Construction and Properties of Box-Behnken Designs

by

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(ABSTRACT)

Box-Behnken designs are used to estimate parameters in a second-order response surface model (Box and Behnken, 1960). These designs are formed by combining ideas from incomplete block designs (BIBD or PBIBD) and factorial experiments, specifically 2^k full or 2^{k-l} fractional factorials.

In this dissertation, a more general mathematical formulation of the Box-Behnken method is provided, a general expression for the coefficient matrix in the least squares analysis for estimating the parameters in the second order model is derived, and the properties of Box-Behnken designs with respect to the estimability of all parameters in a second-order model are investigated when 2^k full factorials are used. The results show that for all pure quadratic coefficients to be estimable, the PBIB(m) design has to be chosen such that its incidence matrix is of full rank, and for all mixed quadratic coefficients to be estimable the PBIB(m) design has to be chosen such that the parameters $\lambda_1, \lambda_2, \dots, \lambda_m$ are all greater than zero.

In order to reduce the number of experimental points the use of 2^{k-l} fractional factorials instead of 2^k full factorials is being considered. Of particular interest and importance are separate considerations of fractions of resolutions III, IV, and V. The

construction of Box-Behnken designs using such fractions is described and the properties of the designs concerning estimability of regression coefficients are investigated. Using designs obtained from resolution V factorials have the same properties as those using full factorials. Resolutions III and IV designs may lead to non-estimability of certain coefficients and to correlated estimators.

The final topic is concerned with Box-Behnken designs in which treatments are applied to experimental units sequentially in time or space and in which there may exist a linear trend effect. For this situation, one wants to find appropriate run orders for obtaining a linear trend-free Box-Behnken design to remove a linear trend effect so that a simple technique, analysis of variance, instead of a more complicated technique, analysis of covariance, to remove a linear trend effect can be used. Construction methods for linear trend-free Box-Behnken designs are introduced for different values of block size (for the underlying PBIB design) k . For $k=2$ or 3, it may not always be possible to find linear trend-free Box-Behnken designs. However, for $k \geq 4$ linear trend-free Box-Behnken designs can always be constructed.

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Chapter 1. Introduction

Response surface methodology is essentially a particular set of mathematical and statistical methods used by researchers to aid in the solution of certain types of problems which are pertinent to scientific or engineering processes (Myers, 1976). The response variable is the measured quantity whose value is assumed to be affected by changing the levels of the factors (or input variables) which are subject to the control of the experimenter. The response surface procedures are a collection involving experimental strategy, mathematical methods, and statistical inference which enable the experimenter to make an efficient empirical exploration of the system in which he is interested. Preceding statistical analysis using the regression method, the experiment must be designed, that is, the input variables must be selected, their values during the actual experimentation designated, and an appropriate model for analysis must be chosen. Generally, the model is fit by the method of least squares. The response surface analysis that follows the experimental strategy revolves around (1) prediction of response values, (2) exploring the response surface in the region of the designated experiment, and (3) possibly finding conditions on the design variables that give rise to optimum response. The most frequently used approximating polynomial models are of degrees one and two. The general form of a first-order model (i.e., models of degree one) in v input variables $x_1, x_2, \ldots, x_v$ is

$$y = \beta_0 + \sum_{i=1}^{v} \beta_i x_i + \varepsilon$$

where y is a response variable, $\beta_0, \beta_i\ (i = 1, \ldots, v)$ are unknown parameters, and ε is a random error term. The 2^k factorial designs, fractional replicates of the 2^k factorial designs, simplex designs, and Plackett-Burman designs are first-order designs. When the first-order model suffers from lack of fit arising from the existence of surface curvature, the first-order model is upgraded by adding higher-order terms to it. The next higher-order model is the second-order model

$$y = \beta_0 + \sum_{i=1}^{v} \beta_i x_i + \sum_{i=1}^{v} \beta_{ii} x_i^2 + \sum_{\substack{i, i' = 1 \\ i < i'}}^{v} \beta_{ii'} x_i x_{i'} + \varepsilon \tag{1.1}$$

where y is a response variable, $\beta_0, \beta_i, \beta_{ii}\ (i = 1, \ldots, v), \beta_{ii'}\ (i, i' = 1, \ldots, v,\ i < i')$ are unknown parameters. A design, by means of which observed values of the response are collected for estimating the parameters in the second-order model is called a second-order design. Experimental designs for fitting a second-order respone surface must involve at least three levels of each variable so that the coefficients in the model can be estimated. Examples of a second-order designs are a 3^k factorial design, central composite designs, equiradial designs, hybrid designs, and so on. Second-order composite designs usually require five levels coded $-\alpha, -1, 0, 1, \alpha$ for each of the variables where α is a positive value. Circumstances occur, however, where second-order arrangements are required which must employ the smallest number of different levels, namely three. One useful class of such designs, which are economical with respect to the number of runs required, is due to Box and Behnken (1960). Box-Behnken designs are formed by combining two level factorial designs with balanced incomplete block designs (BIBD) or partially balanced incomplete block designs (PBIBD) in a particular manner. Box and Behnken showed how to construct the designs, and illustrated the method with some useful designs of second order. In chapter 2 of this dissertation, we

(i) provide a more general mathematical formulation of the Box-Behnken method,

(ii) derive a general expression for the coefficient matrix in the least square analysis for estimating the parameters in model (1.1), and

(iii) investigate the properties of Box-Behnken designs with respect to the estimability of all parameters in a second-order model when we use 2^k full factorials.

In chapter 3, we elucidate the properties of Box-Behnken designs using 2^{k-l} fractional factorials of resolutions III, IV, and V or higher instead of using full factorials. For each case, we obtain the coefficient matrix, and illuminate the properties of the estimators for the parameters in a second order model. And, we investigate the use of appropriate fractional factorials in Box-Behnken designs. Finally, in chapter 4, we consider the situation in which the experiment using a Box-Behnken design is conducted sequentially, one run at a time, and a linear trend is assumed to exist over the experimental plots, i.e. over time. The adjustment of linear trend has been accomplished by the use of analysis of covariance in which covariate is a linear trend. The problem is that we face the complication of analysis of covariance in the presence of linear trend over plots. Instead of using analysis of covariance, we introduce linear trend-free (LTF) Box-Behnken designs to eliminate a linear trend as a solution for simplifying the method. That is, we show how to assign treatment combinations to experimental plots in a particular way in order to remove the linear trend. When the design is linear trend-free, we use an analysis of variance technique which is very simple. That is, sums of squares for the estimates of coefficients we are concerned with are calculated as though there were no linear trend, sums of squares for the estimates of coefficients are calculated easily, variation due to the linear trend may be removed for the error sums of squares, and design efficiencies are increased. Depending on the block size k of PBIB designs, we consider two cases, for $k = 2$ or 3 and for $k \geq 4$ to construct LTF Box-Behnken designs. Linear trend-free Box-Behnken designs may not always exist for $k = 2$ or 3. For $k \geq 4$, however, we can always find LTF Box-Behnken designs.

Chapter 2. Properties of Box-Behnken designs

2.1. Construction of Box-Behnken designs

Box-Behnken designs (Box and Behnken, 1960) are a class of three-level incomplete factorial designs for the estimation of parameters in a second-order response surface model. These designs are formed by combining two-level factorial designs with incomplete block designs in a particular manner. The method can be described as follows:

1. Consider a response surface design with v input variables $x_1, x_2, \ldots, x_v$. Use as an auxiliary design an incomplete block design with v treatments and b blocks of size k, characterized by incidence matrix of the incomplete block design (BIBD or PBIBD) $\underline{N} = (n_{ij})$, with $n_{ij} = 1$ if treatment i occurs in block j and $n_{ij} = 0$ otherwise.

2. Identify the v treatments with the v input variables. and consider the transpose of the incidence matrix $\underline{N}'$. Each row of $\underline{N}'$ contains k unity elements.

3. Suppose in the first row the unity elements occur in columns $l_1, l_2, \ldots, l_k$ ($1 \leq l_1 < l_2 < \cdots < l_k \leq v$). Replace each of those k unity elements by column vectors F_w ($w = 1, 2, \ldots, k$). The elements of F_w are either 1 or -1, and the F_w 's are chosen such that they are orthogonal to each other where the k factors correspond to the input variables numbered $l_1, l_2, \ldots, l_k$. The F_w can be interpreted in two different ways; (i) If the levels of the factors in a 2^k factorial are denoted by -1 and +1 and if the treatment combinations $\underline{z'_i} = (z_{i1}, z_{i2}, \ldots, z_{ik})$ $(i = 1, 2, \ldots, 2^k = s)$ are written in standard order with $z_{ij} = \pm 1$, then

$$F'_w = (z_{1w}, z_{2w}, \ldots, z_{sw})$$

(this is indeed the choice described by Box and Behnken (1960)),

(ii) each F_w represents a vector of the coefficients defining main effects and interactions for the 2^k factorial (there are $2^k - 1$ such vectors but only k are needed, for example the contrast vectors for k independent two-factor interactions as long as one two-factor interaction is not the generalized interaction of the other two-factor interactions).

4. The v - k zeros in each row are replaced by $2^k \times 1$ vectors of zeros.

5. This procedure is repeated for each row of $\underline{N'}$ resulting in $b2^k$ experimental points, using the same vectors $F_1, F_2, \ldots, F_k$.

6. Finally, n_0 center points are added with all elements being zeros to the $b2^k$ experimental points.

If we denote by n the number of observations (runs), we get the Box-Behnken design matrix of size of $n \times v$ where $n = b2^k + n_0$ for a full factorial. The following example will be used to illustrate how a Box-Behnken design can be constructed (see p.457 in Box and Behnken, 1960).

Example 2.1

Below is shown a transpose of the incidence matrix of a balanced incomplete block design for $v = 4$ treatments in $b = 6$ blocks of size $k = 2$. Each treatment appears $r = 3$ times in the design, once with each of the other treatments (i.e. $\lambda = 1$).

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

Since $k = 2$ we consider the 2^2 factorial design, the treatment combinations of which are assigned in standard order as follows:

$$A = \begin{bmatrix} -1 & -1 \\ 1 & -1 \\ -1 & 1 \\ 1 & 1 \end{bmatrix}$$

The contrast vectors for the main effects and two-factor interaction are given by

$$B = \begin{bmatrix} -1 & -1 & 1 \\ 1 & -1 & -1 \\ -1 & 1 & -1 \\ 1 & 1 & 1 \end{bmatrix}$$

A three-level design in four variables (i.e. treatments) is then obtained by combining this incomplete bock design with the 2^2 factorial. The two 1's in every row of the incomplete block design are replaced by either the $k = 2$ columns of the matrix A or any two columns of the matrix B. Wherever a 0 appears a column of zeros with size $2^2 \times 1$ is inserted. The design is completed by the addition of a number n_0 of center points (0, 0, 0, 0), say $n_0 = 1$ center point for this arrangement. The resulting three-level Box-Behnken design in four variables (x_1, x_2, x_3, x_4) is shown in Table 2.1 consists of the following 25 points:

Table 2.1. Box-Behnken design for 4 input variables

x_1	x_2	x_3	x_4
−1	−1	0	0
1	−1	0	0
−1	1	0	0
1	1	0	0
0	0	−1	−1
0	0	1	−1
0	0	−1	1
0	0	1	1
−1	0	0	−1
1	0	0	−1
−1	0	0	1
1	0	0	1
0	−1	−1	0
0	1	−1	0
0	−1	1	0
0	1	1	0
0	−1	0	−1
0	1	0	−1
0	−1	0	1
0	1	0	1
−1	0	−1	0
1	0	−1	0
−1	0	1	0
1	0	1	0
0	0	0	0

Box and Behnken (1960) listed a number of second-order designs for $v = 3, 4, 5, 6, 7, 9, 10, 11, 12$ and 16 variables.

2.2. Box-Behnken design matrix

In order to discuss some of the properties of Box-Behnken designs in general terms it is useful to introduce the following notation and definitions.

Definition 2.1. The vector-valued transformation $\underline{\phi}$ defined on { 0, 1 } into the set of $2^k \times 1$ vectors is given by

$$\underline{\phi}_{ji} = \underline{\phi}(n_{ji}) = n_{ji}\underline{F}_{w(j,i)}$$

where w(j,i) $= n_{j1} + n_{j2} + \cdots + n_{ji}$, with w taking the values 0,1, ... ,k, and $F_{w(j,i)}$ is as defined in Section 2.1, and $\underline{F}_0' = (1, 1, \dots, 1)$.

Definition 2.2. Let $g' = (g_1, g_2, \dots, g_s)$ and $h' = (h_1, h_2, \dots, h_s)$ be $1 \times s$ vectors. The element-wise multiplication of g and h, denoted by goh , is given by the $s \times 1$ vector $goh = (g_1h_1, g_2h_2, \dots, g_sh_s)'$

The design matrix D of the Box-Behnken design consists of two parts, one generated by the incomplete block design and the 2^k factorial as described in Section 2.1, and the other consisting of center points. We write this as

$$D = \begin{bmatrix} D^* \\ 0_{n_0 \times v} \end{bmatrix} \tag{2.1}$$

Using the notation of Definition 2.1. we have

$$D^* = (\underline{\phi}_{ji}) = \begin{bmatrix} \underline{\phi}_{11} & \underline{\phi}_{12} & \cdot & \cdot & \cdot & \underline{\phi}_{1v} \\ \underline{\phi}_{21} & \underline{\phi}_{22} & \cdot & \cdot & \cdot & \underline{\phi}_{2v} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \underline{\phi}_{b1} & \underline{\phi}_{b2} & \cdot & \cdot & \cdot & \underline{\phi}_{bv} \end{bmatrix} = \begin{bmatrix} n_{11}\underline{E}_{w(1,1)} & n_{12}\underline{E}_{w(1,2)} & \cdot & \cdot & \cdot & n_{1v}\underline{E}_{w(1,v)} \\ n_{21}\underline{E}_{w(2,1)} & n_{22}\underline{E}_{w(2,2)} & \cdot & \cdot & \cdot & n_{2v}\underline{E}_{w(2,v)} \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ n_{b1}\underline{E}_{w(b,1)} & n_{b2}\underline{E}_{w(b,2)} & \cdot & \cdot & \cdot & n_{bv}\underline{E}_{w(b,v)} \end{bmatrix} \quad (2.2)$$

consisting of $b2^k$ design points. The matrix $0_{n_0 \times v} = (\underline{0}_{n_0}, \underline{0}_{n_0}, \dots, \underline{0}_{n_0})$ represents $n_0 > 0$ center points. We now write the design matrix as D = ($\underline{x}_1, \underline{x}_2, \dots, \underline{x}_v$) where $\underline{x}_i' = (n_{1i}\underline{E}_{w(1,i)}', n_{2i}\underline{E}_{w(2,i)}', \dots, n_{bi}\underline{E}_{w(b,i)}', \underline{0}_{n_0}')$ is a $1 \times (b2^k + n_0)$ vector.

2.3. Second-order model

Consider the second degree polynomial model

$$y_u = \beta_0 + \sum_{i=1}^{v} \beta_i x_{iu} + \sum_{i=1}^{v} \beta_{ii} x_{iu}^2 + \sum_{\substack{i,i'=1 \\ i<i'}}^{v} \beta_{ii'} x_{iu} x_{i'u} + \varepsilon_u, \quad u = 1,2,\dots,n \qquad (2.3)$$

where y_u is a response variable, $\beta_0, \beta_i, \beta_{ii}$ and $\beta_{ii'}$ are unknown parameters with $i, i' = 1,2,\dots,t$ $i < i'$, and ε_u is an unknown and unobservable random error with mean 0 and variance σ^2 . In matrix notation, we can write (2.3) as

$$\underline{Y} = X\underline{\beta} + \underline{\varepsilon}$$

where $\underline{Y}$ is an $n \times 1$ observation vector, X is an $n \times p$ known matrix, $\underline{\beta}$ is a $p \times 1$ vector of parameters, and $\underline{\varepsilon}$ is an $n \times 1$ vector of unknown and unobservable random errors with mean $\underline{0}$ and variance $\sigma^2 I_{n \times n}$. Here, $p = 1 + 2v + v(v-1)/2$,

$$X = (\underline{1}_n, \underline{x}_1, \underline{x}_2, \dots, \underline{x}_v, \underline{x}_1^{\,2}, \underline{x}_2^{\,2}, \dots, \underline{x}_v^{\,2}, \underline{x}_1\underline{x}_2, \underline{x}_1\underline{x}_3, \dots, \underline{x}_{v-1}\underline{x}_v) \tag{2.4}$$

where $\underline{1}_n$ is an $n \times 1$ vector of unity elements, $\underline{x}_i^2 = \underline{x}_i \circ \underline{x}_i$, $\underline{x}_i\underline{x}_{i'} = \underline{x}_i \circ \underline{x}_{i'}$, and

$$\underline{\beta}' = (\beta_0, \beta_1, \beta_2, \dots, \beta_v, \beta_{11}, \beta_{22}, \dots, \beta_{vv}, \beta_{12}, \beta_{13}, \dots, \beta_{v-1,v}) \tag{2.5}$$

2.4. The coefficient matrix

For the second-order model (2.3), the X matrix in (2.4) can be partitioned as

$$X = (\underline{1}_n, X_1, X_2, X_3)$$

where X_1, X_2 are $n \times v$ matrices, and X_3 is an $n \times v(v-1)/2$ matrix. The coefficient vector $\underline{\beta}$ in (2.5) is partioned correspondingly as

$$\underline{\beta}' = (\beta_0, \underline{\beta}_1', \underline{\beta}_2', \underline{\beta}_3')$$

where $\underline{\beta}_1$, $\underline{\beta}_2$ are $v \times 1$ vectors, representing first and pure quadratic regression coefficients respectively, and $\underline{\beta}_3$ is a $v(v-1)/2 \times 1$ vector, representing the mixed quadratic regression coefficients. We then rewrite model (2.3) in the partitioned form as

$$\underline{Y} = \underline{1}\beta_0 + X_1\underline{\beta}_1 + X_2\underline{\beta}_2 + X_3\underline{\beta}_3 + \underline{\varepsilon} \tag{2.6}$$

The properties of the design are determined essentially by the properties of the coefficient matrix of the normal equations for the model (2.6). This matrix is given by

$$X'X = \begin{bmatrix} n & \underline{1}'X_1 & \underline{1}'X_2 & \underline{1}'X_3 \\ X_1'\underline{1} & X_1'X_1 & X_1'X_2 & X_1'X_3 \\ X_2'\underline{1} & X_2'X_1 & X_2'X_2 & X_2'X_3 \\ X_3'\underline{1} & X_3'X_1 & X_3'X_2 & X_3'X_3 \end{bmatrix}$$

It is proved in Section 2.5 that for a Box-Behnken design constructed by using a PBIB design with m associate classes, denoted by PBIB(m), $X'X$ has the following form

$$X'X = \begin{bmatrix} n & \underline{0}' & r2^k\underline{1}' & \underline{0}' \\ \underline{0} & r2^k I & 0 & 0 \\ r2^k\underline{1} & 0 & 2^k(\underline{NN'}) & 0 \\ \underline{0} & 0 & 0 & G \end{bmatrix} \tag{2.7}$$

In (2.7), the form of the matrix G can be described as follows: If we label the rows and columns of G by (ii') ($i, i' = 1, 2, \dots, v, i < i'$) , and the general element of G by $g_{ii', i''i'''}$, then

$g_{ii', ii'} = \lambda_\gamma 2^k$ if treatments i and i' are γ -th associates ($1 \leq \gamma \leq m$)

and

$g_{ii', i''i'''} = 0$ if (ii') $\neq$ ($i''\,i'''$), i.e. all off-diagonal elements are zero. So, given the values of parameters ($v, r, b, k, \lambda_1, \lambda_2, \dots, \lambda_m$) of the incomplete block design PBIB(m), and the structure of the incidence matrix, we can derive the $X'X$ matrix of the second-order model which contains information about the estimability of the parameters in the second order model (see Section 2.5 for discussion on the estimability).

2.5. Derivation of the coefficient matrix

We first list some properties of the factorial structure and of PBIB(m) designs which will be used to obtain the general form of $X'X$

Property 1. For the $2^k \times 1$ vectors, $F_w, w = 1, 2, \dots, k$, introduced in Section 2.1, we have

$$
\begin{array}{lllll}
(1) & F_w \circ F_w & = & \underline{1}_{2^k} & \textit{all } w \\
(2) & F'_w \cdot F_{w'} & = & 0 & w \neq w' \\
(3) & \underline{1}'_{2^k} \cdot F_w & = & 0 & \textit{all } w \\
(4) & \underline{1}'_{2^k} \cdot (F_w \circ F_w) & = & 2^k & \textit{all } w \\
(5) & \underline{1}'_{2^k} \cdot (F_w \circ F_{w'}) & = & 0 & w \neq w' \\
(6) & F'_w \cdot (F_{w'} \circ F_{w''}) & = & 0 & \textit{all } w,\ w',\ w'' \\
(7) & (F_w \circ F_{w'})'(F_{w''} \circ F_{w'''}) & = & 2^k & w = w',\ w'' = w''' \textit{ or } w = w'',\ w' = w''' \\
 & & = & 0 & \textit{otherwise}
\end{array}
$$

where $\underline{1}_{2^k}$ is a $2^k \times 1$ vector of unity elements, $\underline{0}$ is a $2^k \times 1$ vector of zeros.

Property 2. For the PBIB(m) design with $j = 1, 2, \dots, b,\ i = 1, 2, \dots, \nu$ and parameters $(\nu, b, r, k, \lambda_1, \dots, \lambda_m)$, the elements of $\underline{N'} = (n_{ji})$ satisfy

$$(1)\quad \sum_{j=1}^{b} n_{ji} = \sum_{j=1}^{b}{}^{*} n_{ji} = r$$

$$(2)\quad \sum_{j=1}^{b} n_{ji}n_{ji'} = \sum_{j=1}^{b}{}^{*} n_{ji}n_{ji'} = \lambda_\gamma \qquad \text{if } i, i' \text{ are } \gamma^{th} \text{ associates}$$

where the $\sum_{j=1}^{b}{}^{*}$ notation denotes summation over non-zero elements (this notation will be useful later; see property 3).

In what follows we need to sum over terms like $(n_{ji}F_{w(j,i)})'(n_{ji'}F_{w(j,i')})$ or $(n_{ji}F_{w(j,i)})'(n_{ji'}F_{w(j,i')} \circ n_{ji''}F_{w(j,i'')}), \cdots$, so on. By introducing the $\sum_{j=1}^{b}{}^{*}$ notation, (see above), we exclude terms in which at least one of the n_{ji} - terms is zero. This simplifies the computation of the different parts of $X'X$, because we can take advantage of the following

Property 3.

(1) $\sum_{j=1}^{b}{}^{*}$ is equivalent to $\sum_{j=1}^{b}$

(2) $w(j,i)$ takes values $i = 1, 2, \cdots, k$, greater than zero.

(3) $w(j,i)$ is less than $w' = w(j,i')$ when $i < i'$ since $n_{ji'}$ appearing in $\sum_{j=1}^{b}{}^{*}$ must be one.

