \cdot R.$$
 (10)

Here R is the radius of the sphere of dimension n encircling the simplex of dimension n,  $R_i$  is that of the sphere of dimension i encircling the simplex of dimension i and  $r_i$  is the radius of the sphere of dimension i which can be inscribed in the simplex of dimension i. These are related by

$$R_i = i \cdot r_i \tag{11}$$

$$R_n^2 = \sum_{i=1}^n r_i^2.$$
 (12)

The design constructed in this way contains, according to what has been said in Part 1, an orthogonal system of vectors. This can easily be verified.  $D_1$  is namely trivially orthogonal to n = 2 and in the following the introduction of every new column, i.e. row variable multiplies every column of the previous matrix by identical elements, so orthogonality is maintained again, when

$$\sum_{u=1}^{N} x_{iu} = 0$$
 (13)

which follows from (11). The orthogonality of the rows may also by appreciated in a similar recursive way.

The normalization of the column- and row-vectors of the matrix  $\mathbf{X} = [\mathbf{I}, \mathbf{D}]$  is ensured by the appropriate choice of the value of  $R = R_n$ . By the condition of

$$\sum_{u=1}^{N} x_{iu}^2 = 1 + \sum_{u=1}^{N} x_{iu}^2 = R^2 \frac{n+1}{n} = n+1 = N$$
(14)

we obtain that R, required for the normalization, is:

$$R = \sqrt{n} = \sqrt{N-1} \,. \tag{15}$$

and

By substituting the value of R into (10) we obtain the elements of the orthonormed simplex design:

$$r_i = \sqrt{rac{n+1}{i(i+1)}} \quad ext{and} \quad R_i = \sqrt{rac{i(n+1)}{i+1}} \ .$$
 (16)

For the determination of the coefficients calculable on the basis of the simplex design the extended design matrix is developed, which contains both the possible even product and the square of the columns. This is shown in Table 1. By analysing this table the following conclusions may be drawn:

a) The type *i* columns (i = 0, 1, 2, ..., n) are orthogonal to each other.

b) The type *i* columns (i = 1, 2, ..., n) are orthogonal to every type fg column, for g > f, where  $f \neq i$ .

c) The type ij columns  $(i, j = 1, 2, ..., n; i \neq j)$  are orthogonal to every column of type fg, for j > i, g > f and  $i \neq f$ .

d) The  $0^{th}$  column is orthogonal to every column of type ij, but not so to the columns of type ii. etc.

Studying these properties is important because by regression analysis only coefficients with corresponding columns orthogonal to each other can be determined independently from each other.

As point n + 1 of the simplex of dimension n is suitable only — from the viewpoint of the degrees of freedom — for estimating the coefficient of the linear polynomial (this is the origin of the designation), therefore properties a) and b) are for us the most important ones.

The linear  $b_i$  coefficients may be evaluated on the basis of the simplex design as follows:

$$b_{i} = \frac{\sum_{u=1}^{N} x_{iu} \, \bar{\mathbf{y}}_{u}}{\sum_{u=1}^{N} x_{iu}^{2}} - \frac{\sum_{u=1}^{N} x_{iu} \, \bar{\mathbf{y}}_{u}}{N}; \quad i = 0, 1, 2, ..., n$$
(17)

where  $\bar{y}_u$  is the average of the output value measured at the  $u^{th}$  row of the design matrix. But also the implication of property b) must be remembered, i.e. that for the estimation of  $b_i$  it holds

$$b_{i} = \beta_{i} + c_{2} \beta_{i2} + c_{3} \beta_{i3} + \dots + c_{i} \beta_{ij} + \dots + c_{n} \beta_{in}$$
(18)

where the  $c_j$  values depend on the location of the design. So it may be concluded that first order orthogonal simplex designs give a distorsionless estimate of the  $\beta_i$  coefficients *only* in case of conceivably linear response surfaces.

