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COMPUTER AIDED GENERATION OF LINEAR TREND-FREE RESPONSE SURFACE DESIGNS

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ABSTRACT

The treatment combinations of the ordinary full factorial need not be the best for fitting the relationship. Therefore, it is necessary to search for a suitable set of treatment combinations by using which a stipulated relation can be fitted. The special class of designed experiments for fitting the response surfaces is called response surface design. Response surface designs have wide applications in agricultural, biological and industrial experiments. Similar to factorial experiments, experimental units in response surface design may exhibit trend over space or time. Among response surface designs, Box-Behnken design has been studied and linear trend-free design has been obtained. The developed algorithm helps the experimenters who are conducting quantitative factors using response surface designs. There may be a trend in the experimental material and hence we need trend-free design. It provides a complete solution in the sense that it is capable of generating the trend free Box-Behnken design. Trend-free designs are quite useful for such experimental situations. But the construction for such design is not easily available. It is, therefore, required to give easy method of construction, possibly computer aided for the construction of these designs. Thus algorithms have been developed to generate complete factorial experiments each at two levels with any number of factors k (≥ 4) that are linear trend-free for main effects using the criterion of component-wise product.

***Key Words**:* Response surface designs, linear trend-free designs, orthogonal polynomials, run orders, systematic designs

1. Introduction

Data from experiments with levels or level combinations of one or more factors as treatments are normally investigated to compare level effects of the factors and their interactions. Though such investigations are useful to have objective assessment of the effect of levels tried in the experiment, this seems to have inadequate in nature. The analysis as such does not give any information regarding the possible effects of the intervening levels of the factors or their combinations, *i.e.* one is not able to interpolate the responses at the treatment combinations not tried in the experiment. In such cases, it is more realistic and informative to carry out investigations to determine and quantify the relationship between the values of one or more measurable response variable (s) and the setting of a group of experimental factors presumed to affect the response (s) and to find the settings of the experimental factors that produce the best value or the best set of values of the response(s). Thus if all the factors are quantitative in nature, it is proper to think the response as a function of the factor levels and data from quantitative factorial experiments can be used to fit the response surfaces over the region of interest. Response surfaces besides inferring about the twin purposes can provide information about the rate of change of a response variable. They can also indicate the interactions among the quantitative treatment factors. The special class of designed experiments for fitting the response surfaces is called response surface design. Response surface designs have wide applications in agricultural, biological and industrial experiments. Similar to factorial experiments, experimental units in response surface design may exhibit trend over space or time. Neyman (1929) was the first to realize this problem, Cox (1951, 1952) also illustrated and discussed about this. More recently, these ideas were pursued by Bradley and Yeh (1980) for block designs and Cheng and Jacroux (1988) for factorial experiments. Hinkelmann and Jo (1998) first studied linear trend-free response surface designs. They gave a procedure to construct the linear trend free response surface designs by using the solutions of some of the equations. A class of three-level incomplete factorial designs for the estimation of the parameters in second order model was developed by Box and Behnken (1960). By definition, a three-level incomplete factorial design is a subset of the factorial combinations from a 3^k factorial design. The Box-Behnken designs are formed by combining two-level factorial designs with balanced incomplete block (BIB) designs or partially balanced incomplete block (PBIB) designs in a particular manner. From the last three decades computer aided search/generation/construction has emerged as a powerful tool to obtain designs for various experimental settings. Some of the studies on computer aided designs are available in the literature. Nguyen (1983) developed algorithms for construction of D-optimal fractional factorial plans and MS-optimal incomplete block designs. Studies on development of computer aided search/ construction of optimal block designs and minimal connected D-optimal designs, optimal/ nearly optimal balanced treatment incomplete block designs, designs for making treatment-treatment and treatment-control comparisons and designs for dependent observations, correlated error structure for nested block designs are available in literature (Dwivedi (1997), Rathore

(2004), Rathore *et al.* (2004), Satpati (2006), Satpati *et al.* (2006)). No work seems to be available on computer aided generation on trend-free factorial experiments. In this study attempt has been made to develop the algorithm to generate computer aided complete factorial experiments and that of confounded factorial experiments that are linear trend-free for main effects and identification of two and three factor interactions that are linear trend-free/ nearly linear trend-free in the obtained designs. The working of the algorithms has been illustrated by suitable examples.

A binary incomplete block design with *v* treatments, *b* blocks, *r* replications and k units per block.