Using the notation introduced in Sections 2.2 and 2.3 we now write $X'X$ as

$$X'X = \begin{bmatrix} \underline{1}'\underline{1} & \underline{1}'X_1 & \underline{1}'X_2 & \underline{1}'X_3 \\ X_1'\underline{1} & X_1'X_1 & X_1'X_2 & X_1'X_3 \\ X_2'\underline{1} & X_2'X_1 & X_2'X_2 & X_2'X_3 \\ X_3'\underline{1} & X_3'X_1 & X_3'X_2 & X_3'X_3 \end{bmatrix}$$

$$= \left[\begin{array}{c|ccc|ccc|ccc}
\underline{1}'\underline{1} & \underline{1}'\mathbf{x}_1 & \cdots & \underline{1}'\mathbf{x}_t & \underline{1}'(\mathbf{x}_1\circ\mathbf{x}_1) & \cdots & \underline{1}'(\mathbf{x}_t\circ\mathbf{x}_t) & \underline{1}'(\mathbf{x}_1\circ\mathbf{x}_2) & \cdots & \underline{1}'(\mathbf{x}_{t-1}\circ\mathbf{x}_t) \\ \hline
\mathbf{x}_1'\underline{1} & \mathbf{x}_1'\mathbf{x}_1 & \cdots & \mathbf{x}_1'\mathbf{x}_t & \mathbf{x}_1'(\mathbf{x}_1\circ\mathbf{x}_1) & \cdots & \mathbf{x}_1'(\mathbf{x}_t\circ\mathbf{x}_t) & \mathbf{x}_1'(\mathbf{x}_1\circ\mathbf{x}_2) & \cdots & \mathbf{x}_1'(\mathbf{x}_{t-1}\circ\mathbf{x}_t) \\
\vdots & \vdots & & \vdots & \vdots & & \vdots & \vdots & & \vdots \\
\mathbf{x}_t'\underline{1} & \mathbf{x}_t'\mathbf{x}_1 & \cdots & \mathbf{x}_t'\mathbf{x}_t & \mathbf{x}_t'(\mathbf{x}_1\circ\mathbf{x}_1) & \cdots & \mathbf{x}_t'(\mathbf{x}_t\circ\mathbf{x}_t) & \mathbf{x}_t'(\mathbf{x}_1\circ\mathbf{x}_2) & \cdots & \mathbf{x}_t'(\mathbf{x}_{t-1}\circ\mathbf{x}_t) \\ \hline
(\mathbf{x}_1\circ\mathbf{x}_1)'\underline{1} & (\mathbf{x}_1\circ\mathbf{x}_1)'\mathbf{x}_1 & \cdots & (\mathbf{x}_1\circ\mathbf{x}_1)'\mathbf{x}_t & (\mathbf{x}_1\circ\mathbf{x}_1)'(\mathbf{x}_1\circ\mathbf{x}_1) & \cdots & (\mathbf{x}_1\circ\mathbf{x}_1)'(\mathbf{x}_t\circ\mathbf{x}_t) & (\mathbf{x}_1\circ\mathbf{x}_1)'(\mathbf{x}_1\circ\mathbf{x}_2) & \cdots & (\mathbf{x}_1\circ\mathbf{x}_1)'(\mathbf{x}_{t-1}\circ\mathbf{x}_t) \\
\vdots & \vdots & & \vdots & \vdots & & \vdots & \vdots & & \vdots \\
(\mathbf{x}_t\circ\mathbf{x}_t)'\underline{1} & (\mathbf{x}_t\circ\mathbf{x}_t)'\mathbf{x}_1 & \cdots & (\mathbf{x}_t\circ\mathbf{x}_t)'\mathbf{x}_t & (\mathbf{x}_t\circ\mathbf{x}_t)'(\mathbf{x}_1\circ\mathbf{x}_1) & \cdots & (\mathbf{x}_t\circ\mathbf{x}_t)'(\mathbf{x}_t\circ\mathbf{x}_t) & (\mathbf{x}_t\circ\mathbf{x}_t)'(\mathbf{x}_1\circ\mathbf{x}_2) & \cdots & (\mathbf{x}_t\circ\mathbf{x}_t)'(\mathbf{x}_{t-1}\circ\mathbf{x}_t) \\ \hline
(\mathbf{x}_1\circ\mathbf{x}_2)'\underline{1} & (\mathbf{x}_1\circ\mathbf{x}_2)'\mathbf{x}_1 & \cdots & (\mathbf{x}_1\circ\mathbf{x}_2)'\mathbf{x}_t & (\mathbf{x}_1\circ\mathbf{x}_2)'(\mathbf{x}_1\circ\mathbf{x}_1) & \cdots & (\mathbf{x}_1\circ\mathbf{x}_2)'(\mathbf{x}_t\circ\mathbf{x}_t) & (\mathbf{x}_1\circ\mathbf{x}_2)'(\mathbf{x}_1\circ\mathbf{x}_2) & \cdots & (\mathbf{x}_1\circ\mathbf{x}_2)'(\mathbf{x}_{t-1}\circ\mathbf{x}_t) \\
\vdots & \vdots & & \vdots & \vdots & & \vdots & \vdots & & \vdots \\
(\mathbf{x}_{t-1}\circ\mathbf{x}_t)'\underline{1} & (\mathbf{x}_{t-1}\circ\mathbf{x}_t)'\mathbf{x}_1 & \cdots & (\mathbf{x}_{t-1}\circ\mathbf{x}_t)'\mathbf{x}_t & (\mathbf{x}_{t-1}\circ\mathbf{x}_t)'(\mathbf{x}_1\circ\mathbf{x}_1) & \cdots & (\mathbf{x}_{t-1}\circ\mathbf{x}_t)'(\mathbf{x}_t\circ\mathbf{x}_t) & (\mathbf{x}_{t-1}\circ\mathbf{x}_t)'(\mathbf{x}_1\circ\mathbf{x}_2) & \cdots & (\mathbf{x}_{t-1}\circ\mathbf{x}_t)'(\mathbf{x}_{t-1}\circ\mathbf{x}_t)
\end{array}\right]$$

Then, making use of property 1, property 2, and property 3, we obtain the following expressions for the various section of the $X'X$ matrix:

(a) $\underline{1}'\underline{1}$

$$\underline{1}'\underline{1} = b2^k + n_0 = n$$

(b) $\underline{1}'X_1$

$$\underline{1}'\underline{x_i} = \sum_{j=1}^{b} \underline{1}'(n_{ji}F_{w(j,i)}) = \sum_{j=1}^{b}{}^* n_{ji}(\underline{1}' \cdot F_{w(j,i)}) = 0 \qquad all\ i$$

(c) $\underline{1}'X_2$

$$\begin{aligned}\underline{1}'(\underline{x_i} \circ \underline{x_i}) &= \sum_{j=1}^{b} \underline{1}' \cdot (n_{ji}F_{w(j,i)} \circ n_{ji}F_{w(j,i)}) \qquad all\ i \\ &= \sum_{j=1}^{b}{}^* n_{ji}n_{ji}[\underline{1}' \cdot (F_{w(j,i)} \circ F_{w(j,i)})] \\ &= \sum_{j=1}^{b}{}^* n_{ji}(\underline{1}'\underline{1}) = r2^k\end{aligned}$$

(d) $\underline{1}'X_3$

$$\begin{aligned}1'(\underline{x_i} \circ \underline{x_{i'}}) &= \sum_{j=1}^{b} \underline{1}' \cdot (n_{ji}F_{w(j,i)} \circ n_{ji'}F_{w(j,i')}) \quad i, i' = 1, 2, \ldots, \nu,\ i < i' \\ &= \sum_{j=1}^{b}{}^* n_{ji}n_{ji'}[\underline{1}' \cdot (F_{w(j,i)} \circ F_{w(j,i')})] \\ &= \sum_{j=1}^{b}{}^* n_{ji}n_{ji'}[\underline{1}' \cdot (F_w \circ F_{w'})] = 0 \qquad w < w'\end{aligned}$$

(e) $X_1'X_1$

For $i = i'$ (diagonal elements)

$$\begin{aligned}(\underline{x_i'}\underline{x_i}) &= \sum_{j=1}^{b} (n_{ji}F_{w(j,i)})'(n_{ji}F_{w(j,i)}) \quad i = 1, 2, \ldots, \nu \\ &= \sum_{j=1}^{b}{}^* n_{ji}n_{ji}(F'_{w(j,i)} \cdot F_{w(j,i)})\end{aligned}$$

$$= \sum_{j=1}^{b}{}^{*} n_{ji}(F'_w \cdot F_w) = r2^k$$

For $i \neq i'$ (off-diagonal elements)

$$\begin{aligned}
(\underline{x'_i}\underline{x_{i'}}) &= \sum_{j=1}^{b}(n_{ji}F_{w(j,i)})'(n_{ji'}F_{w(j,i')}) \quad i,i' = 1,2,\ldots,\nu,\ i \neq i' \\
&= \sum_{j=1}^{b}{}^{*} n_{ji}n_{ji'}(F'_{w(j,i)} \cdot F_{w(j,i')}) \\
&= \sum_{j=1}^{b}{}^{*} n_{ji}n_{ji'}(F'_w \cdot F_{w'}) = 0 \quad w \neq w'
\end{aligned}$$

It follows that $(X'_1X_1) = r2^k \cdot I_{\nu\times\nu}$.

(f) X'_1X_2

$$\begin{aligned}
\underline{x'_i}(\underline{x_{i'}} \circ \underline{x_{i'}}) &= \sum_{j=1}^{b}(n_{ji}F_{w(j,i)})'(n_{ji'}F_{w(j,i')} \circ n_{ji'}F_{w(j,i')}) \quad all\ i,\ i' \\
&= \sum_{j=1}^{b}{}^{*} n_{ji}n_{ji'}[F'_{w(j,i)} \cdot (F_{w(j,i')} \circ F_{w(j,i')})] \\
&= \sum_{j=1}^{b}{}^{*} n_{ji}n_{ji'}[F'_w \cdot (F_{w'} \circ F_{w'})] = 0 \quad all\ w,\ w'
\end{aligned}$$

(g) X'_1X_3

$$\begin{aligned}
\underline{x'_i}(\underline{x_{i'}} \circ \underline{x_{i''}}) &= \sum_{j=1}^{b}(n_{ji}F_{w(j,i)})'(n_{ji'}F_{w(j,i')} \circ n_{ji''}F_{w(j,i'')}) \quad i,i',i'' = 1,2,\ldots,\nu,\ i' < i'' \\
&= \sum_{j=1}^{b}{}^{*} n_{ji}n_{ji'}n_{ji''}[F'_{w(j,i)} \cdot (F_{w(j,i')} \circ F_{w(j,i'')})] \\
&= \sum_{j=1}^{b}{}^{*} n_{ji}n_{ji'}n_{ji''}[F'_w \cdot (F_{w'} \circ F_{w''})] = 0 \quad w' < w''
\end{aligned}$$

(h) X'_2X_2

For $i = i'$

$$
\begin{aligned}
(\underline{x_i} \circ \underline{x_i})'(\underline{x_i} \circ \underline{x_i}) &= \sum_{j=1}^{b} (n_{ji} F_{w(j,i)} \circ n_{ji} F_{w(j,i)})'(n_{ji} F_{w(j,i)} \circ n_{ji} F_{w(j,i)}) \quad \textit{all } i \\
&= \sum_{j=1}^{b}{}^{*} n_{ji} n_{ji} (F_{w(j,i)} \circ F_{w(j,i)})'(F_{w(j,i)} \circ F_{w(j,i)}) \\
&= \sum_{j=1}^{b}{}^{*} n_{ji} (F_w \circ F_w)'(F_w \circ F_w) \\
&= \sum_{j=1}^{b}{}^{*} n_{ji} (\underline{1}' \cdot \underline{1}) = r 2^k
\end{aligned}
$$

For $i \neq i'$

$$
\begin{aligned}
(\underline{x_i} \circ \underline{x_i})'(\underline{x_{i'}} \circ \underline{x_{i'}}) &= \sum_{j=1}^{b} (n_{ji} F_{w(j,i)} \circ n_{ji} F_{w(j,i)})'(n_{ji'} F_{w(j,i')} \circ n_{ji'} F_{w(j,i')}) \\
&= \sum_{j=1}^{b}{}^{*} n_{ji} n_{ji'} (F_w \circ F_w)'(F_{w'} \circ F_{w'}) \\
&= \sum_{j=1}^{b}{}^{*} n_{ji} n_{ji'} (\underline{1}' \cdot \underline{1}) = \lambda_\gamma 2^k \quad i,\ i' \quad \gamma^{th} \text{associates}
\end{aligned}
$$

It follows that $X_2' X_2 = 2^k(I + \lambda_1 B_1 + \lambda_2 B_2 + \cdots + \lambda_m B_m) = 2^k(\underline{NN'})$, where B_γ is the γ^{th} association matrix of size $\nu \times \nu$

(i) $X_2 X_3$

$$
\begin{aligned}
(\underline{x_i} \circ \underline{x_i})'(\underline{x_{i'}} \circ \underline{x_{i''}}) &= \sum_{j=1}^{b} (n_{ji} F_{w(j,i)} \circ n_{ji} F_{w(j,i)})'(n_{ji'} F_{w(j,i')} \circ n_{ji''} F_{w(j,i'')}) \quad i' < i'' \\
&= \sum_{j=1}^{b}{}^{*} n_{ji} n_{ji'} n_{ji''} (F_w \circ F_w)'(F_{w'} \circ F_{w''}) \quad w' < w'' \\
&= \sum_{j=1}^{b}{}^{*} n_{ji} n_{ji'} n_{ji''} [\underline{1}' \cdot (F_{w'} \circ F_{w''})] = 0
\end{aligned}
$$

(j) $X_3 X_3$

For $i = i''$, $i' = i'''$ (diagonal elements)

$$
\begin{aligned}
(\underline{x_i} \circ \underline{x_{i'}})'(\underline{x_i} \circ \underline{x_{i'}}) &= \sum_{j=1}^{b}(n_{ji}F_{w(j,i)} \circ n_{ji'}F_{w(j,i')})'(n_{ji}F_{w(j,i)} \circ n_{ji'}F_{w(j,i')}) \quad i < i' \\
&= \sum_{j=1}^{b}{}^{*} n_{ji}n_{ji'}(F_w \circ F_{w'})'(F_w \circ F_{w'}) \quad w < w' \\
&= \sum_{j=1}^{b}{}^{*} n_{ji}n_{ji'}(2^k) = \lambda_\gamma 2^k \quad i,\ i' \quad \gamma^{th}\text{associates}
\end{aligned}
$$

For $i \neq i''$ or $i \neq i'''$ (off-diagonal elements)

$$
\begin{aligned}
(\underline{x_i} \circ \underline{x_{i'}})'(\underline{x_{i''}} \circ \underline{x_{i'''}}) &= \sum_{j=1}^{b}(n_{ji}F_{w(j,i)} \circ n_{ji'}F_{w(j,i')})'(n_{ji''}F_{w(j,i'')} \circ n_{ji'''}F_{w(j,i''')}) \quad i < i',\ i'' < \\
&= \sum_{j=1}^{b}{}^{*} n_{ji}n_{ji'}n_{ji''}n_{ji'''}(F_w \circ F_{w'})'(F_{w''} \circ F_{w'''}) \quad w < w',\ w'' < w''' \\
&= 0
\end{aligned}
$$

Now, let $X_3'X_3 =$ G. Then G is a diagonal matrix with (ii', ii') element equal to $\lambda_\gamma 2^k$ if i and i' are γ^{th} associates, and zero for all off-diagonal elements.

The results (a) - (j) lead then to the form of $X'X$ as given in (2.7). Because the notation is somewhat complex we illustrate the general derivation given above by an example. Consider the Box-Behnken design using the PBIB(2) design with parameters, $\nu = 6,\ r = 2,\ b = 3,\ k = 4,\ \lambda_1 = 2,\ \lambda_2 = 1$ and treatment pairs (1,4), (2,5), and (3,6) being first associates with $\lambda_1 = 2$ and the remaining treatment pairs being second associates with $\lambda_2 = 1$. This PBIB design has incidence matrix

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

(see Design S1 of Clatworthy, 1973).

Then,

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

From this, the design matrix D with 3 center points can be obtained as follows:
$D = (\underline{x}_1, \underline{x}_2, \cdots, \underline{x}_\nu)$

$$= \begin{bmatrix} n_{11}F_{w(1,1)} & n_{12}F_{w(1,2)} & \underline{0} & n_{14}F_{w(1,4)} & n_{15}F_{w(1,5)} & \underline{0} \\ n_{21}F_{w(2,1)} & \underline{0} & n_{23}F_{w(2,3)} & n_{24}F_{w(2,4)} & \underline{0} & n_{26}F_{w(2,6)} \\ \underline{0} & n_{32}F_{w(3,2)} & n_{33}F_{w(3,3)} & \underline{0} & n_{35}F_{w(3,5)} & n_{36}F_{w(3,6)} \\ \underline{0_3} & \underline{0_3} & \underline{0_3} & \underline{0_3} & \underline{0_3} & \underline{0_3} \end{bmatrix}$$

where $\underline{x_i}$ is a $(3 \cdot 2^4 + 3) \times 1$ vector, $i = 1, 2, \cdots, \nu$

Now, consider $\underline{x_i'x_{i'}}$ when $i = 2,\ i' = 5$.

$$\begin{aligned}
\underline{x_2'} \cdot \underline{x_5} &= \sum_{j=1}^{3} (n_{j2}F_{w(j,2)})'(n_{j5}F_{w(j,5)}) + \underline{0_3'0_3} \\
&= (n_{12}F_{w(1,2)})'(n_{15}F_{w(1,5)}) + (n_{22}F_{w(2,2)})'(n_{25}F_{w(2,5)}) + (n_{32}F_{w(3,2)})'(n_{35}F_{w(3,5)}) \\
&= (n_{12}F_{w(1,2)})'(n_{15}F_{w(1,5)}) + \underline{0'0} + (n_{32}F_{w(3,2)})'(n_{35}F_{w(3,5)}) \\
&= n_{12}n_{15}(F_2'F_4) + n_{32}n_{35}(F_1'F_3) \\
&= 1 \times (0) + 1 \times (0) \\
&= 0
\end{aligned}$$

Then, conditions (1), (2) and (3) of property 3 are satisfied since

$$\sum_{j=1}^{3}{}^{*}(n_{j2}F_{w(j,2)})'(n_{j5}F_{w(j,5)}) = (n_{12}F_{w(1,2)})'(n_{15}F_{w(1,5)}) + (n_{32}F_{w(3,2)})'(n_{35}F_{w(3,5)})$$

and

$$\begin{array}{ll} w(1,2) = n_{11} + n_{12} = 2 & w(1,5) = n_{11} + n_{12} + n_{14} + n_{15} = 4 \\ w(3,2) = n_{32} = 1 & w(3,5) = n_{32} + n_{33} + n_{35} = 3 \end{array}$$

which implies that all $w(j,i)$ appearing in $\sum_{j=1}^{b}{}^{*}$ are greater than zero. And $w(1,2)$ is less than $w(1,5)$, And $w(3,2)$ is less than $w(3,5)$ which implies that $w(j,2)$ is less than $w(j,5)$ in $\sum_{j=1}^{b}{}^{*}$.

Let us consider now $\underline{x_i'x_{i'}}$ when $i=1,\ i'=3$.

$$\begin{aligned}\underline{x_1'}\cdot\underline{x_3} &= \sum_{j=1}^{3}(n_{j1}F_{w(j,1)})'(n_{j3}F_{w(j,3)}) + \underline{0_3'0_3} \\ &= (n_{11}F_{w(1,1)})'\cdot\underline{0} + (n_{21}F_{w(2,1)})'(n_{23}F_{w(2,3)}) + \underline{0}'(n_{33}F_{w(3,3)}) \\ &= (n_{21}F_{w(2,1)})'(n_{23}F_{w(2,3)}) \\ &= F_1'F_2 = 0\end{aligned}$$

Also conditions (1), (2) and (3) of Property 3 are satisfied, since

$$\sum_{j=1}^{3}{}^{*}(n_{j1}F_{w(j,1)})'(n_{j3}F_{w(j,3)}) = (n_{21}F_{w(2,1)})'(n_{23}F_{w(2,3)}) = F_1'F_2$$

and

$$w(2,1) = n_{21} = 1 \quad w(2,3) = n_{21} + n_{23} = 2$$

2.6. Estimation of parameters

We now consider estimability of the regression coefficients in model (2.6). For purposes of this discussion we define $\underline{\beta}^*_2 = (\beta_0, \beta_{11}, \beta_{22}, \dots, \beta_{vv})$. Clearly, we can see from (2.7) that the estimates of the parameters $\underline{\beta}_1$ are orthogonal to both the estimates of $\underline{\beta}^*_2$ and to the estimates of the parameters $\underline{\beta}_3$, and the estimates of $\underline{\beta}^*_2$ are also orthogonal to the estimates of the parameters $\underline{\beta}_3$ in the second-order model.

Concerning the estimators for these three sets of parameters we can draw the following conclusions:

(i) X'_1X_1 is of full rank v since rank ($I_{v\times v}$) = v. Accordingly, we get uniformly minimum variance unbiased estimators (UMVUE) for $\underline{\beta}_1$, namely $\hat{\underline{\beta}}_1 = (X_1'X_1)^{-1}X_1'\underline{Y}$.

(ii) The rank of $X_2'X_2$ is less than or equal to v , say s, since rank ($\underline{NN}'$) = s $\leq v$. This implies that we have s estimable functions among $\beta_{11}, \beta_{22}, \dots, \beta_{vv}$. For a given PBIB(m) design the rank of $\underline{NN}'$ can be determined easily from general results about the characteristic roots of $\underline{NN}'$ (see for example, Raghavarao, 1971). Of course, only if rank $(\underline{NN}') = v$ can all $\beta_{ii}(i = 1, 2, \dots, v)$ be estimated.

(iii) Now we consider the estimates of the coefficients $\beta_{ii'}$, $i, i' = 1, 2, \dots, v, i < i'$. For the PBIB(m) design we have $\lambda_\gamma \geq 0$ $(\gamma = 1, 2, \dots, m)$ with at least one $\lambda_\gamma > 0$. If all $\lambda_\gamma > 0$ it is obvious that $X_3'X_3$ is of full rank $v(v-1)/2$ since then rank (G) = $v(v-1)/2$. As a result, we obtain the UMVU estimator of $\underline{\beta}_3$ such that $\hat{\underline{\beta}}_3 = (X_3'X_3)^{-1}X_3'\underline{Y}$, which implies that all $\beta_{ii'}$ are estimable, $i, i' = 1, 2, \dots, v, i < i'$. If $\lambda_\delta = 0$ then all elements $g_{ii', ii'} = 0$ corresponding to those treatments i, i' which are δ -th associates, which implies that the corresponding parameters $\beta_{ii'}$ are not estimable.

2.7. Example

Consider the Box-Behnken design with the cyclic PBIB(2) characterized by the parameters $v = 5, r = 2, b = 5, k = 2, \lambda_1 = 1, \lambda_2 = 0$, and the following association scheme

<u>0.*assoc.*</u>	<u>1.*assoc.*</u>	<u>2.*assoc.*</u>
1	3, 4	2, 5
2	4, 5	3, 1
3	5, 1	4, 2
4	1, 2	5, 3
5	2, 3	1, 4

(Design C1 in Clatworthy, 1973)

with the following incidence matrix $\underset{\sim}{N}$ and its transpose $\underset{\sim}{N}'$:

$$\underset{\sim}{N} = \begin{bmatrix} 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \end{bmatrix}, \qquad \underset{\sim}{N}' = \begin{bmatrix} 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 1 \end{bmatrix}$$

Then we get the following design matrix with $n_0 = 3$

$$D = \begin{bmatrix} \underline{E}_1 & \underline{0} & \underline{E}_2 & \underline{0} & \underline{0} \\ \underline{0} & \underline{E}_1 & \underline{0} & \underline{E}_2 & \underline{0} \\ \underline{0} & \underline{0} & \underline{E}_1 & \underline{0} & \underline{E}_2 \\ \underline{E}_1 & \underline{0} & \underline{0} & \underline{E}_2 & \underline{0} \\ \underline{0} & \underline{E}_1 & \underline{0} & \underline{0} & \underline{E}_2 \\ \underline{0}_3 & \underline{0}_3 & \underline{0}_3 & \underline{0}_3 & \underline{0}_3 \end{bmatrix}$$

where $\underline{E}_w$ is a 4×1 vector with elements of $+1$ and -1, $w = 1, 2$ with e.g., $\underline{E}_1' = (1, 1, -1, -1)$, $\underline{E}_2' = (1, -1, 1, -1)$, $\underline{0}$ is a 4×1 vector of elements being zeros, and $\underline{0}_3$ is a 3×1 vector of elements being zeros.

Then, for the model

$$y_u = \beta_0 + \sum_{i=1}^{5} \beta_i x_{iu} + \sum_{i=1}^{5} \beta_{ii} x_{iu}{}^2 + \sum_{\substack{i, i' = 1 \\ i < i'}}^{5} \beta_{ii'} x_{iu} x_{i'u} + \varepsilon_u, \qquad u = 1,2, \dots, 23,$$

We have

$$
X'X = \begin{array}{c}
\begin{array}{ccccccccccccccccccccc}
\beta_0 & \beta_1 & \beta_2 & \beta_3 & \beta_4 & \beta_5 & \beta_{11} & \beta_{22} & \beta_{33} & \beta_{44} & \beta_{55} & \beta_{12} & \beta_{13} & \beta_{14} & \beta_{15} & \beta_{23} & \beta_{24} & \beta_{25} & \beta_{34} & \beta_{35} & \beta_{45}
\end{array} \\
\left[\begin{array}{c|ccccc|ccccc|cccccccccc}
23 & 0 & 0 & 0 & 0 & 0 & 8 & 8 & 8 & 8 & 8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\hline
0 & 8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\hline
8 & 0 & 0 & 0 & 0 & 0 & 8 & 0 & 4 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
8 & 0 & 0 & 0 & 0 & 0 & 0 & 8 & 0 & 4 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
8 & 0 & 0 & 0 & 0 & 0 & 4 & 0 & 8 & 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
8 & 0 & 0 & 0 & 0 & 0 & 4 & 4 & 0 & 8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
8 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 4 & 0 & 8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\hline
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{array}\right]
\end{array}
$$

The form of $X'X$ implies immediately that all pure quadratic coefficients are estimable since rank $(\underline{NN'}) = 5$ and the mixed quadratic coefficients β_{13}, β_{14}, β_{24}, β_{25}, and β_{35} are estimable, but β_{12}, β_{15}, β_{23}, β_{34}, and β_{45} are not estimable.

2.8. Conclusions

In deriving the general form of the coefficient matrix $X'X$ of the normal equations for estimating the parameters of model (2.3) with a Box-Behnken design we have established the following results:

(i) For all β_{ii} to be estimable the PBIB(m) design has to be chosen such that rank $(\underline{N}\underline{N}') = v$;

(ii) For all $\beta_{ii'}$ $(i < i')$ to be estimable the PBIB(m) design has to be chosen such that all $\lambda_\gamma > 0$ $(\gamma = 1, 2, \dots, m)$.

Chapter 3. Box-Behnken designs using fractional factorials

One practical difficulty with the Box-Behnken design, using an incomplete block design together with the full 2^k factorial, is that the number of design points increases rapidly as k, the block size increases. Instead of using a full factorial, Box and Behnken (1960) advocate using a fractional factorial, say a $\frac{1}{2^l}$ th fraction of the 2^k factorial, hence reducing the number of design points from $b2^k + 1$ to $b2^{k-l} + 1$. Box-Behnken designs using fractional factorials are constructed by combining incomplete block designs with 2^{k-l} fractional factorials. The procedure of constructing such Box-Behnken design is essentially the same as that described in Chapter 2, that is by means of k generators $F_1, F_2, \dots, F_k$. The problem of choosing these generators depends on the resolution of the 2^{k-l} fraction. Generally speaking, we choose $F_1, F_2, \dots, F_{k-l}$ as the first $k-l$ main effect contrasts of the 2^{k-l} factorial. The remaining F 's, i.e. $F_{k-l+1}, F_{k-l+2}, \dots, F_k$ are obtained by appropriate (to be described in subsequent sections) element-wise multiplication of $F_1, F_2, \dots, F_{k-l}$. It will be shown that the F 's obtained in this way satisfy the properties given in Chapter 2. We now explore the possibilities of constructing Box-Behnken designs using fractional factorials of resolution III, IV, and V.