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0		1	2	3 <i>n</i>	12	131 <i>n</i>	23	$24\ldots 2n$	i,i+1i,n	n-1,n	11	22nn
	1	<i>r</i> <sub>1</sub>	- <i>r</i> <sub>2</sub>	$-r_{3}r_{n}$	$r_{1}r_{2}$	$r_1 r_3 \dots r_1 r_{ll}$	$r_{2}r_{3}$	$r_2 r_4 \dots r_2 r_n$	$r_i r_{i+1} \cdots r_i r_n$	$r_{n-1}r_n$	$r_{1}^{2}$	$r_{2}^{2}r_{n}$
	1	$r_1$	$-r_{2}$	$-r_3$ $-r_n$	$-r_1r_2$	$-r_1r_3\dots-r_1r_n$	$r_{2}r_{3}$	$r_2 r_4 \dots r_2 r_n$	$r_i r_{i+1} \dots r_i r_n$	$r_{n-1}r_n$	$r_{1}^{2}$	$r_{2}^{2}r_{n}^{2}$
	1	0	$2r_2$	$-r_3$ $r_n$	0	00	$-2r_{2}r_{3}$	$-2r_2r_4\dots-2r_2r_n$	$r_i r_{i+1} \dots r_i r_n$	$r_{n-1}r_n$	0	$4r_2^2r_n^2$
	1	0	0	$3r_3 - r_n$	0	00	0	00	$r_i r_{i+1} \dots r_i r_n$	$r_{n-1}r_n$	0	$0r_n^2$
<b>X</b> =		•	•					· ·	• •	•		
		•					•	• •	· • •	• .	•	
	1	0	0	$0 - r_n$	0	0 0	0	0 0	$r_i r_{i+1} \dots r_i r_n$	$r_{n-1}r_n$	0	$0 r_{ll}^2$
	1	0	0	$0 - r_n$	0	0 0	0	0 0	$-ir_ir_{i+1}\cdots-ir_ir_n$	$r_{n-1}r_n$	0	$0 r_n^2$
			•		•						•	
	.		•			· · ·	•	• •	• •		•	
	1	0	0	$0 - r_n$	0	0 0	0	0 0	0 0	$r_{n-1}r_n$	0	$0 r_n^2$
	1	0	0	$0 nr_n$	0	0 0	0	0 0	0 0	$-(n-1)r_{n-1}r_n$	0	$0 n^2 r_n^2$

Table 1

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Hence, such plans are not suitable for the estimation of higher degreenumber coefficients, neither as regards the degrees of freedom, nor because of the asymmetric statistical properties.

With all this in view a very important field of application of the linear simplex designs has been found. The sequential evaluation method recommended in [5] and gaining an ever wider ground since, then assumes orthogonal blocks row by row. As this paper deals with two level designs, only saturated designs could be taken into consideration for the preparation of orthogonal blocks by rows. These are however, always bound to problems of mixed effects and their preliminary planning. These problems may be avoided by constructing the design matrix in the following way:

$$\mathbf{X} = \begin{bmatrix} \mathbf{I}, & \mathbf{D}_1 \\ \mathbf{I}, -\mathbf{D}_1 \end{bmatrix}.$$
(19)

Linear plans constructed in this way proved to be very efficient economically. They always help to approximate or obtain the optimum (minimum) number of experiments required for the estimation of the coefficients of the linear polynomial.

# 3. Analysis of quadratic simplex design

The number of the coefficients of a total second order polynomial is (n+1) (n+2)/2. Exactly the same number of experiments is contained in the following simplex-sum design:

$$\mathbf{D} = \begin{bmatrix} \mathbf{D}_1 \\ a\mathbf{D}_2 \end{bmatrix}$$
(20)

where the matrix  $\mathbf{D}_2$  is obtained by the possible pairwise addition of the rows of matrix  $\mathbf{D}_1$ . Here  $\mathbf{D}_1$  is a linear orthogonal simplex design whose number of experiments is denoted in the following by  $N_1$  ( $N_1 = n + 1$ ). Similarly,  $N_2$  is the number of experiments in  $\mathbf{D}_2$ . The number of the experiments of matrix  $\mathbf{D}$ , as already mentioned, is:

$$N = N_1 + N_2 = \binom{n+1}{1} + \binom{n+1}{2} = \binom{n+2}{2} = \frac{(n+1)(n+2)}{2}.$$
 (21)

The design X = [I, D] constructed in this way is optimum — as regards the degrees of freedom — for the determination of the coefficients of the second degree polynomial. In the following the statistical properties of the design will be studied.

