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Construction of Pair-wise Balanced Design

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A new procedure for construction of a pair-wise balanced design with equal replication and un-equal block sizes based on factorial design are presented. Numerical illustration also provided. It was found that the constructed pair-wise balanced design was found to be universal optimal.

Keywords: C-matrix, Balanced Design, Connected, Equal replicated and unequal block sizes, Eigenvalues, Factorial Design.

Introduction

Among all the incomplete block design Balanced Incomplete Block Design (BIBD) is the simply easiest and most suitable incomplete block design in regards of construction and analysis. Because BIBD is binary, connected, proper, equi-replicated, balanced and non orthogonal. However, BIBD is not available for all parameters, because BIBD exist only if

- a) $vr = bk$
- b) $\lambda(v - 1) = r(k - 1)$ and
- c) $b \geq v$

holds true. So in place of BIBD, we need another incomplete block design which is balanced. This type of incomplete block design is called variance balanced; efficiency balanced and pair-wise balanced designs.

In a pair-wise balanced block design, any pair of treatments within the blocks occur equally often. The literature on combinatorial theory contains many

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contributions to the existence and construction of pair-wise balanced designs, including for settings with unequal block sizes.

Bose and Shrikhande (1959a) discussed about the pair-wise balanced design in addition to existence of orthogonal Latin square designs. Bose and Shrikhande (1960a) obtained the various methods for the construction of pair-wise orthogonal sets of Latin square design. However, the detailed discussion and construction on pair-wise balanced design is studied by Bose and Shrikhande (1960a). In other words, we can say that Bose and Shrikhande (1959a, 1959b, 1960a) introduced a general class of incomplete block design which they called pair-wise balanced design of index λ . The pair-wise balanced design also share some of the properties of BIB designs like every pair of treatments occurs together in λ blocks. The concept of pair-wise balanced design is merely the combinatorial interest in block designs. Because with the help of pair-wise balanced design many other incomplete block designs can be constructed. For example, Bose and Shrikhande (1960b) used the pair-wise balanced design in the context of constructing Mutually Orthogonal Latin Square (MOLS). Hedayat and Stufken (1989) showed that the problems of constructing pair-wise balanced designs and variance balanced block designs are equivalent. Effanga, Ugboh, Enang and Eno (2009) developed a non-linear non-preemptive binary integer goal programming model for the construction of D -optimal pair-wise balanced incomplete block designs. The literature on combinatorial theory contains many contributions to the existence and construction of pair-wise balanced designs with un-equal block sizes.

Bose and Shrikhande (1960b) defined pair-wise balanced design as following:

Definition: An arrangement of v treatments in b blocks is defined as pair-wise balanced design of index λ of type $(v; k_1, k_2, \dots, k_m)$ provided

- i) Each set contains (k_1, k_2, \dots, k_m) symbols that are all distinct
- ii) $k_i \leq v; k_i \neq k_j$ and
- iii) every pair of distinct treatments occurs in exactly λ sets of the design.

Further they also showed some of the parametric relation of pair-wise balanced design which is namely:

$$\text{i) } b = \sum_{i=1}^m b_i$$

$$\text{ii) } \lambda v(v-1) = \sum_{i=1}^m b_i k_i (k_i - 1)$$

A characterization of pair-wise balanced design in terms of NN^T matrix can be expressed in the following way.

A block design D is called pair-wise balanced design if all the off diagonal elements of NN^T matrix are same (constant) i.e.,

$$NN^T = (r - \lambda)I_v + \lambda E_{vv} \quad (1)$$

where I_v is an identity matrix of order v and E_{vv} is the unit matrix of order $(v \times v)$.

Methods of Construction

Pair-wise balanced design using 2^n symmetrical factorial design deleting the control treatment and merging all n main effects

Here we discuss the construction of unequal block sizes and equi-replicated binary pair-wise balanced design from symmetrical factorial designs. First of all we will write a lemma without proof.

Lemma. Let us consider a 2^n symmetrical factorial experiment.

- (i) from these 2^n treatment combinations let delete the control treatments.
- (ii) merge all those treatment combinations which represent n main effects and further consider these n merged treatment combinations as one treatment combinations. This way, we have $2^n - n$ treatment combinations
- (iii) finally consider $(2^n - n)$ treatment combinations as the blocks for the required design.

We prove this lemma using following example. Let $n = 3$. The $2^3 = 8$ treatment combinations are

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$$\begin{array}{ccc}
 0 & 0 & 0 \\
 1 & 0 & 0 \\
 0 & 1 & 0 \\
 1 & 1 & 0 \\
 0 & 0 & 1 \\
 1 & 0 & 1 \\
 0 & 1 & 1 \\
 1 & 1 & 1
 \end{array}$$

Delete the control treatment. Next merge all treatment combinations where level of one factor is one while level of other factor is zero. Keep the remaining treatment combinations as such. Finally, the treatment combinations are

$$\begin{array}{ccc}
 1 & 1 & 1 \\
 1 & 1 & 0 \\
 1 & 0 & 1 \\
 0 & 1 & 1 \\
 1 & 1 & 1
 \end{array}$$

Call this matrix as M which is the combinations of $2^n - n$ treatment combinations. The method of constructing pair-wise balanced design is discussed in the following theorem.