3.1. Resolution III Case

We first consider the smallest fraction which is a main effect plan or resolution III design. The basic property of a resolution III design is that main effects are confounded with two-factor interactions. The main effect plan is obtained by specifying the so-called identity relationship. For the 2^{k-l}_{III} we have

$$I = E_1 = E_2 = \cdots = E_l = \text{ all possible generalized interactions}$$

where each of the terms $E_1, E_2, \ldots$ consists of at least 3 letters. The E 's refer to interactions for the 2^k factorial. Now, to choose the generators $F_1, F_2, \ldots, F_k$ for the Box-Behnken design we choose for $F_1, F_2, \ldots, F_{k-l}$ the first $k-l$ main effect contrasts $\mathcal{F}_1, \mathcal{F}_2, \ldots, \mathcal{F}_{k-l}$ for the 2^{k-l} factorial. The remaining $F_{k-l+1}, F_{k-l+2}, \ldots, F_k$ are determined by the alias structure given by the defining relation. More specifically, the E_i 's represent interactions of the 2^k factorial, represented by, say, $F_{i_1} \circ F_{i_2} \circ F_{i_3}$, etc. Then we take each of $\mathcal{F}_{k-l+1}, \mathcal{F}_{k-l+2}, \ldots, \mathcal{F}_k$ as one of alias of the main effects $F_{k-l+1}, F_{k-l+2}, \ldots, F_k$, respectively. A consequence of this is that (6) and (7) of Property 1 (see Section 2.5) do not hold, i.e. we have for some w, w', w'', w''' that $\mathcal{F}_w = \mathcal{F}_{w'} \circ \mathcal{F}_{w''}$ and hence $\mathcal{F}_w' \bullet (\mathcal{F}_{w'} \circ \mathcal{F}_{w''}) \neq 0$, and $(\mathcal{F}_w \circ \mathcal{F}_{w'})' \bullet (\mathcal{F}_{w''} \circ \mathcal{F}_{w'''}) \neq 0$. Consequently, the elements of $X_1'X_3$ are no longer 0 and the off-diagonal elements of $X_3'X_3$ are not 0. In this case, we can write $X'X$ as follows:

$$X'X = \begin{bmatrix} n & \underline{0}' & r2^{k-l}\underline{1}' & \underline{0}' \\ \underline{0} & r2^{k-l}I & 0 & K \\ r2^{k-l}\underline{1} & 0 & 2^{k-l}(\underline{NN'}) & 0 \\ \underline{0} & K' & 0 & G \end{bmatrix} \tag{3.1}$$

where K now is not a 0 matrix and G is not a diagonal matrix. This form of the $X'X$ matrix tells us then that the estimates of $\underline{\beta}^*_2 = (\beta_0, \underline{\beta}_2')'$ are orthogonal to the estimates of $(\underline{\beta}_1', \underline{\beta}_3')'$. Thus, using a resolution III design instead of the full factorial does alter the properties of the estimators in the sense that $\hat{\underline{\beta}}_1$ and $\hat{\underline{\beta}}_3$ are no longer uncorrelated, and the $\hat{\beta}_{ii'}(i < i')$ are no longer uncorrelated. Now, we illustrate the construction of a Box-Behnken design using a resolution III fraction in example 3.1.

Example 3.1.

Consider the Box-Behnken design using a resolution III design with the PBIB(2) based on a Regular group divisible association scheme, with parameters $v = 8, r = 5, b = 8, k = 5, \lambda_1 = 2, \lambda_2 = 3$, and the following association scheme

0.assoc.	1.assoc.	2.assoc.
1	5	2, 3, 4, 6, 7, 8
2	6	3, 4, 5, 7, 8, 1
3	7	4, 5, 6, 8, 1, 2
4	8	5, 6, 7, 1, 2, 3
5	1	6, 7, 8, 2, 3, 4
6	2	7, 8, 1, 3, 4, 5
7	3	8, 1, 2, 4, 5, 6
8	4	1, 2, 3, 5, 6, 7

(Design R134 in Clatworthy, 1973)

with the following incidence matrix $\underline{N}$ and its transpose $\underline{N}'$:

$$\underline{N} = \begin{bmatrix} 1 & 0 & 0 & 1 & 1 & 1 & 1 & 0 \\ 0 & 1 & 0 & 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 1 & 0 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 1 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 & 1 & 1 & 0 & 1 \end{bmatrix}, \quad \underline{N}' = \begin{bmatrix} 1 & 0 & 1 & 1 & 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 1 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & 1 & 1 & 0 & 0 & 1 \end{bmatrix}$$

For the $2^{5-2}{}_{III}$ fractional factorial, we specify the identity relationship as $I = \underline{E}_1 \circ \underline{E}_2 \circ \underline{E}_4 = \underline{E}_1 \circ \underline{E}_3 \circ \underline{E}_5 = \underline{E}_2 \circ \underline{E}_3 \circ \underline{E}_4 \circ \underline{E}_5$. To obtain the generators $\underline{E}_1, \underline{E}_2, \ldots, \underline{E}_5$, we choose for $\underline{E}_1, \underline{E}_2, \underline{E}_3$ the first 3 main effect contrasts $\underline{F}_1, \underline{F}_2, \underline{F}_3$ for the 2^{5-2} factorial. The remaining $\underline{E}_4, \underline{E}_5$ are determined by the defining relation given by $\underline{F}_4, \underline{F}_5$ such that

$\underline{F}_4 = \underline{F}_1 o \underline{F}_2$, $\underline{F}_5 = \underline{F}_1 o \underline{F}_3$, respectively. These main effect contrasts can be written specifically as $\underline{F}_1' = (-1, 1, -1, 1, -1, 1, -1, 1)$, $\underline{F}_2' = (-1, -1, 1, 1, -1, -1, 1, 1)$, $\underline{F}_3' = (-1, -1, -1, -1, 1, 1, 1, 1)$. Thus, $\underline{F}_4' = (1, -1, -1, 1, 1, -1, -1, 1)$, and $\underline{F}_5' = (1, -1, 1, -1, -1, 1, -1, 1)$. Also for $w = 4, w' = 1, w'' = 2$, $F_4' \bullet (F_1 o F_2) = F_4' F_4 = 8$, not 0. Similarly, for $w = 2, w' = 3, w'' = 4, w''' = 5$, $(F_2 o F_3)' \bullet (F_4 o F_5) = (F_2 o F_3)' \bullet (F_1 o F_2 o F_1 o F_3) = (F_2 o F_3)' \bullet (F_2 o F_3) = 8$, again not 0. In order to obtain the Box-Behnken design matrix, we replace the first 3 unity elements of each row by the main effect contrasts $\underline{F}_i\,(i = 1,2,3)$ of the 2^3 factorial. We replace the remaining 2 unity elements of each row by $\underline{F}_4, \underline{F}_5$ Then we obtain a Box-Behnken design matrix using fractional factorial of resolution III, i.e., 2^{5-2}_{III} , adding 3 center point

$$D = \begin{bmatrix} \underline{F}_1 & \underline{0} & \underline{F}_2 & \underline{F}_3 & \underline{F}_4 & \underline{F}_5 & \underline{0} & \underline{0} \\ \underline{0} & \underline{F}_1 & \underline{0} & \underline{F}_2 & \underline{F}_3 & \underline{F}_4 & \underline{F}_5 & \underline{0} \\ \underline{0} & \underline{0} & \underline{F}_1 & \underline{0} & \underline{F}_2 & \underline{F}_3 & \underline{F}_4 & \underline{F}_5 \\ \underline{F}_1 & \underline{0} & \underline{0} & \underline{F}_2 & \underline{0} & \underline{F}_3 & \underline{F}_4 & \underline{F}_5 \\ \underline{F}_1 & \underline{F}_2 & \underline{0} & \underline{0} & \underline{F}_3 & \underline{0} & \underline{F}_4 & \underline{F}_5 \\ \underline{F}_1 & \underline{F}_2 & \underline{F}_3 & \underline{0} & \underline{0} & \underline{F}_4 & \underline{0} & \underline{F}_5 \\ \underline{F}_1 & \underline{F}_2 & \underline{F}_3 & \underline{F}_4 & \underline{0} & \underline{0} & \underline{F}_5 & \underline{0} \\ \underline{0} & \underline{F}_1 & \underline{F}_2 & \underline{F}_3 & \underline{F}_4 & \underline{0} & \underline{0} & \underline{F}_5 \\ \underline{0}_3 & \underline{0}_3 & \underline{0}_3 & \underline{0}_3 & \underline{0}_3 & \underline{0}_3 & \underline{0}_3 & \underline{0}_3 \end{bmatrix}$$

where $\underline{0}$ is a 8×1 vector of elements being zeros.

Then, for the model

$$y_u = \beta_0 + \sum_{i=1}^{8} \beta_i x_{iu} + \sum_{i=1}^{8} \beta_{ii} x_{iu}^2 + \sum_{\substack{i, i' = 1 \\ i < i'}}^{8} \beta_{ii'} x_{iu} x_{i'u} + \varepsilon_u, \qquad u = 1,2, \ldots , 67,$$

We have

$$X'X = \begin{bmatrix} 67 & \underline{0}' & 40\,\underline{1}' & \underline{0}' \\ \underline{0} & 40\,I & 0 & K \\ 40\,\underline{1} & 0 & 8\,(\underline{N}\underline{N}') & 0 \\ \underline{0} & K' & 0 & G \end{bmatrix}$$

with

$$K = \begin{array}{c@{}c} & \begin{array}{ccccccccccccccccccccc} \beta_{12} & \beta_{13} & \beta_{14} & \beta_{15} & \beta_{16} & \beta_{17} & \beta_{18} & \beta_{23} & \beta_{24} & \beta_{25} & \beta_{26} & \beta_{27} & \beta_{28} & \beta_{34} & \beta_{35} & \beta_{36} & \beta_{37} & \beta_{38} & \beta_{45} & \cdots & \beta_{78} \end{array} \\ \begin{array}{c} \beta_1 \\ \beta_2 \\ \beta_3 \\ \beta_4 \\ \beta_5 \\ \beta_6 \\ \beta_7 \\ \beta_8 \end{array} & \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 8 & 0 & 8 & 8 & 0 & 0 & 8 & 0 & 8 & 8 & 0 & \cdots & 0 \\ 0 & 0 & 8 & 0 & 8 & 8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 8 & 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 8 & 0 & 8 & 8 & 0 & 0 & 8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ 8 & 0 & 0 & 0 & 8 & 8 & 0 & 0 & 0 & 0 & 8 & 0 & 8 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 8 & 0 & 0 & 0 & 0 & 8 & 8 & 0 & 0 & 0 & 8 & 0 & 0 & 0 & 0 & 8 & 0 & 0 & \cdots & 0 \\ 8 & 0 & 8 & 0 & 0 & 0 & 8 & 0 & 8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 8 & 0 & \cdots & 0 \\ 8 & 8 & 8 & 0 & 0 & 0 & 0 & 0 & 0 & 8 & 0 & 0 & 0 & 0 & 8 & 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 8 & 0 & 8 & 8 & 0 & 0 & 0 & 8 & 0 & 0 & 0 & 0 & 0 & 0 & 8 & 0 & 0 & 0 & \cdots & 0 \end{bmatrix} \end{array}$$

and

$$
G = \left[\begin{array}{c|ccccccccccccccccccccc}
 & x_{12} & x_{13} & x_{14} & x_{15} & x_{16} & x_{17} & x_{18} & x_{23} & x_{24} & x_{25} & x_{26} & x_{27} & x_{28} & x_{34} & x_{35} & x_{36} & x_{37} & x_{38} & x_{45} & \cdots & x_{78} \\
\hline
x_{12} & 24 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
x_{13} & 0 & 24 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
x_{14} & 0 & 0 & 24 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
x_{15} & 0 & 0 & 0 & 16 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
x_{16} & 0 & 0 & 0 & 0 & 24 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
x_{17} & 0 & 0 & 0 & 0 & 0 & 24 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
x_{18} & 0 & 0 & 0 & 0 & 0 & 0 & 24 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
x_{23} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 24 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
x_{24} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 24 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 8 & 0 & 0 & \cdots & 0 \\
x_{25} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 24 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 8 \\
x_{26} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 16 & 0 & 0 & 0 & 0 & 0 & 0 & 8 & 0 & \cdots & 0 \\
x_{27} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 24 & 0 & 8 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
x_{28} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 24 & 0 & 0 & 8 & 0 & 0 & 0 & \cdots & 0 \\
x_{34} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 8 & 0 & 24 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\
x_{35} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 24 & 0 & 0 & 0 & 0 & \cdots & 0 \\
x_{36} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 8 & 0 & 0 & 24 & 0 & 0 & 8 & \cdots & 0 \\
x_{37} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 16 & 0 & 0 & \cdots & 0 \\
x_{38} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 8 & 0 & 0 & 0 & 0 & 0 & 0 & 24 & 8 & \cdots & 0 \\
x_{45} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 8 & 0 & 8 & 24 & \cdots & 0 \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdots & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdots & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdots & \cdot \\
x_{78} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 8 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 24
\end{array}\right]
$$

From the $X'X$ matrix, we can see that the estimates of $\underline{\beta}^*_2 = (\beta_0, \beta_{11}, \beta_{22}, \dots, \beta_{88})'$ are orthogonal to the estimates of $(\underline{\beta}_1', \underline{\beta}_3')' = (\beta_1, \beta_2, \dots, \beta_8, \beta_{12}, \beta_{13}, \dots, \beta_{78})$. However, $\hat{\underline{\beta}}_1$ and $\hat{\underline{\beta}}_3$ are no longer uncorrelated since K is not 0 matrix. In G, some of off-diagonal elements are not 0. For example, $g_{24,37}$, defined as the element of row x_{24} and column x_{37} in G, is not 0, because the vector for $\underline{x}_{24}$ is given by $\underline{x}_2 \circ \underline{x}_4 = (\underline{0}, \underline{F_1 F_2}, \underline{0}, \underline{0}, \underline{0}, \underline{0}, \underline{F_2 F_4}, \underline{F_1 F_3}, \underline{0}_3)'$, and the vector for $\underline{x}_{37}$ is given by $\underline{x}_3 \circ \underline{x}_7 = (\underline{0}, \underline{0}, \underline{F_1 F_4}, \underline{0}, \underline{0}, \underline{0}, \underline{F_3 F_5}, \underline{0}, \underline{0}_3)'$, $g_{24,37}$ then is obtained by $g_{24,37} = (\underline{x}_{24})'(\underline{x}_{37}) = (\underline{F_2 F_4})'(\underline{F_3 F_5}) = (\underline{F_2 F_1 F_2})' = (\underline{F_3 F_1 F_3}) = \underline{F}_1{}'\underline{F}_1 = 8$. Thus the estimates of mixed quadratic coefficients $\beta_{ii'}$, $i, i' = 1,2, \ldots, 8$, $i < i'$, are no longer uncorrelated each other.

3.2. Resolution IV Case

Next we consider using a resolution IV design, in which two-factor interactions are confounded with each other. For the 2^{k-l}_{IV} we have the identity relationship

$$I = E_1 = E_2 = \cdots = E_l = \text{ all possible generalized interactions}$$

where each of the terms $E_1, E_2, \ldots$ consists of at least 4 letters. The E_i 's refer to interactions for the 2^k factorial, represented by, say, $F_{i_1} \circ F_{i_2} \circ F_{i_3} \circ F_{i_4}$, etc. The procedure for choosing the generators $F_1, F_2, \ldots, F_k$ for the Box-Behnken design is the same as that for the resolution III case. That is, we choose for $F_1, F_2, \ldots, F_{k-l}$ the first $k - l$ main effect contrasts $\boldsymbol{F}_1, \boldsymbol{F}_2, \ldots, \boldsymbol{F}_{k-l}$ for the 2^{k-l} factorial. The remaining $F_{k-l+1}, F_{k-l+2}, \ldots, F_k$ are determined by the alias structure given by the defining relation. Then we regard each of $\boldsymbol{F}_{k-l+1}, \boldsymbol{F}_{k-l+2}, \ldots, \boldsymbol{F}_k$ as alias of the main effects $F_{k-l+1}, F_{k-l+2}, \ldots, F_k$, respectively. A consequence of this is that (7) of Property 1 (see Section 2.5) does not hold, i.e. we have for some w, w', w'', w''' that $(\boldsymbol{F}_w \circ \boldsymbol{F}_{w'})' \bullet (\boldsymbol{F}_{w''} \circ \boldsymbol{F}_{w'''}) \neq 0$. For example, we consider 2^{4-1}_{IV}, i.e. the fractional factorials of resolution IV with 3 contrast vectors for main effects F_1, F_2 and F_3 which are orthogonal to each other, and F_4 being aliased with three-factor interaction $F_1 \circ F_2 \circ F_3$. These main effect contrasts can be written as $\underline{F}_1' = (-1, 1, -1, 1, -1, 1, -1, 1)$, $\underline{F}_2' = (-1, -1, 1, 1, -1, -1, 1, 1)$, $\underline{F}_3' = (-1, -1, -1, -1, 1, 1, 1, 1)$, and $\underline{F}_4' = (F_1 \circ F_2 \circ F_3)' = (-1, 1, 1, -1, 1, -1, -1, 1)$. Thus for $w = 1, w' = 2, w'' = 3, w''' = 4$, $(F_1 \circ F_2)' \bullet (F_3 \circ F_4) = (F_1 \circ F_2)' \bullet (F_3 \circ F_1 \circ F_2 \circ F_3) = (F_1 \circ F_2)' \bullet (F_1 \circ F_2) = 8$ is not 0, which implies that the off-diagonal elements of $X_3'X_3$ are no longer 0 (see (j) X'_3X_3 in Section 2.4). In this case, we can get an $X'X$ matrix similar to (2.7):

$$X'X = \begin{bmatrix} n & \underline{0}' & r2^{k-l}\underline{1}' & \underline{0}' \\ \underline{0} & r2^{k-l}I & 0 & 0 \\ r2^{k-l}\underline{1} & 0 & 2^{k-l}(\underline{NN'}) & 0 \\ \underline{0} & 0 & 0 & G \end{bmatrix} \tag{3.2}$$

except that G is not a diagonal matrix.

From the form of the $X'X$ matrix we can see that the estimates of $\underline{\beta_1}$ and $\underline{\beta_2}$ have the same properties as those with the full factorial. But the estimates of the mixed quadratic coefficients $\underline{\beta_3}$ do not have the same property as those with the full factorial since G is no longer diagonal. In addition, for some PBIB designs some columns of G can be a linear combination of other columns with the result that G is less than full rank (Table 3.1). This means that for some Box-Behnken designs even when all $\lambda_\gamma > 0$ we may not be able to estimate all mixed quadratic coefficients. Thus it may not be advisible to use a resolution IV design. But for some Box-Behnken designs with PBIB(2) when $\lambda_1 > 0$, $\lambda_2 > 0$, G is of full rank (Table 3.2). Then we can estimate all mixed quadratic coefficients such that $\hat{\underline{\beta_3}} = G^{-1}(X_3'\underline{Y})$, which implies that all mixed quadratic coefficients are estimable. In these cases the number of observations can be reduced greatly by making use of fractional factorials.

Table 3.1. PBIB(2) designs in which G is of less than full rank

DesignNo.	t	r	k	b	λ_1	λ_2
*SR*35	6	6	4	9	3	4
*R*94	6	4	4	6	3	2
*T*33	10	4	4	10	1	2
*LS*26	9	4	4	9	1	2
*S*18	8	3	6	4	3	2
*T*57	10	3	6	5	3	1
*S*53	12	2	8	3	2	1

Table 3.2. PBIB(2) designs in which G is of full rank

DesignNo.	t	r	k	b	λ_1	λ_2
*SR*65	9	6	6	9	3	4
*LS*72	9	4	6	6	3	2
*T*71	10	7	7	10	5	4
*R*172	9	7	7	9	6	5
*S*51	10	4	8	5	4	3
*R*186	12	8	8	12	6	5

It does not appear from the Table 3.1 and Table 3.2 that the property of G, i.e. whether it is of full rank or not, is associated with any particular type of PBIB(2) design having $\lambda_1 > 0$ and $\lambda_2 > 0$.

Example 3.2.

Consider the Box-Behnken design using a resolution IV design with the PBIB(2) based on a Latin Square type association scheme, with parameters $v = 9$, $r = 4$, $b = 6$, $k = 6$, $\lambda_1 = 3$, $\lambda_2 = 2$, and the following association scheme

0.assoc.	1.assoc.	2.assoc.
1	2, 3, 4, 7	5, 6, 8, 9
2	1, 3, 5, 8	4, 6, 7, 9
3	1, 2, 6, 9	4, 5, 7, 8
4	1, 5, 6, 7	2, 3, 8, 9
5	2, 4, 6, 8	1, 3, 7, 9
6	3, 4, 5, 9	1, 2, 7, 8
7	1, 4, 8, 9	2, 3, 5, 6
8	2, 5, 7, 9	1, 3, 4, 6
9	3, 6, 7, 8	1, 2, 4, 5

(Design LS72 in Clatworthy, 1973)

with the following incidence matrix $\underline{N}$ and its transpose $\underline{N}'$:

$$\underline{N} = \begin{bmatrix} 0 & 1 & 1 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 & 0 & 1 \\ 0 & 1 & 1 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 & 1 & 0 \\ 1 & 1 & 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 & 1 & 0 \end{bmatrix}, \qquad \underline{N}' = \begin{bmatrix} 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 1 & 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 1 & 0 & 1 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 & 1 & 0 & 1 & 1 & 0 \end{bmatrix}$$

For the 2^{6-2}_{IV} fractional factorial, we specify the identity relationship such that $I = \underset{\sim}{E}_1 \circ \underset{\sim}{E}_2 \circ \underset{\sim}{E}_3 \circ \underset{\sim}{E}_5 = \underset{\sim}{E}_2 \circ \underset{\sim}{E}_3 \circ \underset{\sim}{E}_4 \circ \underset{\sim}{E}_6 = \underset{\sim}{E}_1 \circ \underset{\sim}{E}_4 \circ \underset{\sim}{E}_5 \circ \underset{\sim}{E}_6$. To obtain the generators $\underset{\sim}{E}_1, \underset{\sim}{E}_2, \dots, \underset{\sim}{E}_6$, we choose for $\underset{\sim}{E}_1, \underset{\sim}{E}_2, \underset{\sim}{E}_3, \underset{\sim}{E}_4$ the first 4 main effect contrasts $\underset{\sim}{F}_1, \underset{\sim}{F}_2, \underset{\sim}{F}_3, \underset{\sim}{F}_4$ for the 2^{6-2} factorial. The remaining $\underset{\sim}{E}_5, \underset{\sim}{E}_6$ are determined by the defining relation given by $\underset{\sim}{F}_5, \underset{\sim}{F}_6$ such that $\underset{\sim}{F}_5 = \underset{\sim}{F}_1 \circ \underset{\sim}{F}_2 \circ \underset{\sim}{F}_3$, $\underset{\sim}{F}_6 = \underset{\sim}{F}_2 \circ \underset{\sim}{F}_3 \circ \underset{\sim}{F}_4$, respectively. we then replace the first 4 unity elements of each row by the main effect contrasts $\underset{\sim}{F}_i$ $(i = 1,2,3,4)$ of the 2^4 factorial. We replace the remaining 2 unity elements of each row by $\underset{\sim}{F}_5, \underset{\sim}{F}_6$ Then we obtain a Box-Behnken design matrix using fractional factorial of resolution IV, i.e., 2^{6-2}_{IV} , adding 1 center point such as

$$D = \begin{bmatrix} \underset{\sim}{0} & \underset{\sim}{0} & \underset{\sim}{0} & \underset{\sim}{E}_1 & \underset{\sim}{E}_2 & \underset{\sim}{E}_3 & \underset{\sim}{E}_4 & \underset{\sim}{E}_5 & \underset{\sim}{E}_6 \\ \underset{\sim}{E}_1 & \underset{\sim}{E}_2 & \underset{\sim}{E}_3 & \underset{\sim}{0} & \underset{\sim}{0} & \underset{\sim}{0} & \underset{\sim}{E}_4 & \underset{\sim}{E}_5 & \underset{\sim}{E}_6 \\ \underset{\sim}{E}_1 & \underset{\sim}{E}_2 & \underset{\sim}{E}_3 & \underset{\sim}{E}_4 & \underset{\sim}{E}_5 & \underset{\sim}{E}_6 & \underset{\sim}{0} & \underset{\sim}{0} & \underset{\sim}{0} \\ \underset{\sim}{0} & \underset{\sim}{E}_1 & \underset{\sim}{E}_2 & \underset{\sim}{0} & \underset{\sim}{E}_3 & \underset{\sim}{E}_4 & \underset{\sim}{0} & \underset{\sim}{E}_5 & \underset{\sim}{E}_6 \\ \underset{\sim}{E}_1 & \underset{\sim}{0} & \underset{\sim}{E}_2 & \underset{\sim}{E}_3 & \underset{\sim}{0} & \underset{\sim}{E}_4 & \underset{\sim}{E}_5 & \underset{\sim}{0} & \underset{\sim}{E}_6 \\ \underset{\sim}{E}_1 & \underset{\sim}{E}_2 & \underset{\sim}{0} & \underset{\sim}{E}_3 & \underset{\sim}{E}_4 & \underset{\sim}{0} & \underset{\sim}{E}_5 & \underset{\sim}{E}_6 & \underset{\sim}{0} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

where $\underset{\sim}{E}_w$ $w = 1, 2, \dots, 6$ is a 16×1 vector with
$\underset{\sim}{E}_1' = (1, 1, 1, 1, 1, 1, 1, 1, -1, -1, -1, -1, -1, -1, -1, -1)$,
$\underset{\sim}{E}_2' = (1, 1, 1, 1, -1, -1, -1, -1, 1, 1, 1, 1, -1, -1, -1, -1)$,
$\underset{\sim}{E}_3' = (1, 1, -1, -1, 1, 1, -1, -1, 1, 1, -1, -1, 1, 1, -1, -1)$,
$\underset{\sim}{E}_4' = (1, -1, 1, -1, 1, -1, 1, -1, 1, -1, 1, -1, 1, -1, 1, -1)$, and $\underset{\sim}{E}_5 = \underset{\sim}{E}_1 \circ \underset{\sim}{E}_2 \circ \underset{\sim}{E}_3$,
$\underset{\sim}{E}_6 = \underset{\sim}{E}_2 \circ \underset{\sim}{E}_3 \circ \underset{\sim}{E}_4$, $\underset{\sim}{0}$ is a 16×1 vector of elements being zeros.