On investigating the matrixes  $D_2$  produced for different values of n we discovered a regularity in their construction. The matrix  $D_2$  formed for an arbitrary n is the following:

$$\mathbf{D}_{11} = \begin{bmatrix} \frac{\mathbf{0} + -2r_2 + -2r_3 + -2r_4 + \dots + -2r_n}{\mathbf{D}_{11} + r_2 + -2r_3 + 2r_4 + \dots + -2r_n} \\ \mathbf{D}_{11} + r_2 + -2r_3 + 2r_4 + \dots + -2r_n \\ \mathbf{D}_{12} + 2r_3 + 2r_4 + \dots + 1 \\ \mathbf{D}_{12} + 2r_3 + 2r_4 + \dots + 1 \\ \mathbf{D}_{13} + 2r_4 + 2r_4 + 2r_4 + 2r_4 \\ \mathbf{D}_{13} + 2r_4 + 2r_4 + 2r_4 + 2r_4 \\ \mathbf{D}_{13} + 2r_4 + 2r_4 + 2r_4 \\ \mathbf{D}_{14} + 2r_4 + 2r_4 + 2r_4 + 2r_4 \\ \mathbf{D}_{14} + 2r_4 + 2r_4 + 2r_4 + 2r_4 + 2r_4 \\ \mathbf{D}_{14} + 2r_4 + 2r_$$

Here  $\mathbf{D}_{1i}$  is the linear design of dimension *i* sliced off the linear design of dimension *n*, whose elements are to be evaluated not according to the actual *i*, but always according to *n* from (16). This means that the  $\mathbf{D}_{1i}$  designs remain orthogonal, but the condition of normalization for any *i* will be:

$$\sum_{u=1}^{i+1} x_{iu}^2 = n+1 = N_1.$$
(23)

So the design  $\mathbb{D}_{2n}$  of dimension *n* may be developed from the one of lower dimension by 1, as follows:

$$\mathbf{D}_{2n} = \begin{bmatrix} \mathbf{D}_{2(n-1)} & \vdots & \\ - & - & - & -\frac{2r_n}{n} \\ \mathbf{D}_{1(n-1)} & \vdots & \\ \mathbf{D}_{1(n-1)} & \vdots & \\ (n-1)r_n \end{bmatrix}.$$
(24)

The orthogonality of  $\mathbf{D}_{22}$  is easily appreciated. In the following, when  $\mathbf{D}_{2(n-1)}$  is orthogonal, then  $\mathbf{D}_{2n}$  is also orthogonal, as the orthogonal designs  $\mathbf{D}_{2(n-1)}$  and  $\mathbf{D}_{1(n-1)}$  are multiplied by the column consisting of identical elements. This means that matrix  $\mathbf{D}$  developed according to (20) is also

orthogonal, just as  $D_1$  and  $D_2$  are. Further studies showed that orthogonality exists only for the columns of matrix D, and X = [I, D], resp., but it does not hold for an arbitrary combination of the columns.

As it was shown in Part 1, the points of matrix  $\mathbf{D}_1$  are arranged on a radius  $R = \sqrt{n}$  sphere of dimension n in case of normalized column and row vectors. In the linear orthogonal simplex design  $\cos \Theta_{us} = -\frac{1}{n}$  for any u and s. So the sum of any two row-vectors of  $\mathbf{D}_1$  gives a vector of identical length, which is

$$|\mathbf{d}_{u}^{T} + \mathbf{d}_{s}^{T}| = 2\sqrt{n}\cos\frac{\Theta_{us}}{2} = \sqrt{2(n-1)}.$$
(25)

Therefore point  $\frac{n(n+1)}{2}$  of the quadratic matrix **D** is on a hypersphere of dimension *n* with the radius

$$a\varrho = \sqrt{2(n-1)} \cdot a = Ra \sqrt{2(n-1)}$$
(26)

in the direction of the vectors passing through the centres of the edge-lines of a simplex of dimension n.

Let us investigate the rototability of the design **D**. The necessary and sufficient condition of the second order rototability of the matrix X = [I, D] is that the following conditions for the even momentums are satisfied:

$$\sum_{u=1}^{N} x_{iu}^{2} = \lambda_{2} N = N; \qquad i = 1, 2, ..., n$$

$$\sum_{u=1}^{N} x_{iu}^{4} = 3 \sum_{u=1}^{N} x_{iu}^{2} x_{ju}^{2} = 3 \lambda_{4} N; \qquad i, j = 1, 2, ..., n; i \neq j$$
(27)

and all odd momentums up to the 4<sup>th</sup>-order momentum incl. equal zero [3, 4].