Let $\mathbf{N} = (n_{ij})$ (i = 1, 2, …, *v* ; j = 1, 2, ..., *b*) denotes the incidence matrix of the BIB or PBIB design. Then we prepare a 2^k factorial (where *k* is the same as the block size for the given incomplete block design). The levels of *k* factors are denoted by -1 and +1, representing the low and high level respectively. We write the factorial experiment in standard (lexicographic order). We then write *k* column vectors $\mathbf{A}_i$ (i = 1, 2, …, *k*) of length 2^k with elements ±1 such that the elements of $\mathbf{A}_i$ add to zero and $\mathbf{A}_i$'s are orthogonal to each other.

Box and Behnken (1960) took the $\mathbf{A}_i$ to be the columns of the 2^k factorial treatment combinations; other choices are also possible, such as the coefficient vector for the main effects or interactions for the 2^k factorial. Finally, we substitute in each row of $\mathbf{N}'$ the first 1 by $\mathbf{A}_1$, the second 1 by $\mathbf{A}_2$ and so on the k^{th} 1 by $\mathbf{A}_k$ and all 0's by **0** column vectors of size 2^k. Same procedure will be repeated in all rows of the transpose of incidence matrix *i.e.* $\mathbf{N}'$. So there are total $b2^k$ rows, represents a run for the *v* input variables each taking the values -1, 0, +1. To this obtained design we add n_0 central runs (0, 0, …, 0) to obtain a final design, n_0 should be odd in numbers. The obtained design is Box-Behnken designs with $n = b2^k + n_0$ runs.

2. Linear trend-free response surface designs

The treatments combinations obtained in above section are applied randomly to the *n* experimental units. If it is, however, known or assumed that the experimental units or the experimental material applied to the experimental units exhibit a linear trend over time or space, then it will be more advantageous to choose a systematic arrangement of

For the second order response surface design we consider the model

$$\mathbf{y} = \beta_0\mathbf{1} + \mathbf{X}_1\boldsymbol{\beta}_1 + \mathbf{X}_2\boldsymbol{\beta}_2 + \mathbf{X}_3\boldsymbol{\beta}_3 + \mathbf{T}\boldsymbol{\theta} + \mathbf{e} \qquad (1)$$

where, $\mathbf{y}$ is $n\times 1$ vector of observations, $\mathbf{X}_1$ is $n\times v$ matrix of linear effects, $\mathbf{X}_2$ is $n\times v$ matrix of quadratic effects, $\mathbf{X}_3$ is $n\times v(v-1)/2$ matrix of cross products. β_0 is the vector of a constant, $\boldsymbol{\beta}_1$ is the vector of linear coefficients, $\boldsymbol{\beta}_2$ is the vector of quadratic coefficients, $\boldsymbol{\beta}_3$ is the vector of cross product second order coefficient, **T** is the vector of coefficients of the first-degree orthogonal polynomial of order *n*, **θ** is a regression coefficient, and **e** is a *n* × 1 vector of independently and identically (normally) distributed errors. Based on a more general definition of linear trend-free, the design under model (1) is linear trend free if the conditions $\mathbf{X_i T} = \mathbf{0}$ (i = 1, 2, 3) are satisfied.

We have a Box-Behnken design with n = $b2^k + n_0$ runs, n_0 should be odd in numbers. We can write **T** as

$$\mathbf{T}' = \left(-\frac{n-1}{2}, -\frac{n-1}{2}+1, \ldots, -2, -1, 0, 1, 2, \ldots, \frac{n-1}{2}-1, \frac{n-1}{2}\right) \qquad (2)$$

T is anti-symmetric.

3. Algorithm to generate the linear trend-free Box- Behnken design

For k ≥ 4, the construction

I.1 Take a binary incomplete block (BIB) design with *v* treatments, *b* blocks, *r* replications and *k* units per block. This is stored in a $b\times k$ array.

I.2 Prepare a 2^k factorial (where *k* is the same as the block size for the BIB design) in standard order as follows:

I.3 Let we have *k* factors.

I.4 The number of treatment combinations is $n = 2^k$. Here *n* is an even number.

I.5 Make an array of dimension $n\times k$.

I.6 The first column of the array of size *n* is made such that the entries are -1 and +1 alternatively.

I.7 The second column of the array is made such that the entries are in combinations of two i.e. -1, -1 and +1, +1 alternatively, and so on.