Then, for the model

$$y_u = \beta_0 + \sum_{i=1}^{9} \beta_i x_{iu} + \sum_{i=1}^{9} \beta_{ii} x_{iu}{}^2 + \sum_{\substack{i,\,i'=1 \\ i<i'}}^{9} \beta_{ii'} x_{iu} x_{i'u} + \varepsilon_u, \qquad u = 1,2, \dots, 97,$$

We have

$$X'X = \begin{bmatrix} 97 & \underline{0}' & 64\,\underline{1}' & \underline{0}' \\ \underline{0} & 64\,I & 0 & 0 \\ 64\,\underline{1} & 0 & 16\,(\underline{NN}') & 0 \\ \underline{0} & 0 & 0 & G \end{bmatrix}$$

with

$$G = \begin{array}{c} \\ x_{12} \\ x_{13} \\ x_{14} \\ x_{15} \\ x_{16} \\ x_{17} \\ x_{18} \\ x_{19} \\ x_{23} \\ x_{24} \\ x_{25} \\ \cdot \\ \cdot \\ \cdot \\ x_{89} \end{array} \left[\begin{array}{cccccccccccccc} x_{12} & x_{13} & x_{14} & x_{15} & x_{16} & x_{17} & x_{18} & x_{19} & x_{23} & x_{24} & x_{25} & \cdot\;\cdot\;\cdot & x_{89} \\ 48 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdot\;\cdot\;\cdot & 0 \\ 0 & 48 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 16 & \cdot\;\cdot\;\cdot & 0 \\ 0 & 0 & 48 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdot\;\cdot\;\cdot & 0 \\ 0 & 0 & 0 & 32 & 0 & 0 & 0 & 0 & 16 & 0 & 0 & \cdot\;\cdot\;\cdot & 0 \\ 0 & 0 & 0 & 0 & 32 & 0 & 0 & 0 & 0 & 0 & 0 & \cdot\;\cdot\;\cdot & 0 \\ 0 & 0 & 0 & 0 & 0 & 48 & 0 & 0 & 0 & 16 & 0 & \cdot\;\cdot\;\cdot & 16 \\ 0 & 0 & 0 & 0 & 0 & 0 & 32 & 0 & 16 & 0 & 0 & \cdot\;\cdot\;\cdot & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 32 & 0 & 0 & 0 & \cdot\;\cdot\;\cdot & 0 \\ 0 & 0 & 0 & 16 & 0 & 0 & 16 & 0 & 48 & 0 & 0 & \cdot\;\cdot\;\cdot & 0 \\ 0 & 0 & 0 & 0 & 0 & 16 & 0 & 0 & 0 & 32 & 0 & \cdot\;\cdot\;\cdot & 0 \\ 0 & 16 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 48 & \cdot\;\cdot\;\cdot & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot\;\cdot\;\cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot\;\cdot\;\cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot\;\cdot\;\cdot & \cdot \\ 0 & 0 & 0 & 0 & 0 & 16 & 0 & 0 & 0 & 0 & 0 & \cdot\;\cdot\;\cdot & 48 \end{array} \right]$$

From the $X'X$ matrix, we obtain UMVUE for first order coefficients $\underline{\beta}_1$. We have 5 estimable functions among pure quadratic coefficients $\beta_{11}, \beta_{22}, \dots, \beta_{99}$ since rank $(\underline{N}\underline{N}') = 5$ with

$$(\underline{N}\underline{N}') = \begin{bmatrix} 4 & 3 & 3 & 3 & 2 & 2 & 3 & 2 & 2 \\ 3 & 4 & 3 & 2 & 3 & 2 & 2 & 3 & 2 \\ 3 & 3 & 4 & 2 & 2 & 3 & 2 & 2 & 3 \\ 3 & 2 & 2 & 4 & 3 & 3 & 3 & 2 & 2 \\ 2 & 3 & 2 & 3 & 4 & 3 & 2 & 3 & 2 \\ 2 & 2 & 3 & 3 & 3 & 4 & 2 & 2 & 3 \\ 3 & 2 & 2 & 3 & 2 & 2 & 4 & 3 & 3 \\ 2 & 3 & 2 & 2 & 3 & 2 & 3 & 4 & 3 \\ 2 & 2 & 3 & 2 & 2 & 3 & 3 & 3 & 4 \end{bmatrix}$$

For example, $\beta_{11} - \beta_{55} - \beta_{66} - \beta_{88} - \beta_{99}$, $\beta_{22} + \beta_{55} + \beta_{88}$, $\beta_{33} + \beta_{66} + \beta_{99}$, $\beta_{44} + \beta_{55} + \beta_{66}$, and $\beta_{77} - \beta_{88}$ are estimable functions. In G, some of off-diagonal elements cannot be 0 since two-factor interactions are confounded with each other. For example, the vector for $\underline{x}_{15}$ is given by $\underline{x}_1 \circ \underline{x}_5 = (\underline{0}, \underline{0}, \underline{E_1E_5}, \underline{0}, \underline{0}, \underline{E_1E_4}, 0)'$, the vector for $\underline{x}_{23}$ is given by $x_2 \circ x_3 = (\underline{0}, \underline{E_2E_3}, \underline{E_2E_3}, \underline{E_1E_2}, \underline{0}, \underline{0}, 0)'$, and $g_{15,23}$ represents an element of row x_{15} and column x_{23} in G. Then $g_{15,23}$ can be expressed as $g_{15,23} = (\underline{x}_1 \circ \underline{x}_5)'(\underline{x}_2 \circ \underline{x}_3) = (\underline{E_1E_5})'(\underline{E_2E_3}) = (\underline{E_1E_1E_2E_3})'(\underline{E_2E_3}) = (\underline{E_2E_3})'(\underline{E_2E_3}) = 16$. So $g_{15,23}$ is not 0 due to the confounding of $\underline{E_1E_5}$ with $\underline{E_2E_3}$. However, for this Box-Behnken design using LS72 design, all mixed quadratic coefficients $\beta_{ii'}$, $i, i' = 1,2, \dots, 9$, $i < i'$, are estimable since G is of full rank, i.e. 36.

3.3. Resolution V or Higher

Using fractional factorials of resolution V or higher leads to the same form of $X'X$ as for the full factorial, except that 2^k is replaced by 2^{k-l} ,i.e.,

$$X'X = \begin{bmatrix} n & \underline{0}' & r2^{k-l}\underline{1}' & \underline{0}' \\ \underline{0} & r2^{k-l}I & 0 & 0 \\ r2^{k-l}\underline{1} & 0 & 2^{k-l}(\underline{NN}') & 0 \\ \underline{0} & 0 & 0 & G \end{bmatrix} \tag{3.3}$$

where G is a diagonal matrix with elements being $\lambda_\gamma 2^{k-l}$ if treatments i and i' are γ -th associates ($1 \leq \gamma \leq m$). It is noted that the off-diagonal elements of G are 0 since we use fractional factorials of resolution V, which implies that for off-diagonal elements of G a two-factor interaction $\underline{F}_w\underline{F}_{w'}$ are not confounded with other two-factor interactions $\underline{F}_{w''}\underline{F}_{w'''}$, i.e. (7) $(F_w \circ F_{w'})'(\underline{F}_{w''} \circ \underline{F}_{w'''}) = 0$ of Property 1 in Section 2.5 holds (see (j) X'_3X_3 in Section 2.5). Thus, the estimates of all parameters have the same properties as for the full factorial. But just as the full factorial, the resolution V design leads to a large number of treatment combinations for even moderate values of k, and hence to large n.

3.4. Conclusion

We have seen in this chapter that using fractional factorials instead of full factorials has the following consequences concerning estimability and properties of estimators for the parameters in model (2.3):

(i) For resolution III fractions $\hat{\underline{\beta}}_1$ and $\hat{\underline{\beta}}_3$ are no longer uncorrelated;

(ii) for resolution III and IV fractions the estimators for the elements in $\underline{\beta}_3$ are no longer always uncorrelated;

(iii) for some Box-Behnken designs using resolution IV fractions, not all elements of $\underline{\beta}_3$ are estimable;

(iv) fractions of resolution V or higher lead to designs with the same properties as discussed in Chapter 2.

Chapter 4. Trend-free Box-Behnken designs

In this chapter, we are concerned with Box-Behnken designs in which treatments are applied to experimental units (plots) sequentially in time or space and in which there may exist a linear trend effect. For this situation, the objective is to find appropriate run orders such that the estimates of the parameters in model (2.3) are not affected by such a trend. These designs will be referred to as trend-free Box-Behnken designs.

4.1. Background

First, we consider experimental situations in which a run order is to be conducted over time or space and in which there may be unknown variables influencing the experimental process that are highly correlated with the order in which the observations are obtained. In the experimental designs to be used in some time order sequence, the results obtained may be affected by the particular time order chosen, and we should take this into consideration when the experiment is planned. Time order itself is seldom an important variable, but it frequently serves as a proxy for other important lurking variables such as temperature, humidity, changing operator, materials and so on.

We present a few examples to illustrate this point.

(i) In an experiment to evaluate the accuracy of a facility to calibrate meters for use with sales of cryogenic fluids (liquid nitrogen, liquid oxygen, and so on), the meters at particular point in time represent the experimental units. It is known that the meters, i.e. the experimental units deteriorate over time due to the temperature of the liquid being measured (Joiner and Campbell, 1976).

(ii) if a batch of material is created at the beginning of an experiment and treatments are to be applied to experimental units formed from the material over time, then there could be an unknown effect due to aging of the material which influences the observations obtained (Jacroux, 1990).

It might be suggested that the treatment assignment be made in random order to remove a time effect. But it may be that randomization will lead to a run order that is undesirable. It is sometimes preferable in such situations to use a systematic , rather than a randomized , ordering of the treatments. It is often possible to find an ordering which will allow estimation of treatment effects independently of any polynomial time trends or spatial trends that might be present in the experiment. Such an ordering of the treatments is known as a trend-free design.

Experimental designs to be used in the presence of trends to avoid the complication of analysis of covariance and to increase design efficiencies have been developed.

Cox (1951, 1952) initiated the study of trend-free and nearly trend-free designs for the efficient estimation of treatment effects in the presence of a smooth polynomial trend. He considered the assignment of treatments to plots ordered in space or time without blocking and with a trend extending over the entire sequence of plots. Box (1952) and Box and Hay (1953) in similar experimental sequences investigated choices of levels of quantitative factors. Hill (1960) combined the designs of Cox and Box to form new designs to study the effects of both qualitative and quantitative facors in the presence of trends. Daniel and Wilcoxon (1966) and Daniel (1976) provided methods of sequencing the assignments of fractional treatments combinations to experimental units to achieve better estimates in the presence of a trend in time. Bradley and Yeh (1980) introduced trend-free block designs to eliminate a time effect for block designs in the presence of common polynomial trends over plots within blocks. Cheng and Jacroux (1988) gave some methods for complete and fractional factorial designs in which the estimates of main effects and two-factor interactions are othogonal to some polynomial trends. Lin and Dean (1991) gave some general results on the existence of trend-free and partially trend free designs for both varietal and factorial experiments, and investigated trend-free properties of cyclic and generalized cyclic designs.

4.2. Trend-free block designs

We review the trend-free block (TFB) designs introduced by Bradley and Yeh (1980) to remove a time effect for block designs since Box-Behnken designs are constructed by combining incomplete block designs with 2^k factorial designs. These designs can completely eliminate the effects of defined components of a common trend over plots within blocks. We use TF_pCB for a complete block design free of a common trend of degree p within blocks, and TF_pBIB and TF_pPBIB for similar balanced and partially balanced incomplete block designs. The usual additive model for a block design with polynomial trend is written in terms of plot position t and block designation j as

$$y_{jt} = \mu + \sum_{i=1}^{v} \delta_{jt}^{i} \tau_i + \beta_j + \sum_{a=1}^{p} \theta_a \phi_a(t) + \varepsilon_{jt} \tag{4.1}$$

$j = 1, \ldots, b,\ \ t = 1, \ldots, k$, where y_{jt} is the observation on plot t of block j; μ, τ_i, β_j are respectively the usual mean, treatment, and block parameters; $\sum_{a=1}^{p} \theta_a \phi_a(t)$ is the trend effect on plot t, with θ_a being the regression coefficient of the orthogonal polynomial $\phi_a(t)$ of degree a; the designation of the treatment applied to plot (j, t) is effected through indicator variables, $\delta_{jt}^{i} = 1$ or 0 as treatment i is or is not applied on plot (j, t), $i = 1, \ldots, v$. The model (4.1) in matrix notation is

$$Y = X_{\mu}\mu + X_{\tau}\tau + X_{\beta}\beta + X_{\theta}\theta + \varepsilon \tag{4.2}$$

where Y is a $bk \times 1$ observation vector, $\tau' = (\tau_1, \ldots, \tau_v)$, $\beta' = (\beta_1, \ldots, \beta_b)$, $\theta' = (\theta_1, \ldots, \theta_p)$. Bradley and Yeh (1980) defined trend-free block designs such that a block design modelled by (4.2) is trend-free if

$$R(\tau|\mu, \beta, \theta) = R(\tau|\mu, \beta)$$

where $R(\tau|\mu, \beta, \theta)$ represents the treatment sum of squares adjusted for block effects and trend effects and $R(\tau|\mu, \beta)$ represents the corresponding sum of squares with the trend effect deleted (i.e. ignored). And they showed that a necessary and sufficient condition for a block design to be trend-free is that each trend component is orthogonal to the treatment allocations throughout the experiment; that is,

$$\sum_{j=1}^{b} \sum_{t=1}^{k} \delta_{jt}^{i} \phi_a(t) = 0, \quad a = 1, \ldots, p, \quad i = 1, \ldots, v$$

or, equivalently,

$$X_\tau{}' X_\theta = 0$$

For example, we consider the balanced incomplete block design (BIBD) characterized by the parameters $v = 5, b = 10, k = 3, r = 6, \lambda = 3$ with the given incidence matrix

$$\underline{N} = \begin{array}{c} A \\ B \\ C \\ D \\ E \end{array} \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 & 1 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 & 1 & 0 & 1 & 1 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 & 1 & 1 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 & 1 & 1 & 0 & 1 & 1 & 1 \end{bmatrix}$$

And we assume that a linear trend (i.e. p= 1) exists over experimental units within the blocks, taking values $\phi_1(t) = -1, 0, 1$. Now we assign treatments to plots within blocks not at random (as is usually done) but in the following manner (where -1, 0, 1 refer to positions 1, 2, 3, respectively, in a block):

block	-1	0	1
*block*1	*A*	*B*	*C*
*block*2	*A*	*B*	*D*
*block*3	*A*	*B*	*E*
*block*4	*C*	*D*	*A*
*block*5	*C*	*E*	*A*
*block*6	*D*	*E*	*A*
*block*7	*D*	*B*	*C*
*block*8	*E*	*B*	*C*
*block*9	*E*	*B*	*D*
*block*10	*C*	*D*	*E*

This design satisfies the condition $\sum_{j=1}^{10}\sum_{t=1}^{3}\delta_{jt}^{i}\phi_1(t)=0$, for all treatments since

$\sum_{j=1}^{10}\sum_{t=1}^{3}\delta_{jt}^{A}\phi_1(t)=-1-1-1+1+1+1=0$, $\sum_{j=1}^{10}\sum_{t=1}^{3}\delta_{jt}^{B}\phi_1(t)=0+0+0+0+0+0=0$,
$\sum_{j=1}^{10}\sum_{t=1}^{3}\delta_{jt}^{C}\phi_1(t)=1-1-1+1+1-1=0$, $\sum_{j=1}^{10}\sum_{t=1}^{3}\delta_{jt}^{D}\phi_1(t)=1+0-1-1+1+0=0$,
$\sum_{j=1}^{10}\sum_{t=1}^{3}\delta_{jt}^{E}\phi_1(t)=1+0+0-1-1+1=0$,

or equivalently satisfies the condition $X_\tau{}'X_\theta=\underline{0}=(0,0,0,0,0)'$ since

$$X_\tau = \begin{array}{c} \begin{array}{ccccc} A & B & C & D & E \end{array} \\ \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \end{array} \qquad X_\theta = \begin{array}{c} \theta_1 \\ \begin{bmatrix} -1 \\ 0 \\ 1 \\ -1 \\ 0 \\ 1 \\ -1 \\ 0 \\ 1 \\ -1 \\ 0 \\ 1 \\ -1 \\ 0 \\ 1 \\ -1 \\ 0 \\ 1 \\ -1 \\ 0 \\ 1 \\ -1 \\ 0 \\ 1 \\ -1 \\ 0 \\ 1 \\ -1 \\ 0 \\ 1 \end{bmatrix} \end{array}$$

Thus, we obtain a balanced incomplete block design free of a common trend of degree 1 within blocks (TF_1BIB). That is, each treatment is orthogonal to a linear trend (for more examples see Bradley and Yeh, 1980).

The selection of X_τ may be viewed as a two stage process. The first stage is the determination of a way of blocking specified by the incidence matrix $\underline{N} = X'_\tau X_\beta$, and the second stage is the allocation of treatments to plots within blocks. Then we have the following properties of trend-free block designs:

(i) Let $a'\tau$ be any estimable function of treatment effects for the block design. Then $a'\tau$ is also estimable for the TFB design.

(ii) Let $\hat{\tau}_o$ and $\hat{\tau}$ be the least squares estimators of τ under model (4.2) for the TFB design, and the corresponding block design with within-block treatment randomization respectively. Then $var(a'\hat{\tau}_o) \leq var(a'\hat{\tau})$

(iii) The ordinary analysis of variance sums of squares for treatments and blocks are preserved and variation due to the trend may be removed from the error sum of squares. These properties assures us that TFB designs will be optimal in comparison with the analysis of covariance for the corresponding block design with treatments randomized over plots within blocks.

Yeh and Bradley (1983) also have discussed the existence and construction of TFB designs. Sometimes a TFB design does not exist, and this provides the motivation for considering a nearly trend-free block (NTFB) design. For given design parameters, $v, b, k, r_1, \ldots, r_v$, r_i being the number of replications of treatment i, a block design under model (4.1) is said to be a NTFB design of type A if

$$\sum_{a=1}^{p} \sum_{i=1}^{v} \left[\sum_{j=1}^{b} \sum_{t=1}^{k} \delta_{jt}^{i} \phi_a(t) \right]^2$$

is minimum among the class of connected designs with the same incidence matrix.

Under model (4.1), the information matrix for a design is

$$C = R - (1/k)\underline{N}\underline{N}' - (1/b)X_\tau' X_\theta X_\theta' X_\tau \tag{4.3}$$

where R = diag $(r_1, \dots, r_v)$, X_τ is the $bk \times v$ matrix with $\sum_{j=1}^{b} \delta_{jt}^{i}$ (the number of times that treatment i appears on plot t, $i = 1, 2, \dots, v$, $t = 1, 2, \dots, k$) in row t and column i, and X_θ is the $bk \times p$ matrix with $\phi_a(t)$ in row t and column a.

The matrix C in (4.3), obtained from the reduced normal equations for estimating the treatment parameters in model (4.1), is central to the analysis and the efficiency of a design. When the design is trend-free, $C = R - (1/k)\underline{N}\underline{N}'$ depends only on the incidence matrix $\underline{N}$ and the analysis is simple. When the design is not trend-free, the usual analysis of covariance using trend terms as covariates must be employed to remove the confounding between treatments and trend terms. It is shown that NTFB designs for first- and second-order trends can be constructed with good efficiency properties (Yeh, Bradley, and Notz, 1985). NTFB designs do have the disadvantages of requiring somewhat more complicated covariance analysis computations.

4.3. Property of the factorial design

The properties of 2^k factorial designs are useful to find a LTF Box-Behnken design. We define symmetric and anti-symmetric properties of a vector before we discuss the property of the 2^k factorial design.

<u>Definition 4.1.</u> The vector $(a_1, a_2, \dots, a_s, a_{s+1}, a_{s+2}, \dots, a_{2s})$ or $(a_1, a_2, \dots, a_s, 0, a_{s+1}, a_{s+2}, \dots, a_{2s})$ is said to be symmetric if $a_j = a_{2s-j+1}$, $j = 1,2, \dots, s$

Definition 4.2. The vector $(a_1, a_2, \dots, a_s, a_{s+1}, a_{s+2}, \dots, a_{2s})$ or $(a_1, a_2, \dots, a_s, 0, a_{s+1}, a_{s+2}, \dots, a_{2s})$ is said to be anti-symmetric if $a_j = -a_{2s-j+1}$, $j = 1,2, \dots, s$

We apply the notions of symmetric and anti-symmetric vectors now to the contrast vectors of main effects and two-factor interactions for the 2^k factorial. In what follows we always assume that the 2^k treatment combinations are assigned in standard order (see Section 2.1). It is then easy to write down the contrast vectors for the main effects $A_1, A_2, \dots, A_k$. The contrast vectors for the two-factor interactions A_{ij}, i.e. the interaction between the i-th and j-th factor, is then given by $A_{ij} = A_i \circ A_j$. This is illustrated for $k = 3$ in Table 4.1. Even though it has no meaning in the context of the 2^k factorial itself but only in the context of the Box-Behnken design, we also define pure quadratic effects for the i-th factors by $A_i^2 = A_i \circ A_i$.

Table 4.1. STANDARD ORDERING OF THE 2^3 FACTORIAL

.	A_1	A_2	A_3	A_1^2	A_2^2	A_3^2	A_{12}	A_{13}	A_{23}
1	−1	−1	−1	1	1	1	1	1	1
a_1	1	−1	−1	1	1	1	−1	−1	1
a_2	−1	1	−1	1	1	1	−1	1	−1
a_1a_2	1	1	−1	1	1	1	1	−1	−1
a_3	−1	−1	1	1	1	1	1	−1	−1
a_1a_3	1	−1	1	1	1	1	−1	1	−1
a_2a_3	−1	1	1	1	1	1	−1	−1	1
$a_1a_2a_3$	1	1	1	1	1	1	1	1	1

From the Table 4.1, we observe that the main effect contrasts are anti-symmetric. However, the pure quadratic terms and two-factor interactions are symmetric. The anti-symmetric property for the main effect contrasts A_i, $i = 1,2, \dots, k$, and the symmetric property for the pure quadratic terms A_i^2, $i = 1,2, \dots, k$, and two-factor interactions A_{ij}, $i,j = 1,2, \dots k$, $i < j$, holds for all 2^k factorials.

Next, we consider the case where one center point is inserted into the middle of the 2^k treatment combinations in standard order. For example, when k = 3, the 2^3 treatment combinations can be written as $(1, a_1, a_2, a_1a_2, 0, a_3, a_1a_3, a_2a_3, a_1a_2a_3)$ where 0 is an inserted center point. Then, the main effect contrasts A_1, A_2, A_3 are written as $A_1 = (-1, 1, -1, 1, 0, -1, 1, -1, 1)'$, $A_2 = (-1, -1, 1, 1, 0, -1, -1, 1, 1)'$, $A_3 = (-1, -1, -1, -1, 0, 1, 1, 1, 1)'$. The pure quadratic terms A_1^2, A_2^2, A_3^2 and the two-factor interactions A_{12}, A_{13}, A_{12} are shown in Table 4.2.

Table 4.2. STANDARD ORDERING OF THE 2^3 FACTORIAL with a center point

.	A_1	A_2	A_3	A_1^2	A_2^2	A_3^2	A_{12}	A_{13}	A_{23}
1	−1	−1	−1	1	1	1	1	1	1
a_1	1	−1	−1	1	1	1	−1	−1	1
a_2	−1	1	−1	1	1	1	−1	1	−1
a_1a_2	1	1	−1	1	1	1	1	−1	−1
0	0	0	0	0	0	0	0	0	0
a_3	−1	−1	1	1	1	1	1	−1	−1
a_1a_3	1	−1	1	1	1	1	−1	1	−1
a_2a_3	−1	1	1	1	1	1	−1	−1	1
$a_1a_2a_3$	1	1	1	1	1	1	1	1	1

From Table 4.2, we see, of course, that just as in Table 4.1 the main effect contrasts under standard ordering are anti-symmetric with respect to 0, and the pure quadratic terms and the two-factor interactions are also symmetric with respect 0. We consider now the coefficients for a linear trend, $\phi_1(t) \equiv T$ say, they are given by the coefficients of the orthogonal polynomial of degree 1 and order s equal to number of experimental runs. Specifically, if s = 2q, then

$$T' = (- (s-1), - (s-3), \dots , -3, -1, 1, 3, \dots , s-3, s-1)$$

and if s = 2q + 1, then

$$T' = (-q, - (q-1), \dots , -1, 0, 1, \dots , q-1, q)$$

In both cases, T is anti-symmetric. As a consequence, we see, for example, that for $s = 2^3$ as in Table 4.1 and for $s = 2^3 + 1$ as in Table 4.2 the pure quadratic terms and the two-factor interactions are orthogonal to the linear trend, i.e. $(A_1^2)'\underline{T} = 0$, $(A_2^2)'\underline{T} = 0$, $(A_2^3)'\underline{T} = 0$ and $(A_{12})'\underline{T} = 0$, $(A_{13})'\underline{T} = 0$, $(A_{23})'\underline{T} = 0$. These properties can obviously be generalized for all 2^k factorial designs without or with a center point inserted in the middle of the treatment combinations of the standard order. We take advantage of these properties in Section 4.4 to construct a LTF Box-Behnken designs when there exists a linear trend over experimental plots. At this point we introduce some further notation which will simplify the description of LTF Box-Behnken designs. For any of the coefficient vectors A for a 2^k factorial, similar to those given in Table 4.1, define

$$A = \begin{bmatrix} A^U \\ A^L \end{bmatrix} \tag{4.4}$$

where A^U is called the upper half and A^L is called the lower half of the vector A. A^U and A^L are of course $2^{k-1} \times 1$ vectors.