The study of matrix X at the second order orthogonal simplex designs supplied the following results:

The quadratic momentums are independent of *i* and their values are:

$$\sum_{u=1}^{N} x_{iu}^{2} = (n+1) [1 + a^{2}(n-1)]; \quad i = 1, 2, ..., n.$$
(28)

Hence the value

$$a = \sqrt{\frac{n}{2(n-1)}} \tag{29}$$

is obtained, if condition (27a) is to be ensured. This means then that the radius  $a\varrho$  of the quadratic part is coincident with radius R of the linear part.

i.e. the whole set of points is situated on a hypersphere of radius R. Yet in [3] it has been proved that a set of points distributed uniformly on a hypersphere of radius R cannot constitute a rototable design, because the matrix  $\mathbf{X}^T \mathbf{X}$  of the momentums belonging to it would be then a degenerated matrix. By this we proved that the economically optimum simplex-sum designs with the minimum number of experiments *cannot form* a rototable arrangement.

This statement is supported by the fact that the pure and mixed  $4^{th}$  degree momentums of the matrix X are not independent of i and j, so the conditions (27) cannot be satisfied.

$$\sum_{u=1}^{N} x_{iu}^{4} = (n+1)^{2} \left[ \frac{i^{2}-i+1}{i(i+1)} + \frac{i^{4}-i^{3}+6i^{2}+4i-6}{i(i+1)^{2}} \right]$$

$$\sum_{u=1}^{N} x_{iu}^{2} x_{ju}^{2} = \frac{(n+1)^{2}}{j(j+1)}, \quad \text{where} \quad i < j.$$
(30)

The value of  $\sum_{u=N_1+1}^{N_1+N_2} x_{iu}^2 x_{ju}^2$  depends in a very complicated manner on *i* and *j*.

Note that the quadratic simplex design can be made rototable by the introduction of central points n = 2.

In [2] it has been proved that if **D** is constructed according to (7), then the arrangement can be made rototable by the appropriate choice of the radial constants  $a_1, a_2, \ldots, a_s, \ldots, a_n$ . But the number of the experiments corresponds to that of the constants to be determined, cannot be constructed according to the pattern of the simplex-sum designs. Accordingly economical optimation may be ensured by such designs only approximately at the most.

For the construction of economically nearly optimum rototable simplexsum designs the following may be recommended:

1. If n + 1 can be described as  $p^{ih}$  integer power of 2, then choose for  $\mathbf{D}_1$  a type  $2^p = 2^{n-q}$  fractional factor design [6] and form  $\mathbf{D}_2$  by the possible addition of the rows by pairs. Let us choose here the value of a in (20) on the basis of the rototability conditions (27). This is the case for values of  $n = 3,7,15,31,\ldots$ , etc.

2. If n is divisible by 4, then use for  $\mathbf{D}_1$  a Hadamardian matrix. These are  $(n \times n)$  type matrices with identical numbers of +1 and -1 in each column and the columns are orthogonal to each other [7]. The existence of such matrices has been proved up to n = 200, with the exception of the values n = 92, 116, 156, 184 and 188. In reality 1 is a specific case of the Hadamardian matrices. PLACKETT and BURMAN developed even a particular procedure for the construction of such designs for n = 12, 20, 24, and 36. [3, 8].

Matrix  $D_2$  is constructed as in the previous case. The rototability condition must be examined in each case and the value of a is to be chosen

accordingly. The economically optimum design can only be approximated by preparing a Hadamardian matrix for the variable

$$n' = [n \div 4) + 1] 4 \tag{31}$$

and by completing this by the simplex-sum (here  $\div$  means integer division).

3. Attention must be drawn to the fact that if a regular simplex for  $\mathbf{D}_1$  is dispensed with, it makes feasible to construct an economically optimum second order simplex design. Research is being carried out in this direction.

## Summary

In this paper first and second order simplex designs were analysed.

In Part 1 simplex-sum designs were described in short and the purpose of this study was outlined.

In Part 2 the analysis of the linear simplex design was discussed. It was proved that these designs give a distorsionless estimation of the coefficients of type  $b_i$  only in case of response functions which may be well approximated. The orthogonality by rows of the designs was admitted and thereupon a design of the form (19) was recommended as a basis for the sequential evaluation, as no design problems connected with mixing arise here.

In Part 3 the quadratic simplex design was studied. The regularity found in the design was shown **u**p and it was proved that with the exception of n = 2 it cannot be made rototable for any n. By this it was also proved that an economically optimum second order rototable design (i.e. with minimum number of experiments) cannot be conceived according to the pattern of the simplex-sum design from a regular simplex.

Thereafter recommendations were suggested for the construction of designs with an economically nearly optimum number of experiments on the basis of two level designs.

Finally a tendency was pointed out in the form of asymmetrical simplex designs, the further study of which will permit the development of economically optimum second order simplex-sum designs.

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