I.8 The k^{th} column is made such that the first n/2 places are filled with -1 and last n/2 places with +1.

I.9 In the obtained $n\times k$ matrix, each column is the coefficient of contrast of main effects separately and thus *k* columns are coefficients of contrast of *k* factors.

I.10 'he *n* rows of $n\times k$ matrix represent *n* $(=2^k)$ treatment combinations in lexicographic order.

I.11 The levels of k factors are denoted by -1 and +1, representing the low and high level respectively

I.12 From the above mentioned binary incomplete block (BIB) design in $b \times k$ array, prepare incidence matrix in $v \times b$ array, by reading the values block wise and putting the value 1 in the columns which are the treatment number. The obtained matrix is incidence matrix **N** of binary incomplete block (BIB) design.
N = (n_{ij}) (i = 1, 2, . . ., v ; j = 1, 2, . . ., b).

I.13 Take transpose of the incidence matrix **N,** *i.e.* $\mathbf{N}'$. The matrix $\mathbf{N}'$ has as many ones in each row as number of columns in 2^k factorial experiment.

I.14 Let A_i, i = 1, 2, …, k represent the coefficient of the contrasts of the k main effects. Perform component-wise product within each of b blocks separately. Similar to complete factorial experiment, there are two procedures of component-wise product. The procedure of component-wise product is as given below:
For *k* is odd: When k is odd the new coefficient vectors for main effects will be obtained as:
Let A_i be the new coefficient vectors for main effects for i[th] factor, $i = 1, 2, \ldots, k$

$F_i = A_1 \circ A_2 \circ \cdots \circ A_{i-1} \circ A_{i+1} \circ \cdots \circ A_k$; $(i = 1, 2, \ldots, k-1)$

and $F_k = A_1 \circ A_2 \circ \cdots \circ A_k$; $(i = k)$

For *k* is even: When k is even the new coefficient vectors for main effects will be obtained as:

$F_i = A_1 \circ A_2 \circ \cdots \circ A_{i-1} \circ A_{i+1} \circ \cdots \circ A_k$; $(i = 1, 2, \ldots, k)$.

I.15 Replace each 1 in $\mathbf{N}'$ by obtained F_i, such that first 1 by first column (F_1) second 1 by second column (F_2) and so on, 0's by a columns of zero.

I.16 This choice of F_i ensures that they are independent in the sense that no F_i is the generalized interaction of F_j 's. Also, since $k \geq 4$ it follows that each F_i corresponds to at least a three factor interaction.

I.17 The treatment combinations of the 2^k factorial in standard order and the result of Cheng and Jacroux(1988) this implies that each half is F_i, F_i^U and F_i^L for $(i = 1, 2, \ldots, k)$ orthogonal to a linear trend. Say this design is **D***

I.18 We can write **D*** as:

$\mathbf{D}^* = (\mathbf{B}_1, \mathbf{B}_2, \ldots, \mathbf{B}_b)'$, Each B_i $(i = 1, 2, \ldots, b)$ contains $F_1, F_2, \ldots, F_K$ exactly once, and v – k **0**'s

Partition of each B_i is done into an upper part and a lower part as:

$$\mathbf{B}_i = \begin{bmatrix} \mathbf{B}_i^U \\ \mathbf{B}_i^L \end{bmatrix} (i = 1, 2, \ldots, b)$$

Arrange all $\mathbf{B}_i^U$ in $\mathbf{P_1}$ and $\mathbf{B}_i^L$ in $\mathbf{P}_2$ and $\mathbf{P}_0$ is the central runs (in odd number) partitioning the design matrix **D***, we obtain a design matrix **D** as

$$\mathbf{D} = \begin{bmatrix} P_1 \\ P_0 \\ P_2 \end{bmatrix}$$

Where P_1 represents the first $b2^{k-1}$ runs, P_2 represents the last $b2^{k-1}$ runs and P_0 is the central runs (in odd number).

I.19 The resultant design is trend free Box-Behnken Design. Theses designs are linear trend-free for all effects: (a) linear effects are linear trend-free as shown in Section 2.4, hence, $\mathbf{X}_1'\mathbf{T} = \mathbf{0}$. (b) F_{ii} and $F_{ii'}$ are symmetric, so $\mathbf{X}_2'\mathbf{T} = \mathbf{0}$ and $\mathbf{X}_3'\mathbf{T} = \mathbf{0}$ implies that quadratic and cross product effects are also linear trend-free.

the n run, such that the resulting design is a linear trend-free design.