When there exists a polynomial trend in a complete 2^k factorial design, Cheng and Jacroux (1988) showed that for the standard order of a complete 2^k design, any h-factor interaction is orthogonal to a (h-1)-degree polynomial trend. Consequently, in the standard order of a complete 2^k design, two or more factor interactions are orthogonal to a linear trend t taking values $1+a, 2+a, \dots, 2^k+a$, where a is an arbitrary integer. i.e. , $(A_{12})'\underline{T}=0$, $(A_{13})'\underline{T}=0, \dots,$ $(A_{k-1,k})'\underline{T}=0$, $(A_{123})'\underline{T}=0, \dots,$ $(A_{12\dots k})'\underline{T}=0$. For example, when $k=3$, $a=-17$, we have $(A_{12})'\underline{T}=0$, since $A_{12}=(1,-1,-1,1,1,-1,-1,1)'$ and $\underline{T}=(-16,-15,-14,-13,-12,-11,-10,-9)'$. The main effect contrasts $A_1, A_2, \dots, A_k$, however, are not orthogonal because $A_1'\underline{T}=2^k/2$, $A_2'\underline{T}=2^k$, $A_3'\underline{T}=2 \bullet 2^k, \dots$, and so on where $\underline{T}=(1,2,\dots,2^k)'$ for $a=0$.

The same property holds for the upper half or the lower half of the h-factor interactions $(h \geq 3)$:

Property 4.1. For the standard ordering of a complete 2^k designs, any half of an h-factor interaction contrast vector $(h \geq 3)$ is orthogonal to a linear trend t taking values $1+a, 2+a, \dots, 2^{k-1}+a$ where a is an arbitrary integer, i.e. $(A_{123}{}^U)'\underline{T}=0$, $(A_{123}{}^L)'\underline{T}=0, \dots,$ $(A_{k-2,k-1,k}{}^U)'\underline{T}=0$, $(A_{k-2,k-1,k}{}^L)'\underline{T}=0, \dots,$ $(A_{123\dots k}{}^U)'\underline{T}=0$, $(A_{123\dots k}{}^L)'\underline{T}=0$.

For example, when $k=4$, the various A^U and A^L vectors are given in Table 4.3. Choosing, for example, $a=-9$, the corresponding linear trend t takes the values

$\underline{T} = (-8, -7, -6, -5, -4, -3, -2, -1)'$. We then obtain $(A_{123}{}^{U})'\underline{T} = 0$, $(A_{123}{}^{L})'\underline{T} = 0, \ldots,$ $(A_{234}{}^{U})'\underline{T} = 0$, $(A_{234}{}^{L})'\underline{T} = 0$, $(A_{1234}{}^{U})'\underline{T} = 0$, $(A_{1234}{}^{L})'\underline{T} = 0$.

Property 4.1 is used in Section 4.5.2 to construct linear trend free Box-Behnken designs for $k \geq 4$.

Table 4.3. STANDARD ORDERING OF THE 2^4 FACTORIAL

.	A_1	A_2	A_3	A_4	A_{123}	A_{124}	A_{134}	A_{234}	A_{1234}
1	−1	−1	−1	−1	−1	−1	−1	−1	1
a_1	1	−1	−1	−1	1	1	1	−1	−1
a_2	−1	1	−1	−1	1	1	−1	1	−1
a_1a_2	1	1	−1	−1	−1	−1	1	1	1
a_3	−1	−1	1	−1	1	−1	1	1	−1
a_1a_3	1	−1	1	−1	−1	1	−1	1	1
a_2a_3	−1	1	1	−1	−1	1	1	−1	1
$a_1a_2a_3$	1	1	1	−1	1	−1	−1	−1	−1
a_4	−1	−1	−1	1	−1	1	1	1	−1
a_1a_4	1	−1	−1	1	1	−1	−1	1	1
a_2a_4	−1	1	−1	1	1	−1	1	−1	1
$a_1a_2a_4$	1	1	−1	1	−1	1	−1	−1	−1
a_3a_4	−1	−1	1	1	1	1	−1	−1	1
$a_1a_3a_4$	1	−1	1	1	−1	−1	1	−1	−1
$a_2a_3a_4$	−1	1	1	1	−1	−1	−1	1	−1
$a_1a_2a_3a_4$	1	1	1	1	1	1	1	1	1

4.4. Linear trend-free Box-Behnken designs

We now consider Box-Behnken designs in which a linear trend is assumed over experimental units, and each observation is designated to one experimental unit sequentially. We write the model as follows:

$$y_u = \beta_0 + \sum_{i=1}^{v} \beta_i x_{iu} + \sum_{i=1}^{v} \beta_{ii} x_{iu}^2 + \sum_{\substack{i,i'=1 \\ i<i'}}^{v} \beta_{ii'} x_{iu} x_{i'u} + \theta t_u + \varepsilon_u \tag{4.5}$$

$u = 1,2, \dots, n$, where y_u is a response variable, β_0, β_i, β_{ii} and $\beta_{ii'}$ are unknown parameters with $i, i' = 1,2, \dots, v$ $i < i'$, θ is the regression coefficient of the linear trend t over experimental units, i.e. , a polynomial trend of degree 1, and ε_u is a random error with mean 0 and variance σ^2 . It is noted that a linear trend t takes values $-\frac{n-1}{2}, -\frac{n-1}{2}+1, \dots, -1,0,1, \dots, \frac{n-1}{2}-1, \frac{n-1}{2}$ if t (or n) is odd, and $-n+1, -n+3, \dots, -1,1, \dots, n-3, n-1$ if t (or n) is even.

In matrix notation, we can write

$$\underline{Y} = \underline{1}\beta_0 + X_1\underline{\beta}_1 + X_2\underline{\beta}_2 + X_3\underline{\beta}_3 + \underline{T}\theta + \underline{\varepsilon} \tag{4.6}$$

where $\underline{T} = (t_1, t_2, \dots, t_n)'$ is a $n \times 1$ linear trend vector.

Now, we define a linear trend-free Box-Behnken design as follows:

Definition 4.1. A Box-Behnken design under model (4.5) is said to be linear trend-free (LTF) if

$$\sum_{u=1}^{n} x_{iu} t_u = 0, \quad \sum_{u=1}^{n} x_{iu}^2 t_u = 0, \quad \sum_{u=1}^{n} x_{iu} x_{i'u} t_u = 0, \quad i, i' = 1, \dots, v \tag{4.7}$$

or, equivalently

$$X_1'\underline{T}=\underline{0},\quad X_2'\underline{T}=\underline{0},\quad X_3'\underline{T}=\underline{0}.$$

The main objective then is to obtain a run order such that the design is a linear trend-free Box-Behnken design. Such a method will be described in Section 4.5.

For LTF Box-Behnken designs using the model

$$\underline{Y}=\underline{1}\beta_0+X_1\underline{\beta}_1+X_2\underline{\beta}_2+X_3\underline{\beta}_3+\underline{T}\theta+\underline{\varepsilon}$$

and using a full 2^k factorial we have, according to Definition 4.1, the following $X'X$ matrix:

$$X'X=\begin{bmatrix} n & \underline{1}'X_1 & \underline{1}'X_2 & \underline{1}'X_3 & \underline{1}'\underline{T} \\ X_1'\underline{1} & X_1'X_1 & X_1'X_2 & X_1'X_3 & X_1'\underline{T} \\ X_2'\underline{1} & X_2'X_1 & X_2'X_2 & X_2'X_3 & X_2'\underline{T} \\ X_3'\underline{1} & X_3'X_1 & X_3'X_2 & X_3'X_3 & X_3'\underline{T} \\ \underline{T}\underline{1} & \underline{T}X_1 & \underline{T}X_2 & \underline{T}X_3 & \underline{T}\underline{T} \end{bmatrix}=\begin{bmatrix} n & \underline{0}' & r2^k\underline{1}' & \underline{0}' & 0 \\ \underline{0} & r2^kI & 0 & 0 & \underline{0} \\ r2^k\underline{1} & 0 & 2^k(\underline{N}\underline{N}') & 0 & \underline{0} \\ \underline{0} & 0 & 0 & G & \underline{0} \\ 0 & \underline{0}' & \underline{0}' & \underline{0}' & \underline{T}\underline{T} \end{bmatrix} \quad (4.8)$$

We can see from the $X'X$ matrix that the estimates of the first-order coefficients $\underline{\beta}_1$, and the second-order coefficients $\underline{\beta}_2$, $\underline{\beta}_3$ are orthogonal to the estimates of the estimate of the linear trend coefficient θ. Concerning the estimators of these parameters we can state the following properties:

(i) The estimates of the first-order coefficients β_i, $i=1,2,\ldots,v$, the pure quadratic coefficients β_{ii}, $i=1,2,\ldots,v$, and the mixed quadratic coefficients $\beta_{ii'}$, $i,i'=1,2,\ldots,v$, $i<i'$ are not affected by a linear trend. The properties of these estimators are same as those discussed in Section 2.5.

(ii) We obtain the UMVUE of the linear trend coefficient θ as $\hat{\theta}=(\underline{T}\underline{T})^{-1}\underline{T}\underline{Y}$.

4.5. Construction of LTF Box-Behnken Designs

We now consider Box-Behnken designs when there exists a linear trend over experimental plots. We consider first a design with one center point, which implies that we have an odd number of design points (observations), i.e. $n = b2^k + 1$. Thus, we use a linear trend t taking values $-\frac{n-1}{2}, -\frac{n-1}{2}+1, \ldots, -1, 0, 1, \ldots, \frac{n-1}{2}-1, \frac{n-1}{2}$ over n experimental units. We first modify the Box-Behnken design matrix D^* , given by (2.1) and (2.2). Without loss of generality, we replace the F_w by main effect contrasts under standard ordering A_w , for the factorial part of Box-Behnken design matrix D^* in (2.2). Then we rewrite D^* as

$$D^* = \begin{bmatrix} B_1 \\ B_2 \\ \cdot \\ \cdot \\ \cdot \\ B_b \end{bmatrix} = \begin{bmatrix} n_{11}A_{w(1,1)} & n_{12}A_{w(1,2)} & \cdots & n_{1v}A_{w(1,v)} \\ n_{21}A_{w(2,1)} & n_{22}A_{w(2,2)} & \cdots & n_{2v}A_{w(2,v)} \\ \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdots & \cdot \\ n_{b1}A_{w(b,1)} & n_{b2}A_{w(b,2)} & \cdots & n_{bv}A_{w(b,v)} \end{bmatrix} \tag{4.9}$$

where B_i is a $2^k \times v$ matrix, w(j,i) $= n_{j1} + n_{j2} + \cdots + n_{ji}$, with w taking values $0, 1, \ldots, k$, and $A_{w(j,i)}$ is a 2^k main effect contrast of the standard ordering (i.e. $2^k \times 1$ vector), and $A_0' = (1, 1, \ldots, 1)$. We divide the B_i, $i = 1, 2, \ldots, b$, into two parts, the upper half of B_i, and the lower half of B_i, denoted by B_i^U and B_i^L, respectively, so that

$$B_i = \begin{bmatrix} B_i^U \\ B_i^L \end{bmatrix} = \begin{bmatrix} n_{i1}A_{w(i,1)}^U & n_{i2}A_{w(i,2)}^U & \cdots & n_{iv}A_{w(i,v)}^U \\ n_{i1}A_{w(i,1)}^L & n_{i2}A_{w(i,2)}^L & \cdots & n_{iv}A_{w(i,v)}^L \end{bmatrix} \tag{4.10}$$

where B_i^U, B_i^L are $2^{k-1} \times v$ matrices.

We then write the Box-Behnken design matrix D augmented with linear trend $\underline{T}$,say S, as

$$S \equiv (D, T) = \begin{bmatrix} B_1^{\ U} & \\ B_1^{\ L} & \\ B_2^{\ U} & \\ B_2^{\ L} & \\ . & \\ . & \underline{T} \\ . & \\ B_b^{\ U} & \\ B_b^{\ L} & \\ \underline{0} & \end{bmatrix} = \begin{bmatrix} n_{11}A_{w(1,1)}^{\ \ U} & n_{12}A_{w(1,2)}^{\ \ U} & . \ . \ . & n_{1v}A_{w(1,v)}^{\ \ U} & \\ n_{11}A_{w(1,1)}^{\ \ L} & n_{12}A_{w(1,2)}^{\ \ L} & . \ . \ . & n_{1v}A_{w(1,v)}^{\ \ L} & \\ n_{21}A_{w(2,1)}^{\ \ U} & n_{22}A_{w(2,2)}^{\ \ U} & . \ . \ . & n_{2v}A_{w(2,v)}^{\ \ U} & \\ n_{21}A_{w(2,1)}^{\ \ L} & n_{22}A_{w(2,2)}^{\ \ L} & . \ . \ . & n_{2v}A_{w(2,v)}^{\ \ L} & \\ . & . & . \ . \ . & . & \\ . & . & . \ . \ . & . & \underline{T} \\ . & . & . \ . \ . & . & \\ n_{b1}A_{w(b,1)}^{\ \ U} & n_{b2}A_{w(b,2)}^{\ \ U} & . \ . \ . & n_{bv}A_{w(b,v)}^{\ \ U} & \\ n_{b1}A_{w(b,1)}^{\ \ L} & n_{b2}A_{w(b,2)}^{\ \ L} & . \ . \ . & n_{bv}A_{w(b,v)}^{\ \ L} & \\ 0 & 0 & . \ . \ . & 0 & \end{bmatrix} \quad (4.11)$$

and $\underline{T} = (-\frac{n-1}{2}, -\frac{n-1}{2}+1, \dots, -1, 0, 1, \dots, \frac{n-1}{2}-1, \frac{n-1}{2})'$.

For example, for the Box-Behnken design (No.1 in Box and Behnken, 1960) with the BIBD with the parameters $v = 3, r = 2, b = 3, k = 2, \lambda = 1$, and the transpose of the incidence matrix given by

$$\underline{N} = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{bmatrix}, \qquad \underline{N}' = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{bmatrix},$$

we obtain Box-Behnken design matrix D with one center point as

$$D = \begin{bmatrix} B_1 \\ B_2 \\ B_3 \\ \underline{0} \end{bmatrix} = \begin{bmatrix} A_1 & A_2 & \underline{0}_4 \\ A_1 & \underline{0}_4 & A_2 \\ \underline{0}_4 & A_1 & A_2 \\ 0 & 0 & 0 \end{bmatrix} = \begin{bmatrix} -1 & -1 & 0 \\ 1 & -1 & 0 \\ -1 & 1 & 0 \\ 1 & 1 & 0 \\ -1 & 0 & -1 \\ 1 & 0 & -1 \\ -1 & 0 & 1 \\ 1 & 0 & 1 \\ 0 & -1 & -1 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \end{bmatrix}$$

where

$$B_1 = \begin{bmatrix} -1 & -1 & 0 \\ 1 & -1 & 0 \\ -1 & 1 & 0 \\ 1 & 1 & 0 \end{bmatrix}, \quad B_2 = \begin{bmatrix} -1 & 0 & -1 \\ 1 & 0 & -1 \\ -1 & 0 & 1 \\ 1 & 0 & 1 \end{bmatrix}, \quad B_3 = \begin{bmatrix} 0 & -1 & -1 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \\ 0 & 1 & 1 \end{bmatrix}$$

are $2^2 \times 3$ matrices, the 2^2 main effect contrasts of the standard ordering A_1, A_2 are defined as $A_1 = (-1, 1, -1, 1)'$, $A_2 = (-1, -1, 1, 1)'$, and $\underline{0}_4$ is a 4×1 zero vector.

Thus, we can express the upper half of B_i, and the lower half of B_i, $i = 1,2,3$ as

$$B_1^U = \begin{bmatrix} -1 & -1 & 0 \\ 1 & -1 & 0 \end{bmatrix} \quad B_2^U = \begin{bmatrix} -1 & 0 & -1 \\ 1 & 0 & -1 \end{bmatrix} \quad B_3^U = \begin{bmatrix} 0 & -1 & -1 \\ 0 & 1 & -1 \end{bmatrix}$$

$$B_1^L = \begin{bmatrix} -1 & 1 & 0 \\ 1 & 1 & 0 \end{bmatrix} \quad B_2^L = \begin{bmatrix} -1 & 0 & 1 \\ 1 & 0 & 1 \end{bmatrix} \quad B_3^L = \begin{bmatrix} 0 & -1 & 1 \\ 0 & 1 & 1 \end{bmatrix}$$

Consequently, $A_i, i = 1,2$ are divided into A_i^U, A_i^L with $A_1^U = (-1, 1)'$, $A_1^L = (-1, 1)'$, $A_2^U = (-1, -1)'$, $A_2^L = (1, 1)'$.

Hence, we can write the Box-Behnken design matrix with a center point as follows:

$$D = \begin{bmatrix} B_1^U \\ B_1^L \\ B_2^U \\ B_2^L \\ B_3^U \\ B_3^L \\ \underline{0} \end{bmatrix} = \begin{bmatrix} A_1^U & A_2^U & \underline{0}_2 \\ A_1^L & A_2^L & \underline{0}_2 \\ A_1^U & \underline{0}_2 & A_2^U \\ A_1^L & \underline{0}_2 & A_2^L \\ \underline{0}_2 & A_1^U & A_2^U \\ \underline{0}_2 & A_1^L & A_2^L \\ 0 & 0 & 0 \end{bmatrix} = \begin{bmatrix} -1 & -1 & 0 \\ 1 & -1 & 0 \\ -1 & 1 & 0 \\ 1 & 1 & 0 \\ -1 & 0 & -1 \\ 1 & 0 & -1 \\ -1 & 0 & 1 \\ 1 & 0 & 1 \\ 0 & -1 & -1 \\ 0 & 1 & -1 \\ 0 & -1 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \end{bmatrix}$$

where $\underline{0}_2$ is a 2×1 zero vector.

Now, we consider the situation of Box-Behnken experimental design in which a run order is to be conducted in time order sequence over the experimental plots, assuming that there exists a linear trend t taking values $-6, -5, \dots, -1, 0, 1, \dots, 5, 6$ over the 13 experimental units. Writing the Box-Behnken design in the usual way we have

$$
S \equiv (D, T) = \begin{bmatrix} A_1^{\,U} & A_2^{\,U} & \underset{\sim}{0}_2 & \\ A_1^{\,L} & A_2^{\,L} & \underset{\sim}{0}_2 & \\ A_1^{\,U} & \underset{\sim}{0}_2 & A_2^{\,U} & \\ A_1^{\,L} & \underset{\sim}{0}_2 & A_2^{\,L} & \underset{\sim}{T} \\ \underset{\sim}{0}_2 & A_1^{\,U} & A_2^{\,U} & \\ \underset{\sim}{0}_2 & A_1^{\,L} & A_2^{\,L} & \\ 0 & 0 & 0 & \end{bmatrix} = \begin{bmatrix} -1 & -1 & 0 & -6 \\ 1 & -1 & 0 & -5 \\ -1 & 1 & 0 & -4 \\ 1 & 1 & 0 & -3 \\ -1 & 0 & -1 & -2 \\ 1 & 0 & -1 & -1 \\ -1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 1 \\ 0 & -1 & -1 & 2 \\ 0 & 1 & -1 & 3 \\ 0 & -1 & 1 & 4 \\ 0 & 1 & 1 & 5 \\ 0 & 0 & 0 & 6 \end{bmatrix}
$$

The problem then is how to arrange treatment combinations so that the resulting design is a LTF Box-Behnken design. We shall take advantage of the symmetric property of the second order terms (pure quadratic terms and the two-factor interactions) and anti-symmetric property of the main effect contrasts of the 2^k factorials shown in Section 4.3 in order to construct a LTF Box-Behnken designs by putting a center point on the middle of the experimental units associated with the 0-value of the linear trend, and placing the halves of each B_i, $i = 1,2, \ldots , b$ symmetrically with respect to the center point since the structure of the Box-Behnken designs is based on the 2^k factorial designs. We consider two cases (i) for $k=2$ or 3 and (ii) $k \geq 4$ to arrange run orders.

4.5.1. Construction method of LTF Box-Behnken designs for k=2 or 3

For $k=2$ or 3, a LTF Box-Behnken design can be constructed by the following method:

1. In (4.11), we place a center point in the middle of the experimental units associated with 0-value of $\mathcal{T}$.

   For convenience of describing the following method we partition the Box-Behnken design then into three parts: P_1 consists of the first $b2^{k-1}$ runs, P_0 consists of the center point, and P_2 consists of the last $b2^{k-1}$ runs, i.e.

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

   Written in this order P_1 is associated with the negative values of $\mathcal{T}$, P_0 is associated with the 0-value of $\mathcal{T}$, and P_2 is associated with the positive values of $\mathcal{T}$. We partition $\mathcal{T}$ correspondingly into

$$\mathcal{T} = \begin{bmatrix} \mathcal{T}_1 \\ T_0 \\ \mathcal{T}_2 \end{bmatrix}.$$

2. For each B_i, $i = 1,2, \dots, b$, we put B_i^U in P_1 and B_i^L in P_2 symmetrically with respect to the center point (P_0) or vice versa.

   Obviously, there exist 2^b such arrangements. We call them $D_1, D_2, \dots, D_{2^b}$. In all cases, the vectors for the pure quadratic terms $\underline{x}_1^2, \underline{x}_2^2, \dots, \underline{x}_v^2$, and for the mixed quadratic terms $\underline{x}_{12}, \underline{x}_{13}, \dots, \underline{x}_{v-1,v}$ are symmetric. This implies that the pure quadratic terms and mixed quadratic terms are orthogonal to a linear trend $\underline{T}$, i.e. $(\underline{x}_1^2)'\underline{T} = 0$, $(\underline{x}_2^2)'\underline{T} = 0, \dots, (\underline{x}_v^2)'\underline{T} = 0$, and $(\underline{x}_{12})'\underline{T} = 0$, $(\underline{x}_{13})'\underline{T} = 0, \dots, (\underline{x}_{v-1,v})'\underline{T} = 0$. And the vectors for the first-order terms $\underline{x}_1, \underline{x}_2, \dots, \underline{x}_v$ are anti-symmetric. We thus have to consider run orders such that also the vectors for the first-order terms $\underline{x}_1, \underline{x}_2, \dots, \underline{x}_v$ are orthogonal to $\underline{T}$ i.e. $(\underline{x}_1)'\underline{T} = 0, (\underline{x}_2)'\underline{T} = 0, \dots, (\underline{x}_v)'\underline{T} = 0$.

3. We choose any one of the 2^b arrangements $D_1, D_2, \dots, D_{2^b}$.

4. For the given D_i we number the individual design points in P_2 starting from the center point (i.e. P_0) as design point 1, design point 2, ..., design point $b2^{k-1}$ since P_2 contains $b2^{k-1}$ design points. Similarly, we number the individual design points in P_1, starting again from the center point P_0 as design point $\overline{1}$, design point $\overline{2}, \dots$, design point $\overline{b2^{k-1}}$.

   The next problem is to position the individual $b2^{k-1}$ design points associated with P_2 to obtain $(\underline{x}_1^+)'\underline{T}_2 = 0, (\underline{x}_2^+)'\underline{T}_2 = 0, \dots, (\underline{x}_v^+)'\underline{T}_2 = 0$ where $\underline{x}_j^+, j = 1,2, \dots, v$ represents the vector of $\underline{x}_j$ associated with P_2 , and is to position the individual $b2^{k-1}$ design points associated with P_1 to obtain $(\underline{x}_1^-)'\underline{T}_1 = 0, (\underline{x}_2^-)'\underline{T}_1 = 0, \dots, (\underline{x}_v^-)'\underline{T}_1 = 0$ where $\underline{x}_j^-, j = 1,2, \dots, v$ represents the vector of $\underline{x}_j$ associated with P_1 .

5. Let $\{c_i,\ i = 1, 2, \dots, b2^{k-1}\}$ represent a permutation of the integers $1, 2, \dots, b2^{k-1}$. And let $\{ c_i,\ i = 1, 2, \dots, b2^{k-1} \}$ represent the values of the positions of experimental

units in which the corresponding design point i, $i = 1,2 \dots , b2^{k-1}$ in P_2 should be placed to obtain a LTF Box-Behnken design; that is, the design point 1 moves to c_1 position, the design point 2 moves to c_2 position, ... , the design point $b2^{k-1}$ moves to c_{b2^k-1} position of the experimental unit. Similarly, let $\{ -c_i,\ i = 1, 2, \dots , b2^{k-1}\}$ also represent a permutation of the integers $-1, -2, \dots , -b2^{k-1}$. And let $\{ -c_i,\ i = 1, 2, \dots , b2^{k-1}\}$ represent the values of the positions of experimental units in which the corresponding design point $\bar{i}$, $\bar{i} = -1, -2, \dots , -b2^{k-1}$ in P_1 should be placed; that is, the design point $\bar{1}$ moves to $-c_1$ position, the design point $\bar{2}$ moves to $-c_2$ position, ... , the design point $\overline{b2^{k-1}}$ moves to $-c_{b2^k-1}$ position of the experimental unit. We then obtain a LTF Box-Behnken design.

If we define $\underline{C}^+ = (c_1, c_2, \dots , c_{b2^k-1})$ and $\underline{C}^- = (-c_1, -c_2, \dots , -c_{b2^k-1})$ we want to find $\underline{C}^+$ and $\underline{C}^-$ such that

$$\underline{x}_j^{+\prime} \underline{C}^+ = 0, \quad j = 1, 2, \dots , v, \tag{4.12}$$

and

$$\underline{x}_j^{-\prime} \underline{C}^- = 0, \quad j = 1, 2, \dots , v, \tag{4.12a}$$

i.e. find permutations $\{c_i\}$ and $\{ -c_i\}$ such that the v equations above are satisfied. If we find a solution to (4.12) then we also satisfy (4.12a).

6. Suppose we have found $\underline{C}^+$ such that the equations (4.12) are satisfied. Denote the solution by $C_0^+ = \{c_i\}_0$. Then C_0^+ represents the orders of the runs $1, 2, \dots , b2^k$ (numbered in standard order). Let $C_0^+(D_1)$ denote the rearrangement of the runs D_1 according to the permutation C_0^+. Also, let $C_0^- = \{ -c_i\}_0$. Then the LTF Box-Behnken design is given by

$$D = \begin{bmatrix} C_0^-(P_1) \\ P_0 \\ C_0^+(P_2) \end{bmatrix}$$

7. If we cannot find solutions for equation (4.12) we choose another D_j from the remaining arrangements, and repeat the whole procedure.

If we cannot find solutions for equation (4.12) for any of the 2^b arrangements, then there does not exist a run order which yields a LTF Box-Behnken design. On the other hand, if we can find a $\underline{C}^+$ satisfying equation (4.12), then the design constructed by this method is not unique since there may be other solutions.

Example 4.5.1

We refer to the previous example of a Box-Behnken design in this section (Design No.1 in Box and Behnken, 1960). Again we rewrite the design matrix S with $\underline{T}$

$$S = (D, T) = \begin{bmatrix} B_1{}^U & \\ B_1{}^L & \\ B_2{}^U & \\ B_2{}^L & \underline{T} \\ B_3{}^U & \\ B_3{}^L & \\ \underline{0} & \end{bmatrix} = \begin{bmatrix} A_1{}^U & A_2{}^U & \underline{0}_2 & \\ A_1{}^L & A_2{}^L & \underline{0}_2 & \\ A_1{}^U & \underline{0}_2 & A_2{}^U & \\ A_1{}^L & \underline{0}_2 & A_2{}^L & \underline{T} \\ \underline{0}_2 & A_1{}^U & A_2{}^U & \\ \underline{0}_2 & A_1{}^L & A_2{}^L & \\ 0 & 0 & 0 & \end{bmatrix} = \begin{bmatrix} -1 & -1 & 0 & -6 \\ 1 & -1 & 0 & -5 \\ -1 & 1 & 0 & -4 \\ 1 & 1 & 0 & -3 \\ -1 & 0 & -1 & -2 \\ 1 & 0 & -1 & -1 \\ -1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 1 \\ 0 & -1 & -1 & 2 \\ 0 & 1 & -1 & 3 \\ 0 & -1 & 1 & 4 \\ 0 & 1 & 1 & 5 \\ 0 & 0 & 0 & 6 \end{bmatrix}$$

By following step 1 and step 2, we have 2^3 arrngements.

$$D_1 = \begin{bmatrix} B_1{}^U \\ B_2{}^U \\ B_3{}^U \\ \underline{0} \\ B_3{}^L \\ B_2{}^L \\ B_1{}^L \end{bmatrix}, \quad D_2 = \begin{bmatrix} B_1{}^U \\ B_2{}^U \\ B_3{}^L \\ \underline{0} \\ b_3{}^U \\ b_2{}^L \\ b_1{}^L \end{bmatrix}, \quad D_3 = \begin{bmatrix} B_1{}^U \\ B_2{}^L \\ B_3{}^U \\ \underline{0} \\ B_3{}^L \\ B_2{}^U \\ B_1{}^L \end{bmatrix}, \quad D_4 = \begin{bmatrix} B_1{}^L \\ B_2{}^U \\ B_3{}^U \\ \underline{0} \\ B_3{}^L \\ B_2{}^L \\ B_1{}^U \end{bmatrix}$$

$$
D_5 = \begin{bmatrix} B_1{}^U \\ B_2{}^L \\ B_3{}^L \\ \underline{0} \\ B_3{}^U \\ B_2{}^U \\ B_1{}^L \end{bmatrix}, \quad
D_6 = \begin{bmatrix} B_1{}^L \\ B_2{}^U \\ B_3{}^L \\ \underline{0} \\ B_3{}^U \\ B_2{}^L \\ B_1{}^U \end{bmatrix}, \quad
D_7 = \begin{bmatrix} B_1{}^L \\ B_2{}^L \\ B_3{}^U \\ \underline{0} \\ B_3{}^L \\ B_2{}^U \\ B_1{}^U \end{bmatrix}, \quad
D_8 = \begin{bmatrix} B_1{}^L \\ B_2{}^L \\ B_3{}^L \\ \underline{0} \\ B_3{}^U \\ B_2{}^U \\ B_1{}^U \end{bmatrix}
$$

i.e.,

$$
D_1 = \begin{array}{c} \begin{array}{ccc} x_1 & x_2 & x_3 \end{array} \\ \begin{bmatrix} -1 & -1 & 0 \\ 1 & -1 & 0 \\ -1 & 0 & -1 \\ 1 & 0 & -1 \\ 0 & -1 & -1 \\ 0 & 1 & -1 \\ 0 & 0 & 0 \\ 0 & -1 & 1 \\ 0 & 1 & 1 \\ -1 & 0 & 1 \\ 1 & 0 & 1 \\ -1 & 1 & 0 \\ 1 & 1 & 0 \end{bmatrix} \end{array}
\quad
D_2 = \begin{array}{c} \begin{array}{ccc} x_1 & x_2 & x_3 \end{array} \\ \begin{bmatrix} -1 & -1 & 0 \\ 1 & -1 & 0 \\ -1 & 0 & -1 \\ 1 & 0 & -1 \\ 0 & -1 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \\ 0 & -1 & -1 \\ 0 & 1 & -1 \\ -1 & 0 & 1 \\ 1 & 0 & 1 \\ -1 & 1 & 0 \\ 1 & 1 & 0 \end{bmatrix} \end{array}
\quad
D_3 = \begin{array}{c} \begin{array}{ccc} x_1 & x_2 & x_3 \end{array} \\ \begin{bmatrix} -1 & -1 & 0 \\ 1 & -1 & 0 \\ -1 & 0 & 1 \\ 1 & 0 & 1 \\ 0 & -1 & -1 \\ 0 & 1 & -1 \\ 0 & 0 & 0 \\ 0 & -1 & 1 \\ 0 & 1 & 1 \\ -1 & 0 & -1 \\ 1 & 0 & -1 \\ -1 & 1 & 0 \\ 1 & 1 & 0 \end{bmatrix} \end{array}
\quad
D_4 = \begin{array}{c} \begin{array}{ccc} x_1 & x_2 & x_3 \end{array} \\ \begin{bmatrix} -1 & 1 & 0 \\ 1 & 1 & 0 \\ -1 & 0 & -1 \\ 1 & 0 & -1 \\ 0 & -1 & -1 \\ 0 & 1 & -1 \\ 0 & 0 & 0 \\ 0 & -1 & 1 \\ 0 & 1 & 1 \\ -1 & 0 & 1 \\ 1 & 0 & 1 \\ -1 & -1 & 0 \\ 1 & -1 & 0 \end{bmatrix} \end{array}
$$

$$
D_5 = \begin{array}{c} \begin{array}{ccc} x_1 & x_2 & x_3 \end{array} \\ \begin{bmatrix} -1 & -1 & 0 \\ 1 & -1 & 0 \\ -1 & 0 & 1 \\ 1 & 0 & 1 \\ 0 & -1 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \\ 0 & -1 & -1 \\ 0 & 1 & -1 \\ -1 & 0 & -1 \\ 1 & 0 & -1 \\ -1 & 1 & 0 \\ 1 & 1 & 0 \end{bmatrix} \end{array}
\quad
D_6 = \begin{array}{c} \begin{array}{ccc} x_1 & x_2 & x_3 \end{array} \\ \begin{bmatrix} -1 & 1 & 0 \\ 1 & 1 & 0 \\ -1 & 0 & -1 \\ 1 & 0 & -1 \\ 0 & -1 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \\ 0 & -1 & -1 \\ 0 & 1 & -1 \\ -1 & 0 & 1 \\ 1 & 0 & 1 \\ -1 & -1 & 0 \\ 1 & -1 & 0 \end{bmatrix} \end{array}
\quad
D_7 = \begin{array}{c} \begin{array}{ccc} x_1 & x_2 & x_3 \end{array} \\ \begin{bmatrix} -1 & 1 & 0 \\ 1 & 1 & 0 \\ -1 & 0 & 1 \\ 1 & 0 & 1 \\ 0 & -1 & -1 \\ 0 & 1 & -1 \\ 0 & 0 & 0 \\ 0 & -1 & 1 \\ 0 & 1 & 1 \\ -1 & 0 & -1 \\ 1 & 0 & -1 \\ -1 & -1 & 0 \\ 1 & -1 & 0 \end{bmatrix} \end{array}
\quad
D_8 = \begin{array}{c} \begin{array}{ccc} x_1 & x_2 & x_3 \end{array} \\ \begin{bmatrix} -1 & 1 & 0 \\ 1 & 1 & 0 \\ -1 & 0 & 1 \\ 1 & 0 & 1 \\ 0 & -1 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \\ 0 & -1 & -1 \\ 0 & 1 & -1 \\ -1 & 0 & -1 \\ 1 & 0 & -1 \\ -1 & -1 & 0 \\ 1 & -1 & 0 \end{bmatrix} \end{array}
$$

For all cases, the generated pure quadratic terms $\underline{x}_1^2$, $\underline{x}_2^2$, $\underline{x}_3^2$ and the mixed quadratic terms $\underline{x}_1\underline{x}_2$, $\underline{x}_1\underline{x}_3$, $\underline{x}_2\underline{x}_3$ are symmetric, implying that $(\underline{x}_i^2)'\underline{T} = 0$, $(\underline{x}_i\underline{x}_{i'})'\underline{T} = 0$, $i, i' = 1,2,3$, $i < i'$. The first-order terms $\underline{x}_1$, $\underline{x}_2$, $\underline{x}_3$ are anti-symmetric with respect to the center point. So, we consider run orders for the first order terms, while keeping the symmetric property of the second order terms.

Choose D_1 . In this case, we have $b2^{k-1} = 6$ design points in P_2 associated with positive values of $\underline{T}$ starting from the center point, i.e. (0, -1, 1) is called a design point 1, (0, 1, 1) is called a design point 2, ... , and (1, 1, 0) is called a design point 6. Similarly, we define design points in P_1 associated with negative values of $\underline{T}$ starting from the center point. i.e. (0, 1, -1) is called a design point $\bar{1}$, (0, -1, -1) is called a design point $\bar{2}$, ... , and (-1, -1, 0) is called a design point $\bar{6}$. And we have $v = 3$ equations.

Find $\underline{C}^+ = (c_1, c_2, \ldots, c_6)'$ to satisfy $(\underline{x}_1^+)'\underline{C}^+ = 0$, $(\underline{x}_2^+)'\underline{C}^+ = 0$, $(\underline{x}_3^+)'\underline{C}^+ = 0$. But, we cannot find solutions $\underline{C}^+$ due to the fact that all elements of $\underline{C}^+$ take positive integer values, ranging from 1 to 6, resulting that $(\underline{x}_3^+)'\underline{C}^+ \geq 0$.

Choose D_2. In the same way as D_1 we have $b2^{k-1} = 6$ design points in P_2 associated with $\underline{T}_2$ starting from the center point, i.e. a design point 1 is given by (0, -1, -1). a design point 2 is given by (0, 1, -1), ... , a design point 6 is given by (1, 1, 0). Likewise, we define design points in P_1 associated with $\underline{T}_1$ starting from the center point. i.e. (0, 1, 1) is called a design point $\bar{1}$, (0, -1, 1) is called a design point $\bar{2}$, ... , and (-1, -1, 0) is called a design point $\bar{6}$. And we have $v = 3$ equations.

We next Find $\underline{C}^+ = (c_1, c_2, \ldots, c_6)'$ to satisfy $(\underline{x}_1^+)'\underline{C}^+ = 0$, $(\underline{x}_2^+)'\underline{C}^+ = 0$, $(\underline{x}_3^+)'\underline{C}^+ = 0$. Then, we have X matrix with $\underline{T}$ as follows:

$$
(X, \underline{T}) = \begin{bmatrix} B_1{}^U \\ B_2{}^U \\ B_3{}^L \\ \underline{0} \quad \underline{T} \\ B_3{}^U \\ B_2{}^L \\ B_1{}^L \end{bmatrix} =
\begin{array}{cc}
\begin{array}{cccccccccc} x_1 & x_2 & x_3 & x_1^2 & x_2^2 & x_3^3 & x_1x_2 & x_1x_3 & x_2x_3 & \underline{T} \end{array} & \underline{C} \\
\left[\begin{array}{cccccccccc}
-1 & -1 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & -6 \\
1 & -1 & 0 & 1 & 1 & 0 & -1 & 0 & 0 & -5 \\
-1 & 0 & -1 & 1 & 0 & 1 & 0 & 1 & 0 & -4 \\
1 & 0 & -1 & 1 & 0 & 1 & 0 & -1 & 0 & -3 \\
0 & -1 & 1 & 0 & 1 & 1 & 0 & 0 & -1 & -2 \\
0 & 1 & 1 & 0 & 1 & 1 & 0 & 0 & 1 & -1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & -1 & 0 & 1 & 1 & 0 & 0 & 1 & 1 \\
0 & 1 & -1 & 0 & 1 & 1 & 0 & 0 & -1 & 2 \\
-1 & 0 & 1 & 1 & 0 & 1 & 0 & -1 & 0 & 3 \\
1 & 0 & 1 & 1 & 0 & 1 & 0 & 1 & 0 & 4 \\
-1 & 1 & 0 & 1 & 1 & 0 & -1 & 0 & 0 & 5 \\
1 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 6
\end{array}\right] &
\begin{array}{c}
-c_6 \\ -c_5 \\ -c_4 \\ -c_3 \\ -c_2 \\ -c_1 \\ \\ c_1 \\ c_2 \\ c_3 \\ c_4 \\ c_5 \\ c_6
\end{array}
\end{array}
$$

According to step 4, we want to find $\underline{C}^+ = (c_1, c_2, c_3, c_4, c_5, c_6)'$ satisfying $(\underline{x}_1{}^+)'\underline{C}^+ = 0$, $(\underline{x}_2{}^+)'\underline{C}^+ = 0$, $(\underline{x}_3{}^+)'\underline{C}^+ = 0$, i.e.

$$- c_3 + c_4 - c_5 + c_6 = 0 \tag{4.13}$$

$$- c_1 + c_2 + c_5 + c_6 = 0$$

$$- c_1 - c_2 + c_3 + c_4 = 0$$

We use the LINDO programming package (Schrage, 1984) to solve these equations (Appendix). We obtain one of the possible solutions as $\underline{C}^+ = (6, 3, 4, 5, 2, 1)'$. But, this is not unique since $\underline{C}^{+} = (6, 3, 5, 4, 1, 2)'$ is another solution. Following step 6, we arrange run orders according to $\underline{C}^{+} = (6, 3, 4, 5, 2, 1)'$ such that for P_2 associated with $\underline{T}_2$, design point 1 = (0, -1, -1) is placed on the position of $c_1 = 6$ value of $\underline{T}_2$, design point 2 = (0, 1, -1) is placed on the position of $c_2 = 3$ value of $\underline{T}_2$, and so on. Finally, design point 6 = (1, 1, 0) is placed on the position of $c_6 = 1$ value of $\underline{T}_2$. We also arrange run orders according to $\underline{C}^{-} = (-6, -3, -4, -5, -2, -1)'$ such that for P_1 associated with $\underline{T}_1$ design point $\bar{1}$ = (0, 1, 1) is placed on the position of $-c_1 = -6$ value of $\underline{T}_1$, design point $\bar{2}$ = (0, -1, 1) is placed on the position of $-c_2 = -3$ value of $\underline{T}_1$, and so on. Finally, design point 6 = (-1, -1, 0) is placed on the position of $-c_6 = -1$ value of $\underline{T}_1$. Then we obtain LTF Box-Behnken design such as

$$D_{LTF} = \begin{bmatrix} C_0^{-}(P_1) \\ P_0 \\ C_0^{+}(P_2) \end{bmatrix} = \begin{bmatrix} 0 & 1 & 1 \\ -1 & 0 & -1 \\ 1 & 0 & -1 \\ 0 & -1 & 1 \\ 1 & -1 & 0 \\ -1 & -1 & 0 \\ 0 & 0 & 0 \\ 1 & 1 & 0 \\ -1 & 1 & 0 \\ 0 & 1 & -1 \\ -1 & 0 & 1 \\ 1 & 0 & 1 \\ 0 & -1 & -1 \end{bmatrix}$$

We then write the X matrix with $\underline{T}$ for LTF Box-Behnken design such as

$$(X, T) = \begin{array}{c} \begin{array}{cccccccccc} x_1 & x_2 & x_3 & x_1^2 & x_2^2 & x_3^2 & x_1x_2 & x_1x_3 & x_2x_3 & T \end{array} \\ \begin{bmatrix} 0 & 1 & 1 & 0 & 1 & 1 & 0 & 0 & 1 & -6 \\ -1 & 0 & -1 & 1 & 0 & 1 & 0 & 1 & 0 & -5 \\ 1 & 0 & -1 & 1 & 0 & 1 & 0 & -1 & 0 & -4 \\ 0 & -1 & 1 & 0 & 1 & 1 & 0 & 0 & -1 & -3 \\ 1 & -1 & 0 & 1 & 1 & 0 & -1 & 0 & 0 & -2 \\ -1 & -1 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 1 \\ -1 & 1 & 0 & 1 & 1 & 0 & -1 & 0 & 0 & 2 \\ 0 & 1 & -1 & 0 & 1 & 1 & 0 & 0 & -1 & 3 \\ -1 & 0 & 1 & 1 & 0 & 1 & 0 & -1 & 0 & 4 \\ 1 & 0 & 1 & 1 & 0 & 1 & 0 & 1 & 0 & 5 \\ 0 & -1 & -1 & 0 & 1 & 1 & 0 & 0 & 1 & 6 \end{bmatrix} \end{array}$$

Hence, for the model

$$y_u = \beta_0 + \sum_{i=1}^{3} \beta_i x_{iu} + \sum_{i=1}^{3} \beta_{ii} x_{iu}{}^2 + \sum_{\substack{i, i' = 1 \\ i < i'}}^{3} \beta_{ii'} x_{iu} x_{i'u} + \theta t_u + \varepsilon_u, \qquad u = 1,2, \dots, 13$$

we have the following coefficient matrix

$$\begin{bmatrix} X'X & X'\underline{T} \\ \underline{T}'X & \underline{T}'\underline{T} \end{bmatrix} = \begin{bmatrix} n & \underline{0}' & r2^k\underline{1}' & \underline{0}' & 0 \\ \underline{0} & r2^k I & 0 & 0 & \underline{0} \\ r2^k\underline{1} & 0 & 2^k(\underline{N}\underline{N}') & 0 & \underline{0} \\ \underline{0} & 0 & 0 & G & \underline{0} \\ 0 & \underline{0}' & \underline{0}' & \underline{0}' & \underline{T}'\underline{T} \end{bmatrix} = \begin{bmatrix} 13 & \underline{0}' & 8\underline{1}' & \underline{0}' & 0 \\ \underline{0} & 8I & 0 & 0 & \underline{0} \\ 8\underline{1} & 0 & 4(\underline{N}\underline{N}') & 0 & \underline{0} \\ \underline{0} & 0 & 0 & 4I & \underline{0} \\ 0 & \underline{0}' & \underline{0}' & \underline{0}' & 182 \end{bmatrix}$$

From the $X'X$ matrix, we can obtain a UMVUE of the linear trend coefficient θ such as $\hat{\theta} = (\frac{1}{182})\underline{T}'\underline{Y}$, without affecting the other coefficients.

Example 4.5.2

The following example shows that there may not exist a LTF Box-Behnken Design. We consider the Box-Behnken design with the PBIB(2) characterized by the parameters $v = 6, r = 2, b = 4, k = 3, \lambda_1 = 0, \lambda_2 = 1$, and treatment combinations (1,4), (2,5), (3,6) being first associates with $\lambda_1 = 0$ and the remaining treatment combinations being second associates with $\lambda_2 = 1$, (Design SR18 in Clatworthy, 1973). Then the transpose of the incidence matrix is:

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

The Box-Behnken design matrix D with a linear trend $\underline{T}$ can be written as

$$S \equiv (D, \underset{\sim}{T}) = \begin{bmatrix} B_1{}^U \\ B_1{}^L \\ B_2{}^U \\ B_2{}^L \\ B_3{}^U \\ B_3{}^L \\ B_4{}^U \\ B_4{}^L \\ \underset{\sim}{0} \end{bmatrix} \underset{\sim}{T} = \begin{bmatrix} A_1{}^U & A_2{}^U & A_3{}^U & \underset{\sim}{0} & \underset{\sim}{0} & \underset{\sim}{0} \\ A_1{}^L & A_2{}^L & A_3{}^L & \underset{\sim}{0} & \underset{\sim}{0} & \underset{\sim}{0} \\ A_1{}^U & \underset{\sim}{0} & \underset{\sim}{0} & \underset{\sim}{0} & A_2{}^U & A_3{}^U \\ A_1{}^L & \underset{\sim}{0} & \underset{\sim}{0} & \underset{\sim}{0} & A_2{}^L & A_3{}^L \\ \underset{\sim}{0} & A_1{}^U & \underset{\sim}{0} & A_2{}^U & \underset{\sim}{0} & A_3{}^U \\ \underset{\sim}{0} & A_1{}^L & \underset{\sim}{0} & A_2{}^L & \underset{\sim}{0} & A_3{}^L \\ \underset{\sim}{0} & \underset{\sim}{0} & A_1{}^U & A_2{}^U & A_3{}^U & \underset{\sim}{0} \\ \underset{\sim}{0} & \underset{\sim}{0} & A_1{}^L & A_2{}^L & A_3{}^L & \underset{\sim}{0} \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \underset{\sim}{T}$$

where

$A_1{}^U = (-1,1,-1,1)'$, $A_1{}^L = (-1,1,-1,1)'$, $A_2{}^U = (-1,-1,1,1)'$, $A_2{}^L = (-1,-1,1,1)'$, $A_3{}^U = (-1,-1,-1,-1)'$, $A_3{}^L = (1,1,1,1)'$ are 2^2 factorials, $\underset{\sim}{0}$ is a 4×1 vector of elements being zeros, $\underset{\sim}{T} = (-16, -15, \dots, -1, 0, 1, \dots, 15, 16)$.

There are 2^4 possible ways to arrange by step 1 and step 2.

$$D_1 = \begin{bmatrix} B_1{}^U \\ B_2{}^U \\ B_3{}^U \\ B_4{}^U \\ \underset{\sim}{0} \\ B_4{}^L \\ B_3{}^L \\ B_2{}^L \\ B_1{}^L \end{bmatrix} \quad D_2 = \begin{bmatrix} B_1{}^U \\ B_2{}^U \\ B_3{}^U \\ b_4{}^L \\ \underset{\sim}{0} \\ B_4{}^U \\ B_3{}^L \\ B_2{}^L \\ B_1{}^L \end{bmatrix} \quad D_3 = \begin{bmatrix} B_1{}^U \\ B_2{}^U \\ B_3{}^L \\ B_4{}^U \\ \underset{\sim}{0} \\ B_4{}^U \\ B_3{}^L \\ B_2{}^L \\ B_1{}^L \end{bmatrix} \quad D_4 = \begin{bmatrix} B_1{}^U \\ B_2{}^L \\ B_3{}^U \\ B_4{}^U \\ \underset{\sim}{0} \\ B_4{}^L \\ B_3{}^L \\ B_2{}^U \\ B_1{}^L \end{bmatrix}$$

$$D_5 = \begin{bmatrix} B_1^{\ L} \\ B_2^{\ U} \\ B_3^{\ U} \\ B_4^{\ U} \\ \underline{0} \\ B_4^{\ L} \\ B_3^{\ L} \\ B_2^{\ L} \\ B_1^{\ U} \end{bmatrix} \quad D_6 = \begin{bmatrix} B_1^{\ U} \\ B_2^{\ U} \\ B_3^{\ L} \\ B_4^{\ L} \\ \underline{0} \\ B_4^{\ U} \\ B_3^{\ U} \\ B_2^{\ L} \\ B_1^{\ L} \end{bmatrix} \quad D_7 = \begin{bmatrix} B_1^{\ U} \\ B_2^{\ L} \\ B_3^{\ U} \\ B_4^{\ U} \\ \underline{0} \\ B_4^{\ U} \\ B_3^{\ L} \\ B_2^{\ U} \\ B_1^{\ L} \end{bmatrix} \quad D_8 = \begin{bmatrix} B_1^{\ U} \\ B_2^{\ L} \\ B_3^{\ L} \\ B_4^{\ U} \\ \underline{0} \\ B_4^{\ L} \\ B_3^{\ U} \\ B_2^{\ U} \\ B_1^{\ L} \end{bmatrix}$$

$$D_9 = \begin{bmatrix} B_1^{\ L} \\ B_2^{\ U} \\ B_3^{\ U} \\ B_4^{\ L} \\ \underline{0} \\ B_4^{\ U} \\ B_3^{\ L} \\ B_2^{\ L} \\ B_1^{\ U} \end{bmatrix} \quad D_{10} = \begin{bmatrix} B_1^{\ L} \\ B_2^{\ U} \\ B_3^{\ L} \\ B_4^{\ U} \\ \underline{0} \\ B_4^{\ L} \\ B_3^{\ U} \\ B_2^{\ L} \\ B_1^{\ U} \end{bmatrix} \quad D_{11} = \begin{bmatrix} B_1^{\ L} \\ B_2^{\ L} \\ B_3^{\ U} \\ B_4^{\ U} \\ \underline{0} \\ B_4^{\ L} \\ B_3^{\ L} \\ B_2^{\ U} \\ B_1^{\ U} \end{bmatrix} \quad D_{12} = \begin{bmatrix} B_1^{\ U} \\ B_2^{\ L} \\ B_3^{\ L} \\ B_4^{\ L} \\ \underline{0} \\ B_4^{\ U} \\ B_3^{\ U} \\ B_2^{\ U} \\ B_1^{\ L} \end{bmatrix}$$

$$D_{13} = \begin{bmatrix} B_1{}^L \\ B_2{}^U \\ B_3{}^L \\ B_4{}^L \\ \underline{0} \\ B_4{}^U \\ B_3{}^U \\ B_2{}^L \\ B_1{}^U \end{bmatrix} \quad D_{14} = \begin{bmatrix} B_1{}^L \\ B_2{}^L \\ B_3{}^U \\ B_4{}^L \\ \underline{0} \\ B_4{}^U \\ B_3{}^L \\ B_2{}^U \\ B_1{}^U \end{bmatrix} \quad D_{15} = \begin{bmatrix} B_1{}^L \\ B_2{}^L \\ B_3{}^L \\ B_4{}^U \\ \underline{0} \\ B_4{}^L \\ B_3{}^U \\ B_2{}^U \\ B_1{}^U \end{bmatrix} \quad D_{16} = \begin{bmatrix} B_1{}^L \\ B_2{}^L \\ B_3{}^L \\ B_4{}^L \\ \underline{0} \\ B_4{}^U \\ B_3{}^U \\ B_2{}^U \\ B_1{}^U \end{bmatrix}$$

For all cases, the second order terms are orthogonal to a linear trend $\underline{T} = (-16, \ -15, \dots, 16)'$, since $\underline{x}_1{}^2$, $\underline{x}_2{}^2, \dots, \underline{x}_6{}^2$ and $\underline{x}_1\underline{x}_2$, $\underline{x}_1\underline{x}_3, \dots, \underline{x}_5\underline{x}_6$ are symmetric. But the first order terms $\underline{x}_1$, $\underline{x}_2, \dots, \underline{x}_6$ are anti-symmetric.