4. Working of algorithm

For $k \geq 4$ Let we have a BIB design with parameters (v = 5, b = 5, r = 4, k = 4, λ = 3).

$$\mathbf{N} = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 1 & 2 & 3 & 5 \\ 1 & 2 & 4 & 5 \\ 1 & 3 & 4 & 5 \\ 2 & 3 & 4 & 5 \end{bmatrix}$$

Generate incidence matrix from step I.4

$$\mathbf{N} = \begin{bmatrix} 1 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 & 1 \end{bmatrix}$$

generate its transpose matrix N′

Since block size is 4 hence 2^4 factorial design in lexicographic order is generated using steps I.1 to II.8 under Section 2.3

Design – 1

Treatment combinations	A_a	A_b	A_c	A_d
(1)	-1	-1	-1	-1
a	1	-1	-1	-1
b	-1	1	-1	-1
ab	1	1	-1	-1
c	-1	-1	1	-1
ac	1	-1	1	-1
bc	-1	1	1	-1
abc	1	1	1	-1
d	-1	-1	-1	1
ad	1	-1	-1	1
bd	-1	1	-1	1
abd	1	1	-1	1
cd	-1	-1	1	1
acd	1	-1	1	1
bcd	-1	1	1	1
abcd	1	1	1	1

Using computer program of algorithm-II of section II, perform the component-wise product of A_i and A_j by using step II.4. Here *k* (= 4) is even so A has been generated using component-wise product of A_b, A_c and A_d as: $A_a = A_b \circ A_b \circ A_c$.

A_b	A_c	A_d	$A_b \circ A_c \circ A_d$		A_a
-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	-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

Further B, C and D are generated using the formula:
$F_i = A_1 \circ A_2 \circ \cdots \circ A_{i-1} \circ A_{i+1} \circ \cdots \circ A_k$;
$(i = a, b, c,$ and *d*). Thus we get the Design-2

Design-2

Treatment combinations	A (F_a)	B (F_b)	C (F_c)	D (F_d)
(1)	-1	-1	-1	-1
bcd	-1	1	1	1
acd	1	-1	1	1
ab	1	1	-1	-1
abd	1	1	-1	1
ac	1	-1	1	-1
bc	-1	1	1	-1
d	-1	-1	-1	1
abc	1	1	1	-1
ad	1	-1	-1	1
bd	-1	1	-1	1
c	-1	-1	1	-1
cd	-1	-1	1	1
b	-1	1	-1	-1
a	1	-1	-1	-1
abcd	1	1	1	1

Substituting each column of factorial experiment in transpose incidence matrix, we get the Box Behnken design in five factors each at three levels

A	**B**	**C**	**D**	**E**	**A**	**B**	**C**	**D**	**E**
-1	-1	-1	-1	0	1	1	0	1	-1
-1	1	1	1	0	1	-1	0	-1	1
1	-1	1	1	0	-1	1	0	-1	1
1	1	-1	-1	0	-1	-1	0	1	-1
1	1	-1	1	0	-1	-1	0	1	1
1	-1	1	-1	0	-1	1	0	-1	-1
-1	1	1	-1	0	1	-1	0	-1	-1
-1	-1	-1	1	0	1	1	0	1	1
1	1	1	-1	0	-1	0	-1	-1	-1
1	-1	-1	1	0	-1	0	1	1	1
-1	1	-1	1	0	1	0	-1	1	1
-1	-1	1	-1	0	1	0	1	-1	-1
-1	-1	1	1	0	1	0	1	-1	1
-1	1	-1	-1	0	1	0	-1	1	-1
1	-1	-1	-1	0	-1	0	1	1	-1
1	1	1	1	0	-1	0	-1	-1	1
-1	-1	-1	0	-1	1	0	1	1	-1
-1	1	1	0	1	1	0	-1	-1	1
1	-1	1	0	1	-1	0	1	-1	1
1	1	-1	0	-1	-1	0	-1	1	-1
1	1	-1	0	1	-1	0	-1	1	1
1	-1	1	0	-1	-1	0	1	-1	-1
-1	1	1	0	-1	1	0	-1	-1	-1
-1	-1	-1	0	1	1	0	1	1	1
1	1	1	0	-1	0	-1	-1	-1	-1
1	-1	-1	0	1	0	-1	1	1	1
-1	1	-1	0	1	0	1	-1	1	1
-1	-1	1	0	-1	0	1	1	-1	-1
-1	-1	1	0	1	0	1	1	-1	1
-1	1	-1	0	-1	0	1	-1	1	-1
1	-1	-1	0	-1	0	-1	1	1	-1
1	1	1	0	1	0	-1	-1	-1	1
-1	-1	0	-1	-1	0	1	1	1	-1
-1	1	0	1	1	0	1	-1	-1	1
1	-1	0	1	1	0	-1	1	-1	1