We exclude the cases D_1, D_2, D_5, D_8, D_9, D_{12}, D_{15}, and D_{16} since $\underline{x}_6{}^+$ consists of 1 and 0, or -1 and 0 so that they will not satisfy the equation $(\underline{x}_6{}^+)'\underline{C}^+ = 0$, due to the fact that all elements of $\underline{C}^+$ take positive integer values, ranging from 1 to 16.

Choose any case, say, D_3. Then, we rewrite D_3 as

$$
D_3 = \begin{bmatrix} B_1{}^U \\ B_2{}^U \\ B_3{}^L \\ B_4{}^U \\ \underline{0} \\ B_4{}^L \\ B_3{}^U \\ B_2{}^L \\ B_1{}^L \end{bmatrix} = \begin{array}{cc}
\begin{matrix} x_1 & x_2 & x_3 & x_4 & x_5 & x_6 & \underline{T} \end{matrix} & \underline{C} \\
\begin{bmatrix}
-1 & -1 & -1 & 0 & 0 & 0 & -16 \\
1 & -1 & -1 & 0 & 0 & 0 & -15 \\
-1 & 1 & -1 & 0 & 0 & 0 & -14 \\
1 & 1 & -1 & 0 & 0 & 0 & -13 \\
-1 & 0 & 0 & 0 & -1 & -1 & -12 \\
1 & 0 & 0 & 0 & -1 & -1 & -11 \\
-1 & 0 & 0 & 0 & 1 & -1 & -10 \\
1 & 0 & 0 & 0 & 1 & -1 & -9 \\
0 & -1 & 0 & -1 & 0 & 1 & -8 \\
0 & 1 & 0 & -1 & 0 & 1 & -7 \\
0 & -1 & 0 & 1 & 0 & 1 & -6 \\
0 & 1 & 0 & 1 & 0 & 1 & -5 \\
0 & 0 & -1 & -1 & -1 & 0 & -4 \\
0 & 0 & 1 & -1 & -1 & 0 & -3 \\
0 & 0 & -1 & 1 & -1 & 0 & -2 \\
0 & 0 & 1 & 1 & -1 & 0 & -1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & -1 & -1 & 1 & 0 & 1 \\
0 & 0 & 1 & -1 & 1 & 0 & 2 \\
0 & 0 & -1 & 1 & 1 & 0 & 3 \\
0 & 0 & 1 & 1 & 1 & 0 & 4 \\
0 & -1 & 0 & -1 & 0 & -1 & 5 \\
0 & 1 & 0 & -1 & 0 & -1 & 6 \\
0 & -1 & 0 & 1 & 0 & -1 & 7 \\
0 & 1 & 0 & 1 & 0 & -1 & 8 \\
-1 & 0 & 0 & 0 & -1 & 1 & 9 \\
1 & 0 & 0 & 0 & -1 & 1 & 10 \\
-1 & 0 & 0 & 0 & 1 & 1 & 11 \\
1 & 0 & 0 & 0 & 1 & 1 & 12 \\
-1 & -1 & 1 & 0 & 0 & 0 & 13 \\
1 & -1 & 1 & 0 & 0 & 0 & 14 \\
-1 & 1 & 1 & 0 & 0 & 0 & 15 \\
1 & 1 & 1 & 0 & 0 & 0 & 16
\end{bmatrix} &
\begin{matrix}
-c_{16} \\ -c_{15} \\ -c_{14} \\ -c_{13} \\ -c_{12} \\ -c_{11} \\ -c_{10} \\ -c_9 \\ -c_8 \\ -c_7 \\ -c_6 \\ -c_5 \\ -c_4 \\ -c_3 \\ -c_2 \\ -c_1 \\ \\ c_1 \\ c_2 \\ c_3 \\ c_4 \\ c_5 \\ c_6 \\ c_7 \\ c_8 \\ c_9 \\ c_{10} \\ c_{11} \\ c_{12} \\ c_{13} \\ c_{14} \\ c_{15} \\ c_{16}
\end{matrix}
\end{array}
$$

Now, we want to find $\underline{C}^+ = (c_1, c_2, \dots, c_{16})'$ satisfying $\underline{x}_1^{+\prime}\underline{C}^+ = 0,\ \underline{x}_2^{+\prime}\underline{C}^+ = 0, \dots, \underline{x}_6^{+\prime}\underline{C}^+ = 0$, resulting that

$$-c_9 + c_{10} - c_{11} + c_{12} - c_{13} + c_{14} - c_{15} + c_{16} = 0$$

$$-c_5 + c_6 - c_7 + c_8 - c_{13} - c_{14} + c_{15} + c_{16} = 0$$

$$-c_1 + c_2 - c_3 + c_4 + c_{13} + c_{14} + c_{15} + c_{16} = 0$$

$$-c_1 - c_2 + c_3 + c_4 - c_5 - c_6 + c_7 + c_8 = 0$$

$$c_1 + c_2 + c_3 + c_4 - c_9 - c_{10} + c_{11} + c_{12} = 0$$

$$-c_5 - c_6 - c_7 - c_8 + c_9 + c_{10} + c_{11} + c_{12} = 0$$

Again, we use LINDO to solve the case of 16 variables with 6 equations in similar way to example 4.6.1. We , however, could not find a set of the solutions which satisfies the constraints. There does not exist a solution for the other arrangements D_4, D_6, D_7, D_{10}, D_{11}, D_{13}, and D_{14}, either. So, in this design, there does not exist a LTF Box-Behnken design for the model

$$y_u = \beta_0 + \sum_{i=1}^{6} \beta_i x_{iu} + \sum_{i=1}^{6} \beta_{ii} x_{iu}{}^2 + \sum_{\substack{i,i'=1 \\ i<i'}}^{6} \beta_{ii'} x_{iu} x_{i'u} + \theta t_u + \varepsilon_u, \qquad u = 1,2,\dots,33$$

4.5.2. Construction method of LTF Box-Behnken designs for $k \geq 4$

Before we construct LTF Box-Behnken designs for $k \geq 4$. we investigate the properties of $F_1, F_2, \dots, F_k$ such that $F_i = A_1 \circ A_2 \circ \dots \circ A_{i-1} \circ A_{i+1} \circ \dots \circ A_k$, $i = 1,2,\dots,k$ when k is even, $F_i = A_1 \circ A_2 \circ \ldots \circ A_{i-1} \circ A_{i+1} \circ \ldots \circ A_{k-1}$, $i = 1,2, \ldots, k-1$, and $F_k = A_1 \circ A_2 \circ \ldots \circ A_k$ when k is odd where F_i is a $2^k \times 1$ vector, A_i is a main effect contrasts of the standard ordering. We let F_i^U be the upper half of F_i, F_i^L be the lower half of F_i, where F_i^U, F_i^L are $2^{k-1} \times 1$ vector. Then these F_i and F_i^U, F_i^L satisfies the following properties:

(i) The k F_i, $i = 1,2, \ldots, k$

are independent in the sense that no F_i is the generalized interaction of other F_j 's.

(ii) both F_i^U and F_i^L, $i = 1,2, \ldots, k$ are orthogonal to a linear trend taking values $\underline{T} = (1 + a, 2 + a, \ldots, 2^{k-1} + a)$ in which a is an arbitrary integer, i.e., $(F_i^U)'\underline{T} = 0$, $(F_i^L)'\underline{T} = 0$, $i = 1,2, \ldots, k$ because of property 4.1,

(iii) the generated two-factor interaction terms with an inserted center point $F_iF_j = A_iA_j$, defined as $F_iF_j = F_i \circ F_j$, $A_iA_j = A_i \circ A_j$, are symmetric, implying that F_iF_j are orthogonal to a linear trend $\underline{T}$ which is anti-symmetric as we have shown earlier in Section 4.1.

For example, when k = 4, we choose $F_1 = A_2 \circ A_3 \circ A_4$, $F_2 = A_1 \circ A_3 \circ A_4$, $F_3 = A_1 \circ A_2 \circ A_4$, $F_4 = A_1 \circ A_2 \circ A_3$, where F_i is a $2^k \times 1$ vector, A_i is a main effect contrast of the standard ordering of 2^4 factorial (Table 4.4). Then, these factorials satisfy the following properties:

(i) These F_1, F_2, F_3, F_4 are independent such that no F_i is the generalized interaction of others in the set.

(ii) Both F_i^U and F_i^L, $i = 1,2,3,4$ are orthogonal to a corresponding linear trend, which was already discussed in the same example of Section 4.3.

(iii) The two-factor interaction terms with an inserted center point F_1F_2, F_1F_3, F_1F_4, F_2F_3, F_2F_4, F_3F_4 are symmetric with respect to 0 (Table 4.6). Hence, these interaction terms are orthogonal to a linear trend $\underline{T}$ which is anti-symmetric with respect to 0 since $F_iF_j = A_i \circ A_j$.

Table 4.4. 2^4 FACTORIAL

F_1	F_2	F_3	F_4	F_1F_2	F_1F_3	F_1F_4	F_2F_3	F_2F_4	F_3F_4
−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	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

where $F_1 = A_2 \circ A_3 \circ A_4$, $F_2 = A_1 \circ A_3 \circ A_4$, $F_3 = A_1 \circ A_2 \circ A_4$, $F_4 = A_1 \circ A_2 \circ A_3$,

Table 4.5. The UPPER HALF and LOWER HALF OF 2^4 FACTORIAL

F_1^U	F_2^U	F_3^U	F_4^U	$F_1F_2^U$	$F_1F_3^U$	$F_1F_4^U$	$F_2F_3^U$	$F_2F_4^U$	$F_3F_4^U$
−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

F_1^L	F_2^L	F_3^L	F_4^L	$F_1F_2^L$	$F_1F_3^L$	$F_1F_4^L$	$F_2F_3^L$	$F_2F_4^L$	$F_3F_4^L$
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

Table 4.6. Two-factor interactions of 2^4 factorial with an inserted center point

F_1F_2	F_1F_3	F_1F_4	F_2F_3	F_2F_4	F_3F_4
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	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

Now, we are in position to construct LTF Box-Behnken designs for $k \geq 4$ by the following method:

1. For k is even, choose $F_i = A_1 \circ A_2 \circ \ldots \circ A_{i-1} \circ A_{i+1} \circ \ldots \circ A_k$, $i = 1,2, \ldots, k$. When k is odd, choose $F_i = A_1 \circ A_2 \circ \ldots \circ A_{i-1} \circ A_{i+1} \circ \ldots \circ A_{k-1}$, $i = 1,2, \ldots, k-1$, and $F_k = A_1 \circ A_2 \circ \ldots \circ A_k$.

2. Replace A_i, $i = 1,2, \dots, k$ by F_i, $i = 1,2, \dots, k$ into the Box-Behnken design matrix (4.9) or (4.11).

3. In (4.11), position a center point on the middle of the experimental units associated with 0-value of $\underline{T}$.

4. For each B_i, $i = 1,2, \dots, b$, put B_i^U in the experimental units associated with the negative values of $\underline{T}$ and B_i^L in the experimental units associated with the positive values of $\underline{T}$ symmetrically with respect to the center point or vice versa.

Then we obtain a LTF Box-Behnken design since the first order terms $\underline{x}_1, \underline{x}_2, \dots, \underline{x}_v$ are orthogonal to a linear trend, and the second order terms are also orthogonal to a linear trend because all pure quadratic terms $\underline{x}_1^2, \underline{x}_2^2, \dots, \underline{x}_v^2$, and the mixed quadratic terms $\underline{x}_{12}, \underline{x}_{13}, \dots, \underline{x}_{v-1,v}$ are symmetric with respect to the center point. Here is one of LTF Box-Behnken design matrices constructed by the above method.

$$
S \equiv (D, \underline{T}) = \begin{bmatrix} B_1^{\ U} & \\ B_2^{\ U} & \\ \cdot & \\ \cdot & \\ \cdot & \\ B_b^{\ U} & \\ \underline{0} & \underline{T} \\ B_b^{\ L} & \\ \cdot & \\ \cdot & \\ \cdot & \\ B_2^{\ L} & \\ B_1^{\ L} & \end{bmatrix} = \begin{bmatrix} n_{11}F_{w(1,1)}^{\ \ U} & n_{12}F_{w(1,2)}^{\ \ U} & \cdots & n_{1v}F_{w(1,v)}^{\ \ U} & \\ n_{21}F_{w(2,1)}^{\ \ U} & n_{22}F_{w(2,2)}^{\ \ U} & \cdots & n_{2v}F_{w(2,v)}^{\ \ U} & \\ \cdot & \cdot & \cdots & \cdot & \\ \cdot & \cdot & \cdots & \cdot & \\ \cdot & \cdot & \cdots & \cdot & \\ n_{b1}F_{w(b,1)}^{\ \ U} & n_{b2}F_{w(b,2)}^{\ \ U} & \cdots & n_{bv}F_{w(b,v)}^{\ \ U} & \\ 0 & 0 & \cdots & 0 & \underline{T} \\ n_{b1}F_{w(b,1)}^{\ \ L} & n_{b2}F_{w(b,2)}^{\ \ L} & \cdots & n_{bv}F_{w(b,v)}^{\ \ L} & \\ \cdot & \cdot & \cdots & \cdot & \\ \cdot & \cdot & \cdots & \cdot & \\ \cdot & \cdot & \cdots & \cdot & \\ n_{21}F_{w(2,1)}^{\ \ L} & n_{22}F_{w(2,2)}^{\ \ L} & \cdots & n_{2v}F_{w(2,v)}^{\ \ L} & \\ n_{11}F_{w(1,1)}^{\ \ L} & n_{12}F_{w(1,2)}^{\ \ L} & \cdots & n_{1v}F_{w(1,v)}^{\ \ L} & \end{bmatrix} \quad (4.14)
$$

where $F_i = A_1 \circ A_2 \circ \dots \circ A_{i-1} \circ A_{i+1} \circ \dots \circ A_k,\ i = 1,2,\dots,k.$ when k is even, $F_i = A_1 \circ A_2 \circ \dots \circ A_{i-1} \circ A_{i+1} \circ \dots \circ A_{k-1},\ i = 1,2,\dots,k-1$, and $F_k = A_1 \circ A_2 \circ \dots \circ A_k$ when k is odd.

Example 4.5.3

Consider the Box-Behnken design with the PBIB(2) characterized by the parameters $v = 6, r = 2, b = 3, k = 4, \lambda_1 = 2, \lambda_2 = 1$, and treatment combinations (1,4), (2,5), (3,6) being first associates with $\lambda_1 = 2$ and the remaining treatment combinations being second associates with $\lambda_2 = 1$, (Design S1 in Clatworthy, 1973). Then the transpose of the incidence matrix is:

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

Thus, the Box-Behnken design matrix D with linear trend vector $\underline{T}$ can be written as

$$(D, \underline{T}) = \begin{bmatrix} B_1^{\ U} & \\ B_1^{\ L} & \\ B_2^{\ U} & \\ B_2^{\ L} & \underline{T} \\ B_3^{\ U} & \\ B_3^{\ L} & \\ \underline{0} & \end{bmatrix} = \begin{bmatrix} A_1^{\ U} & A_2^{\ U} & \underline{0} & A_3^{\ U} & A_4^{\ U} & \underline{0} & \\ A_1^{\ L} & A_2^{\ L} & \underline{0} & A_3^{\ L} & A_4^{\ L} & \underline{0} & \\ A_1^{\ U} & \underline{0} & A_2^{\ U} & A_3^{\ U} & \underline{0} & A_4^{\ U} & \\ A_1^{\ L} & \underline{0} & A_2^{\ L} & A_3^{\ L} & \underline{0} & A_4^{\ L} & \underline{T} \\ \underline{0} & A_1^{\ U} & A_2^{\ U} & \underline{0} & A_3^{\ U} & A_4^{\ U} & \\ \underline{0} & A_1^{\ L} & A_2^{\ L} & \underline{0} & A_3^{\ L} & A_4^{\ L} & \\ 0 & 0 & 0 & 0 & 0 & 0 & \end{bmatrix}$$

where $A_1^U = (-1, 1, -1, 1, -1, 1, -1, 1)'$, $A_1^L = (-1, 1, -1, 1, -1, 1, -1, 1)'$, ... , $A_4^U = (-1, -1, -1, -1, -1, -1, -1, -1)'$, $A_4^L = (1, 1, 1, 1, 1, 1, 1, 1)'$ are 2^4 factorials (see Table 4.4), $\underline{0}$ is an 8×1 zero vector, and $\underline{T}' = (-24, -23, \ldots, -1, 0, 1, \ldots, 23, 24)$.

Now, we want to construct a LTF Box-Behnken design using the method for $k \geq 4$.

1. Choose $F_1 = A_2 \circ A_3 \circ A_4$, $F_2 = A_1 \circ A_3 \circ A_4$, $F_3 = A_1 \circ A_2 \circ A_4$, $F_4 = A_1 \circ A_2 \circ A_3$ since $k = 4$ is even, where

$$A_i = \begin{bmatrix} A_i^{\ U} \\ A_i^{\ L} \end{bmatrix} \quad i = 1,2,3,4$$

2. Using F_1, F_2, F_3, F_4, as the generators of the Box-Behnken design, we then rewrite the design matrix D with $\underline{T}$ as

$$(D, \underline{T}) = \begin{bmatrix} B_1{}^U & \\ B_1{}^L & \\ B_2{}^U & \\ B_2{}^L & \underline{T} \\ B_3{}^U & \\ B_3{}^L & \\ \underline{0} & \end{bmatrix} = \begin{bmatrix} F_1{}^U & F_2{}^U & \underline{0} & F_3{}^U & F_4{}^U & \underline{0} & \\ F_1{}^L & F_2{}^L & \underline{0} & F_3{}^L & F_4{}^L & \underline{0} & \\ F_1{}^U & \underline{0} & F_2{}^U & F_3{}^U & \underline{0} & F_4{}^U & \\ F_1{}^L & \underline{0} & F_2{}^L & F_3{}^L & \underline{0} & F_4{}^L & \underline{T} \\ \underline{0} & F_1{}^U & F_2{}^U & \underline{0} & A_3{}^U & F_4{}^U & \\ \underline{0} & F_1{}^L & F_2{}^L & \underline{0} & F_3{}^L & F_4{}^L & \\ 0 & 0 & 0 & 0 & 0 & 0 & \end{bmatrix}$$

3. Place a center point in the middle of the experimental units.

4. Move B_1^U, B_2^U, B_3^U in the experimental units associated with the negative values of $\underline{T}$, and the corresponding B_1^L, B_2^L, B_3^L are placed on the experimental units associated with the positive values of $\underline{T}$ symmetrically with respect to the center point.

Then, we obtain a LTF Box-Behnken design matrix as follows:

$$D_{LTF} = \begin{bmatrix} B_1{}^U \\ B_2{}^U \\ B_3{}^U \\ \underline{0} \\ B_3{}^L \\ B_2{}^L \\ B_1{}^L \end{bmatrix} = \begin{bmatrix} F_1{}^U & F_2{}^U & \underline{0} & F_3{}^U & F_4{}^U & \underline{0} \\ F_1{}^U & \underline{0} & F_2{}^U & F_3{}^U & \underline{0} & F_4{}^U \\ \underline{0} & F_1{}^U & F_2{}^U & \underline{0} & F_3{}^U & F_4{}^U \\ 0 & 0 & 0 & 0 & 0 & 0 \\ \underline{0} & F_1{}^L & F_2{}^L & \underline{0} & F_3{}^L & F_4{}^L \\ F_1{}^L & \underline{0} & F_2{}^L & F_3{}^L & \underline{0} & F_4{}^L \\ F_1{}^L & F_2{}^L & \underline{0} & F_3{}^L & F_4{}^L & \underline{0} \end{bmatrix}$$

Accordingly, we obtain X matrix for LTF Box-Behnken design with $\underline{T}$ such as

$$X = [\, D_{LTF} \quad X^* \quad \underline{T} \,]$$

where

$$X^* = \begin{array}{c} \\ \left[\begin{array}{cccccccccccc} x_{11} & x_{22} & x_{33} & x_{44} & x_{55} & x_{66} & x_{12} & x_{13} & x_{14} & \cdots & x_{56} \\ \underline{1} & \underline{1} & \underline{0} & \underline{1} & \underline{1} & \underline{0} & F_1F_2^U & \underline{0} & F_1F_3^U & \cdots & \underline{0} \\ \underline{1} & \underline{0} & \underline{1} & \underline{1} & \underline{0} & \underline{1} & \underline{0} & F_1F_2^U & F_1F_3^U & \cdots & \underline{0} \\ \underline{0} & \underline{1} & \underline{1} & \underline{0} & \underline{1} & \underline{1} & \underline{0} & \underline{0} & \underline{0} & \cdots & F_3F_4^U \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \cdots & 0 \\ \underline{0} & \underline{1} & \underline{1} & \underline{0} & \underline{1} & \underline{1} & \underline{0} & \underline{0} & \underline{0} & \cdots & F_3F_4^L \\ \underline{1} & \underline{0} & \underline{1} & \underline{1} & \underline{0} & \underline{1} & \underline{0} & F_1F_2^L & F_1F_3^L & \cdots & \underline{0} \\ \underline{1} & \underline{1} & \underline{0} & \underline{1} & \underline{1} & \underline{0} & F_1F_2^L & \underline{0} & F_1F_3^L & \cdots & \underline{0} \end{array}\right]\end{array}$$

Here, $F_iF_j^U$ and $F_iF_j^L$ are defined as the upper half and the lower half of F_iF_j respectively, $\underline{1}$ is an 8×1 vector with elements being 1.

Then, for the model

$$y_u = \beta_0 + \sum_{i=1}^{6} \beta_i x_{iu} + \sum_{i=1}^{6} \beta_{ii} {x_{iu}}^2 + \sum_{\substack{i,i'=1 \\ i<i'}}^{6} \beta_{ii'} x_{iu} x_{i'u} + \theta t_u + \varepsilon_u, \qquad u = 1,2, \dots, 49$$

we have the $X'X$ matrix

$$X'X = \begin{bmatrix} n & \underline{0}' & r2^k\underline{1}' & \underline{0}' & \underline{1}'\underline{T} \\ \underline{0} & r2^k I & 0 & 0 & \underline{0} \\ r2^k\underline{1} & 0 & 2^k(\underline{NN}') & 0 & \underline{0} \\ \underline{0} & 0 & 0 & G & \underline{0} \\ \underline{1}'\underline{T} & \underline{0}' & \underline{0}' & \underline{0}' & \underline{T}'\underline{T} \end{bmatrix} = \begin{bmatrix} 49 & \underline{0}' & 32\underline{1}' & \underline{0}' & 0 \\ \underline{0} & 32I & 0 & 0 & \underline{0} \\ 32\underline{1} & 0 & 16(\underline{NN}') & 0 & \underline{0} \\ \underline{0} & 0 & 0 & G & \underline{0} \\ 0 & \underline{0}' & \underline{0}' & \underline{0}' & 9800 \end{bmatrix}$$

where G is a diagonal matrix with diagonal elements being 32 or 16.