1	1	0	-1	-1	0	-1	-1	1	-1
1	1	0	-1	1	0	-1	-1	1	1
1	-1	0	1	-1	0	-1	1	-1	-1
-1	1	0	1	-1	0	1	-1	-1	-1
-1	-1	0	-1	1	0	1	1	1	1

We can write **D*** as:

$$\mathbf{D^*} = \left(\mathbf{B}_1, \mathbf{B}_2, \ldots, \mathbf{B}_4\right)'$$

Each $B_i \; (i = a, b, c, d, e)$ contains $F_a, F_b \ldots, F_d$ exactly once, and one column of zero.

Now partition of each B_i is done into an upper part and a lower part as:

$$B_i = \begin{bmatrix} B_i^U \\ B_i^L \end{bmatrix} (i = 1, 2, \ldots, 5)$$

Rearranging and partitioning the design matrix **D***, we obtain a design matrix **D** as

$$\mathbf{D} = \begin{bmatrix} P_1 \\ P_0 \\ P_2 \end{bmatrix}$$

where P_1 represents the first 40 runs, P_2 represents the last 40 runs and P_0 has one central runs. Thus the obtained Box-Behnken design is linear trend-free for all linear effects, quadratic effects and cross products.

A	B	C	D	E	A	B	C	D	E
1	-1	-1	-1	0	0	1	1	1	-1
-1	1	1	1	0	0	1	-1	-1	1
1	-1	1	1	0	0	-1	1	-1	1
1	1	-1	-1	0	0	-1	-1	1	-1
1	1	-1	1	0	0	-1	-1	1	1
1	-1	1	-1	0	0	-1	1	-1	-1
-1	1	1	-1	0	0	1	-1	-1	-1
-1	-1	-1	1	0	0	1	1	1	1
-1	-1	-1	0	-1	1	0	1	1	-1
-1	1	1	0	1	1	0	-1	-1	1
1	-1	1	0	1	-1	0	1	-1	1
1	1	-1	0	-1	-1	0	-1	1	-1
1	1	-1	0	1	-1	0	-1	1	1
1	-1	1	0	-1	-1	0	1	-1	-1
-1	1	1	0	-1	1	0	-1	-1	-1
-1	-1	-1	0	1	1	0	1	1	1
-1	-1	0	-1	-1	1	1	0	1	-1
-1	1	0	1	1	1	-1	0	-1	1
1	-1	0	1	1	-1	1	0	-1	1
1	1	0	-1	-1	-1	-1	0	1	-1
1	1	0	-1	1	-1	-1	0	1	1
1	-1	0	1	-1	-1	1	0	-1	-1
-1	1	0	1	-1	1	-1	0	-1	-1
-1	-1	0	-1	1	1	1	0	1	1
-1	0	-1	-1	-1	1	1	1	0	-1
-1	0	1	1	1	1	-1	-1	0	1
1	0	-1	1	1	-1	1	-1	0	1
1	0	1	-1	-1	-1	-1	1	0	-1
1	0	1	-1	1	-1	-1	1	0	1
1	0	-1	1	-1	-1	1	-1	0	-1
-1	0	1	1	-1	1	-1	-1	0	-1
-1	0	-1	-1	1	1	1	1	0	1
0	-1	-1	-1	-1	1	1	1	-1	0
0	-1	1	1	1	1	-1	-1	1	0
0	1	-1	1	1	-1	1	-1	1	0
0	1	1	-1	-1	-1	-1	1	-1	0
0	1	1	-1	1	-1	-1	1	1	0
0	1	-1	1	-1	-1	1	-1	-1	0
0	-1	1	1	-1	1	-1	-1	-1	0
0	-1	-1	-1	1	1	1	1	1	0
0	0	0	0	0					

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