Up to now, we considered linear trend-free (LTF) Box-Behnken designs with one center point. We now consider LTF Box-Behnken designs with an odd number of center points, i.e. $n_0 = 2n' + 1$. Thus, we use a linear trend t taking values $-\frac{n-1}{2}, -\frac{n-1}{2}+1, \dots, -1, 0, 1, \dots, \frac{n-1}{2}-1, \frac{n-1}{2}$ over n experimental units where $n = b2^k + 2n' + 1$ is a number of observations with $b2^k$ experimental points and $2n' + 1$ center points. In this case the construction methods for LTF Box-Behnken designs are the same as those shown in Section 4.5.1 and Section 4.5.2 except that we put n' center points on the first n' experimental units associated with the negative values of $\underline{T}$, i.e $-\frac{n-1}{2}, -\frac{n-1}{2}+1, \dots, -\frac{n-1}{2}+n'-1$ values of the linear trend, 1 center point on the middle of the experimental units associated with the 0-value of $\underline{T}$, and the remaining n' center points on the last n' experimental units associated with the positive values of $\underline{T}$, i.e on the values $\frac{n-1}{2}, \frac{n-1}{2}-1, \dots, \frac{n-1}{2}-n'+1$ of the linear trend. For example, suppose we have $n_0 = 5$ center points. Then we put 2 center points on the first experimental units associated with the $-\frac{n-1}{2}, -\frac{n-1}{2}+1$ values of $\underline{T}$, 1 center point on the middle of the experimental units associated with the 0-value of $\underline{T}$, and 2 center points on the last experimental units associated with the $\frac{n-1}{2}, \frac{n-1}{2}-1$ values of $\underline{T}$

, where $n = b2^k + 5$. And we apply the same procedures of the construction methods in Section 4.5.1 and Section 4.5.2 depending on the value of k .

4.5.3. LTF Box-Behnken designs with orthogonal blocking

Where insufficient homogeneous experimental material is available for all the experimental runs it become desirable to run them blocks. Where possible it is desirable to achieve orthogonal blocking, that is to arrange the runs such that the block contrasts are uncorrelated with all the estimates of the coefficients in the second-order model (Box and Behnken, 1960). Box and Behnken illustrate this with the following example:

Table 4.7. Box-Behnken design No.2 (Box and Behnken, 1960).

$$
D = \begin{bmatrix} Block1 \\ Block2 \\ Block3 \end{bmatrix} = \left[\begin{array}{rrrr}
x_1 & x_2 & x_3 & x_4 \\
-1 & -1 & 0 & 0 \\
1 & -1 & 0 & 0 \\
-1 & 1 & 0 & 0 \\
1 & 1 & 0 & 0 \\
0 & 0 & -1 & -1 \\
0 & 0 & 1 & -1 \\
0 & 0 & -1 & 1 \\
0 & 0 & 1 & 1 \\
0 & 0 & 0 & 0 \\
\hline
-1 & 0 & 0 & -1 \\
1 & 0 & 0 & -1 \\
-1 & 0 & 0 & 1 \\
1 & 0 & 0 & 1 \\
0 & -1 & -1 & 0 \\
0 & 1 & -1 & 0 \\
0 & -1 & 1 & 0 \\
0 & 1 & 1 & 0 \\
0 & 0 & 0 & 0 \\
\hline
0 & -1 & 0 & -1 \\
0 & 1 & 0 & -1 \\
0 & -1 & 0 & 1 \\
0 & 1 & 0 & 1 \\
-1 & 0 & -1 & 0 \\
1 & 0 & -1 & 0 \\
-1 & 0 & 1 & 0 \\
1 & 0 & 1 & 0 \\
0 & 0 & 0 & 0
\end{array}\right]
$$

The Box-Behnken design is a rotatable second order design suitable for studying four variables in 27 trials and is capable of being blocked in three sets of nine trials with one center point in each block.

Now we consider Box-Behnken designs with orthogonal blocking in which a common linear trend is assumed over experimental units within each block and each observation is designated to one experimental unit sequentially. We write the model as follows:

$$y_u = \beta_0 + \sum_{i=1}^{v} \beta_i x_{iu} + \sum_{i=1}^{v} \beta_{ii} x_{iu}^2 + \sum_{\substack{i,i'=1 \\ i<i'}}^{v} \beta_{ii'} x_{iu} x_{i'u} + \sum_{m=1}^{b} \delta_m (z_{mu} - \bar{z}_m) + \theta t_u + \varepsilon_u \quad (4.15)$$

$u = 1,2, \ldots, n$, where $\beta_0, \beta_i, \beta_{ii}$ and $\beta_{ii'}$ are unknown parameters, δ_m is coefficient of corresponding block effect z_m , z_{mu} is unity if the u th observation arises from an experimental run in the m th block, θ is the regression coefficient of the common linear trend t over experimental units in each block, and ε_u is a random error.

In matrix notation, we can write

$$\underline{Y} = \underline{1}\beta_0 + X_1\underline{\beta}_1 + X_2\underline{\beta}_2 + X_3\underline{\beta}_3 + Z\underline{\delta} + \underline{T}\theta + \underline{\varepsilon} \quad (4.16)$$

where $\underline{\delta}$ is a $m \times 1$ block effect vector.

Now, we define a linear trend-free Box-Behnken design with orthogonal blocking as follows:

<u>Definition 4.3.</u> A Box-Behnken design with orthogonal blocking under model (4.15) is said to be linear trend-free (LTF) if

$$\sum_{bl.m} x_{iu} t_u = 0, \quad \sum_{bl.m} x_{iu}^2 t_u = 0, \quad \sum_{bl.m} x_{iu} x_{i'u} t_u = 0, \quad (m = 1, \ldots, b) \quad (4.17)$$

The *bl.m* notation indicates that the sum is being taken over the observations in the m th block. The objective then is to construct a run order within blocks such that the design is a linear trend-free Box-Behnken design. The construction methods are the same as those shown in Sections 4.5.1 and 4.5.2. We apply the method of Section 4.5.1 when k = 2 or 3, and the method of Section 4.5.2 when $k \geq 4$.

Example 4.5.4

We consider the Box-Behnken design No.2 shown in previous example assuming now that there exists a linear trend over experimental units within each block. The design matrix with a linear trend $\underline{T}$ is as follows:

$$
(D, T) = \begin{bmatrix} Block1 \\ Block2 \\ Block3 \end{bmatrix} =
\begin{array}{c}
\begin{array}{cccccccc} x_1 & x_2 & x_3 & x_4 & z_1 & z_2 & z_3 & t \end{array} \\
\left[\begin{array}{cccccccc}
-1 & -1 & 0 & 0 & 1 & 0 & 0 & -4 \\
1 & -1 & 0 & 0 & 1 & 0 & 0 & -3 \\
-1 & 1 & 0 & 0 & 1 & 0 & 0 & -2 \\
1 & 1 & 0 & 0 & 1 & 0 & 0 & -1 \\
0 & 0 & -1 & -1 & 1 & 0 & 0 & 0 \\
0 & 0 & 1 & -1 & 1 & 0 & 0 & 1 \\
0 & 0 & -1 & 1 & 1 & 0 & 0 & 2 \\
0 & 0 & 1 & 1 & 1 & 0 & 0 & 3 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 4 \\
\hline
-1 & 0 & 0 & -1 & 0 & 1 & 0 & -4 \\
1 & 0 & 0 & -1 & 0 & 1 & 0 & -3 \\
-1 & 0 & 0 & 1 & 0 & 1 & 0 & -2 \\
1 & 0 & 0 & 1 & 0 & 1 & 0 & -1 \\
0 & -1 & -1 & 0 & 0 & 1 & 0 & 0 \\
0 & 1 & -1 & 0 & 0 & 1 & 0 & 1 \\
0 & -1 & 1 & 0 & 0 & 1 & 0 & 2 \\
0 & 1 & 1 & 0 & 0 & 1 & 0 & 3 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 4 \\
\hline
0 & -1 & 0 & -1 & 0 & 0 & 1 & -4 \\
0 & 1 & 0 & -1 & 0 & 0 & 1 & -3 \\
0 & -1 & 0 & 1 & 0 & 0 & 1 & -2 \\
0 & 1 & 0 & 1 & 0 & 0 & 1 & -1 \\
-1 & 0 & -1 & 0 & 0 & 0 & 1 & 0 \\
1 & 0 & -1 & 0 & 0 & 0 & 1 & 1 \\
-1 & 0 & 1 & 0 & 0 & 0 & 1 & 2 \\
1 & 0 & 1 & 0 & 0 & 0 & 1 & 3 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 4
\end{array}\right]
\end{array}
$$

We follow the method 4.5.1 to find a run order to be linear trend-free since $k=2$.

By step 1, we put a center point within each block on the middle of the experimental units whose linear trend value is 0. Then, we obtain run orders as follows:

$$(D, T) = \begin{bmatrix} Block1 \\ Block2 \\ Block3 \end{bmatrix} = \begin{array}{c} \begin{array}{cccccccc} x_1 & x_2 & x_3 & x_4 & z_1 & z_2 & z_3 & t \end{array} \\ \left[\begin{array}{cccccccc}
-1 & -1 & 0 & 0 & 1 & 0 & 0 & -4 \\
1 & -1 & 0 & 0 & 1 & 0 & 0 & -3 \\
-1 & 1 & 0 & 0 & 1 & 0 & 0 & -2 \\
1 & 1 & 0 & 0 & 1 & 0 & 0 & -1 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & -1 & -1 & 1 & 0 & 0 & 1 \\
0 & 0 & 1 & -1 & 1 & 0 & 0 & 2 \\
0 & 0 & -1 & 1 & 1 & 0 & 0 & 3 \\
0 & 0 & 1 & 1 & 1 & 0 & 0 & 4 \\
\hline
-1 & 0 & 0 & -1 & 0 & 1 & 0 & -4 \\
1 & 0 & 0 & -1 & 0 & 1 & 0 & -3 \\
-1 & 0 & 0 & 1 & 0 & 1 & 0 & -2 \\
1 & 0 & 0 & 1 & 0 & 1 & 0 & -1 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & -1 & -1 & 0 & 0 & 1 & 0 & 1 \\
0 & 1 & -1 & 0 & 0 & 1 & 0 & 2 \\
0 & -1 & 1 & 0 & 0 & 1 & 0 & 3 \\
0 & 1 & 1 & 0 & 0 & 1 & 0 & 4 \\
\hline
0 & -1 & 0 & -1 & 0 & 0 & 1 & -4 \\
0 & 1 & 0 & -1 & 0 & 0 & 1 & -3 \\
0 & -1 & 0 & 1 & 0 & 0 & 1 & -2 \\
0 & 1 & 0 & 1 & 0 & 0 & 1 & -1 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
-1 & 0 & -1 & 0 & 0 & 0 & 1 & 1 \\
1 & 0 & -1 & 0 & 0 & 0 & 1 & 2 \\
-1 & 0 & 1 & 0 & 0 & 0 & 1 & 3 \\
1 & 0 & 1 & 0 & 0 & 0 & 1 & 4
\end{array}\right] \end{array}$$

Here, we consider the first block to find a run order to be linear trend-free. the first block can be written as

$$Block1 = \begin{array}{c} \begin{matrix} x_1 & x_2 & x_3 & x_4 \end{matrix} \\ \begin{bmatrix} -1 & -1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & -1 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & -1 & 1 \\ 0 & 0 & 1 & 1 \end{bmatrix} \end{array}$$

By step 2, we have 2^2 cases for first block to arrange.

$$Block1(D_1) = \begin{array}{c} \begin{matrix} x_1 & x_2 & x_3 & x_4 \end{matrix} \\ \begin{bmatrix} -1 & -1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & -1 & -1 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 1 \\ 0 & 0 & 1 & 1 \\ -1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{bmatrix} \end{array}, \quad Block1(D_2) = \begin{array}{c} \begin{matrix} x_1 & x_2 & x_3 & x_4 \end{matrix} \\ \begin{bmatrix} -1 & -1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & -1 & 1 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & -1 \\ 0 & 0 & 1 & -1 \\ -1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{bmatrix} \end{array}, \quad \begin{array}{c} \underline{c} \\ -c_4 \\ -c_3 \\ -c_2 \\ -c_1 \\ \\ c_1 \\ c_2 \\ c_3 \\ c_4 \end{array}$$

$$Block1(D_3) = \begin{array}{c} \begin{array}{cccc} x_1 & x_2 & x_3 & x_4 \end{array} \\ \begin{bmatrix} -1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & -1 & -1 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 1 \\ 0 & 0 & 1 & 1 \\ -1 & -1 & 0 & 0 \\ 1 & -1 & 0 & 0 \end{bmatrix} \end{array}, \quad Block1(D_4) = \begin{array}{c} \begin{array}{cccc} x_1 & x_2 & x_3 & x_4 \end{array} \\ \begin{bmatrix} -1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & -1 \\ 0 & 0 & 1 & -1 \\ -1 & -1 & 0 & 0 \\ 1 & -1 & 0 & 0 \end{bmatrix} \end{array}, \quad \begin{array}{c} \underline{C} \\ -c_4 \\ -c_3 \\ -c_2 \\ -c_1 \\ \\ c_1 \\ c_2 \\ c_3 \\ c_4 \end{array}$$

We can see that the all cases $Block1(D_1)$, $Block1(D_2)$, $Block1(D_3)$ and $Block1(D_4)$ will not satisfy the equations $\underline{x}_2^{+\prime}\underline{C}^+ = 0$, $\underline{x}_4^{+\prime}\underline{C}^+ = 0$, since $\underline{x}_2^+$, $\underline{x}_4^+$ consist of 1 and 0, or -1 and 0 due to the fact that all elements of $\underline{C}^+$ take positive integer values, ranging from 1 to 4. So, in this design, there does not exist a LTF Box-Behnken design with orthogonal blocking.

4.6. Conclusions

When a linear trend exists over experimental units in the Box-Behnken designs, we use two different methods for constructing LTF Box-Behnken designs, depending on the value of k . We apply the method of Section 4.5.1 when $k = 2$ or 3, and the method of Section 4.5.2 when $k \geq 4$. We then have the following results:

(i) For k = 2 or 3, we can generally but not always find a LTF Box-Behnken design using the construcion method first described in Section 4.4.

(ii) For $k \geq 4$, there always exist LTF Box-Behnken designs.

(iii) For Box-Behnken designs with orthogonal blocking, there always exist LTF Box-Behnken designs when $k \geq 4$, however, we have not been able to find arrangements that are linear trend-free within blocks when $k = 2$ or 3.

Chapter 5. Summary

Box-Behnken designs (Box and Behnken, 1960) are a class of three-level incomplete factorial designs for the estimation of parameters in a second-order response surface model. These designs are formed by combining two-level factorial designs with incomplete block designs in a particular manner. Box and Behnken showed how to construct the designs, and illustrated the method with some useful designs of second order.

In Chapter 2, we consider the properties of Box-Behnken design with respect to the estimability of all parameters in a second-order model when we use 2^k full factorials. The design matrix of the Box-Behnken design is expressed as a more general mathematical formulation. We can derive the $X'X$ matrix which contains information about the estimability of the parameters in the second order model. The properties of the design are determined essentially by the properties of the coefficient matrix of the normal equations. Concerning the estimators, we can draw the following conclusions from the $X'X$ matrix:

(i) We get uniformly minimum variance unbiased estimators for the first-order coefficients.

(ii) The rank of $X_2'X_2$ is less than or equal to v , say s, since rank ($\underline{N}\underline{N}'$) $=$ s $\leq v$. This implies that we have s estimable functions among $\beta_{11}, \beta_{22}, \ldots, \beta_{vv}$. So, for all β_{ii} to be estimable the PBIB(m) design has to be chosen such that rank $(\underline{N}\underline{N}') = v$.

(iii) If $\lambda_1, \lambda_2, \ldots, \lambda_m$ are all greater than zero, the mixed quadratic coefficients are all estimable. If $\lambda_\delta = 0$ then all elements $g_{ii', ii'} = 0$ corresponding to those treatments i, i' which are δ -th associates, and this implies that the corresponding parameters $\beta_{ii'}$ are not estimable. So, for all $\beta_{ii'}$ $(i < i')$ to be estimable the PBIB(m) design has to be chosen such that all $\lambda_\gamma > 0$ $(\gamma = 1, 2, \ldots, m)$.

In Chapter 3, we consider the properties of Box-Behnken design when we use 2^{k-l} fractional factorials. One practical difficulty with the Box-Behnken design, using an incomplete block design together with the full 2^k factorial, is that the number of design points increases rapidly as k, the block size increases. Instead of using a full factorial, Box and Behnken (1960) advocate using a 2^{k-l} fractional factorial, hence reducing the number of design points from $b2^k + 1$ to $b2^{k-l} + 1$.

We first consider the smallest fraction which is a main effect plan or resolution III design. The basic property of a resolution III design is that main effects are confounded with two-factor interactions. A consequence of this is that for the coefficient matrix the elements of X'_1X_3 are no longer 0 and the off-diagonal elements of X'_3X_3 are not 0. Thus, using a resolution III design instead of the full factorial does alter the properties of the estimators in the sense that the estimates of the first-order coefficients and the estimates of the mixed quadratic coefficients are no longer uncorrelated, and the estimates of the mixed quadratic coefficients are no longer uncorrelated with each other.

Next we consider using a resolution IV design, in which two-factor interactions are confounded with each other. A consequence of this is that X'_3X_3 is not a diagonal matrix. From the form of the $X'X$ matrix we can see that the estimates of the first-order coefficients and the pure qudratic coefficients have the same properties as those with the full factorial. But the estimates of the mixed quadratic coefficients do not have the same property as those with the full factorial since X'_3X_3 is no longer diagonal. In addition, for some PBIB designs X'_3X_3 is less than full rank. This means that for some Box-Behnken designs even when all $\lambda_\gamma > 0$ we may not be able to estimate all mixed quadratic coefficients. Thus it may not be advisible to use a resolution IV design. But for some Box-Behnken designs with PBIB(2) when $\lambda_1 > 0$, $\lambda_2 > 0$, X'_3X_3 is of full rank, which implies that all mixed quadratic coefficients are estimable. Using fractional factorials of resolution V or higher leads to the same form of $X'X$ as for the full factorial, except that 2^k is replaced by 2^{k-l} . Thus, the estimates of all parameters have the same properties as for the full factorial.

In Chapter 4, we are first concerned with Box-Behnken designs using 2^k full factorials in which treatments are applied to experimental units (plots) sequentially in time or space and in which there may exist a linear trend effect. For this situation, the objective is to obtain a linear trend-free Box-Behnken design so that the estimates of the first-order coefficients, the pure quadratic coefficients, and the mixed quadratic coefficients are not affected by such a trend. We take advantage of the symmetric property of the second order terms (pure quadratic terms and the two-factor interactions) and anti-symmetric property of the main effect contrasts of the 2^k factorials in order to construct a LTF Box-Behnken design by putting a center point on the middle of the experimental units associated with the 0-value of the linear trend, and placing the halves of each B_i, $i = 1,2, \ldots , b$ symmetrically with respect to the center point since the structure of the Box-Behnken designs is based on the 2^k factorial designs. We use two different methods for constructing LTF Box-Behnken designs, depending on the value of k. We apply the method of Section 4.5.1 when $k = 2$ or 3, and the method of Section 4.5.2 when $k \geq 4$. We then have the following results:

(i) For $k = 2$ or 3, it may not always be possible to find linear trend-free Box-Behnken designs.

(ii) For $k \geq 4$, there always exist LTF Box-Behnken designs.

We next consider Box-Behnken designs with orthogonal blocking in which a common linear trend is assumed over experimental units within each block and each observation is designated to one experimental unit sequentially. The objective then is to construct a run order within blocks such that the design is a linear trend-free Box-Behnken design. The construction methods are the same as those shown in Sections 4.5.1 and 4.5.2. For Box-Behnken designs with orthogonal blocking, we always find linear trend-free Box-Behnken designs when $k \geq 4$, however, we have not been able to find arrangements that are linear trend-free within blocks when $k = 2$ or 3.

The following topics require further research:

(i) For Box-Behnken designs with orthogonal blocking and $k = 2$ or 3 we want to find run orders within blocks such that the design is a linear trend-free Box-Behnken design.

(ii) In addition to linear trends we may also want to include quadratic trends and construct Box-Behnken designs which are both linear and quadratic trend-free.

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Appendix. The modified LINDO Program

The computer program LINDO (Linear, INteractive, and Discrete Optimizer) was develpoed by Schrage (1981) and updated as recently as 1991 (Release 5.0). It is an interactive linear, quadratic, and integer programming system designed for maximizing or minimizing linear objective functions subject to several linear constraints of equality or/and inequality. In order to use this program in the context of Chapter 4, i.e. to solve equations like (4.13), several modification must be made since (i) equations (4.13) do not have a specific objective function to be optimized, and (ii) the solution $\underset{\sim}{C}^{+} = (c_1, c_2, \dots, c_6)'$ has to be such that the c_i, $i = 1,2, \dots, b2^{k-1}$ are distinct integer values between 1 and $b2^{k-1}$.

To solve linear equations like (4.13), first we assign a dummy objective function (it can be either a minimization or maximization problem). Then we assign our linear system $\underset{\sim}{x}_1^{+\prime}\underset{\sim}{C}^{+} = 0$, $\underset{\sim}{x}_2^{+\prime}\underset{\sim}{C}^{+} = 0, \dots,$ $\underset{\sim}{x}_v^{+\prime}\underset{\sim}{C}^{+} = 0$ as constraints in the optimization problem. Note that $\sum_{i=1}^{b2^{k-1}} c_i = \dfrac{b2^{k-1}(b2^{k-1}+1)}{2}$ since the solutions c_i are distinct integers from 1 to $b2^{k-1}$. To make the solutions c_i distinct, we use standard assignment technique. Define assignment matrix $\{y_{ij}\}$, $i,j = 1, \dots, b2^{k-1}$ such that $\sum_{j=1}^{b2^{k-1}} y_{ij} = 1$ for all i, $\sum_{i=1}^{b2^{k-1}} y_{ij} = 1$ for all j where y_{ij} 's can only take either 0 or 1. Then, each row and each column of the assignment matrix $\{y_{ij}\}$ has only one nonzero element (i.e., 1). After assignment of y_{ij}, we assign actual integers varying from 1 to $b2^{k-1}$ to the c_i's according to the indicator variables y_{ij}'s such that $c_i = \sum_{j=1}^{b2^{k-1}} j y_{ij}$.

We illustrate the procedure for the specific equations (4.13) with 6 variables and 3 equations since $b2^{k-1} = 6$, $v = 3$. We modify the LINDO program as follows:

```
( 1)  MIN C1 + C2 + C3 + C4 + C5 + C6
      ST
( 2)  -C3 + C4 - C5 + C6 = 0
( 3)  -C1 + C2 + C5 + C6 = 0
( 4)  -C1 - C2 + C3 + C4 = 0
( 5)   C1 + C2 + C3 + C4 + C5 + C6 = 21
( 6)   Y11 + Y12 + Y13 + Y14 + Y15 + Y16 = 1
( 7)   Y21 + Y22 + Y23 + Y24 + Y25 + Y26 = 1
( 8)   Y31 + Y32 + Y33 + Y34 + Y35 + Y36 = 1
( 9)   Y41 + Y42 + Y43 + Y44 + Y45 + Y46 = 1
(10)   Y51 + Y52 + Y53 + Y54 + Y55 + Y56 = 1
(11)   Y61 + Y62 + Y63 + Y64 + Y65 + Y66 = 1
(12)   Y11 + Y21 + Y31 + Y41 + Y51 + Y61 = 1
(13)   Y12 + Y22 + Y32 + Y42 + Y52 + Y62 = 1
(14)   Y13 + Y23 + Y33 + Y43 + Y53 + Y63 = 1
(15)   Y14 + Y24 + Y34 + Y44 + Y54 + Y64 = 1
(16)   Y15 + Y25 + Y35 + Y45 + Y55 + Y65 = 1
(17)   Y16 + Y26 + Y36 + Y46 + Y56 + Y66 = 1
(18)  -Y11 - 2Y12 - 3Y13 - 4Y14 - 5Y15 - 6Y16 + C1 = 0
(19)  -Y21 - 2Y22 - 3Y23 - 4Y24 - 5Y25 - 6Y26 + C2 = 0
```

```
(20)  -Y31 - 2Y32 - 3Y33 - 4Y34 - 5Y35 - 6Y36 + C3 = 0
(21)  -Y41 - 2Y42 - 3Y43 - 4Y44 - 5Y45 - 6Y46 + C4 = 0
(22)  -Y51 - 2Y52 - 3Y53 - 4Y54 - 5Y55 - 6Y56 + C5 = 0
(23)  -Y61 - 2Y62 - 3Y63 - 4Y64 - 5Y65 - 6Y66 + C6 = 0
      END
      INTE Y11
      INTE Y12
      INTE Y13
      INTE Y14
      INTE Y15
      INTE Y16
      INTE Y21
      INTE Y22
      INTE Y23
      INTE Y24
      INTE Y25
      INTE Y26
      INTE Y31
      INTE Y32
      INTE Y33
      INTE Y34
      INTE Y35
      INTE Y36
      INTE Y41
      INTE Y42
      INTE Y43
```

INTE Y44

INTE Y45

INTE Y46

INTE Y51

INTE Y52

INTE Y53

INTE Y54

INTE Y55

INTE Y56

INTE Y61

INTE Y62

INTE Y63

INTE Y64

INTE Y65

INTE Y66

Here, line (1) is a dummy objective function, lines (2)-(4) are constrainsts in actual linear equations, i.e., $\underline{x}_1^{+\prime}\underline{C}^+ = 0$, $\underline{x}_2^{+\prime}\underline{C}^+ = 0$, $\underline{x}_3^{+\prime}\underline{C}^+ = 0$, line (5) means that $\sum_{i=1}^{6} c_i = 21$, lines (6)-(17) dictate standard assignment of 6 rows and 6 columns by using indicator variables x_{ij} such that $\sum_{j=1}^{6} y_{ij} = 1$ for all i , $\sum_{i=1}^{6} y_{ij} = 1$ for all j , and lines (18)-(23) will assign to the c_i actual values varying from 1 to 6 according to non-zero y_{ij} values. INTE defines indicator variables y_{ij} as binary (0 or 1). Then we obtain a solution $\underline{C}^+ = (c_1, c_2, c_3, c_{4,}c_5, c_6)' = (6, 3, 4, 5, 2, 1)'$.

Vita

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