Theorem. If there exist 2^n symmetrical factorial experiments then there always exist unequal block sizes, equi-replicated, binary pair-wise balanced design, by deleting the control treatment and merging all the treatment combinations belonging to main effects and then considering these merged n treatment combinations as one, with the following parameters

$$v = n, b = 2^n - n, r = 2^{n-1}, \underline{k} = \left(\underbrace{2, \dots, 2}_{nC_2}; \underbrace{3, \dots, 3}_{nC_3}; \underbrace{n-1, \dots, n-1}_{nC_{n-1}}; n, n \right)' \text{ and } \lambda = 2^{n-2} + 1$$

Proof: Let us consider a 2^n symmetrical factorial experiment. This has 2^n treatment combinations. Consider n factors as rows and 2^n treatment combinations as columns. Now using the above lemma, we have the following incidence matrix N of a design d .

$$N = \begin{bmatrix} 1 & 1 & 1 & 0 & \cdots & \cdots & 0 & 1 \\ 1 & 1 & 0 & 1 & \cdots & \cdots & 1 & 1 \\ 1 & 0 & 1 & 1 & \cdots & \cdots & 1 & 1 \\ 1 & 0 & 0 & 0 & \cdots & \cdots & 1 & 1 \\ 1 & 0 & 0 & 0 & \cdots & \cdots & 1 & 1 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots \\ 1 & 0 & 0 & 0 & \cdots & \cdots & 1 & 1 \\ 1 & 0 & 0 & 0 & \cdots & \cdots & 1 & 1 \end{bmatrix} \quad (2)$$

Since we have n rows and considered these as treatments, obviously $v = n$.

For incidence matrix N , among ${}^n C_2$ columns, in each column element ‘1’ will occur two times and 0 will occur $(n - 2)$ times. Similarly for ${}^n C_3$ columns, element ‘1’ will occur three times and element 0 will occur $(n - 3)$ times in each column, and so on, i.e., for ${}^n C_{n-1}$ columns, element ‘1’ will occur $(n - 1)$ time and element 0 will occur 1 time. Moreover there will be one column whose all elements are unity. Finally one more column, which is obtained by merging n treatment combinations, is having also all elements are ‘1’. Hence numbers of blocks are

$$\begin{aligned} b &= {}^n C_2 + {}^n C_3 + \dots + {}^n C_{n-1} + 1 + 1 \\ &= {}^n C_0 + {}^n C_2 + {}^n C_3 + \dots + {}^n C_{n-1} + {}^n C_n \\ &= {}^n C_0 + {}^n C_1 + {}^n C_2 + {}^n C_3 + \dots + {}^n C_n - {}^n C_1 \end{aligned}$$

Since ${}^n C_0 + {}^n C_2 + {}^n C_3 + \dots + {}^n C_n = 2^n$ and therefore $b = 2^n - {}^n C_1 = 2^n - n$.

Again each row of N contains 2^{n-1} times ‘1’ and $(2^{n-1} - n)$ times “zero” and hence $r = 2^{n-1}$. Obviously block size is

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$$\underline{k} = \left(\underbrace{2, \dots, 2}_{{}^nC_2}; \underbrace{3, \dots, 3}_{{}^nC_3}; \underbrace{n-1, \dots, n-1}_{{}^nC_{n-1}}; n, n \right)'$$

Finally the number of treatments $v = n$, number of blocks $b = 2^n - n$ and the number of replication is $r = 2^{n-1}$.

Using the incidence matrix N shown in (2), we have the following C -matrix.

$$C = \begin{pmatrix} \alpha & \beta & \beta & \beta & \dots & \beta \\ \beta & \alpha & \beta & \beta & \dots & \beta \\ \beta & \beta & \alpha & \beta & \dots & \beta \\ \beta & \beta & \beta & \alpha & \dots & \beta \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \beta & \beta & \beta & \beta & \dots & \alpha \end{pmatrix}_{(vv)} \quad (3)$$

where $\alpha = r - \sum_j \frac{n_{ij}^2}{k_j}$ and $\beta = -\sum_j \frac{n_{ij}n_{ij}}{k_j}$

The eigenvalues of the above C -matrix are obtained as

$$\theta = \alpha \left[\frac{v}{v-1} \right]$$

with multiplicities $(v-1)$. For the design having the incidence matrix N given in equation (2) the NN^T is given below.

$$NN^T = \begin{bmatrix} 2^{n-1} & 2^{n-2} + 1 & \dots & 2^{n-2} + 1 \\ 2^{n-2} + 1 & 2^{n-1} & \dots & 2^{n-2} + 1 \\ \vdots & \vdots & \ddots & \vdots \\ 2^{n-2} + 1 & 2^{n-2} + 1 & \dots & 2^{n-1} \end{bmatrix} \quad (4)$$

In the above matrix all the off diagonal elements are same and it can be expressed

$$(2^{n-1} - 2^{n-2} - 1)I_v + 2^{n-2} + 1E_{vv} \quad (5)$$

Hence it proves that the incidence matrix N in (2) gives unequal block sizes, equi-replicated and binary pair-wise balanced design with parameters

$$v = n, b = 2^n - n, r = 2^{n-1}, \underline{k} = \left(\underbrace{2, \dots, 2}_{{}^nC_2}; \underbrace{3, \dots, 3}_{{}^nC_3}; \underbrace{n-1, \dots, n-1}_{{}^nC_{n-1}}; n, n \right)' \text{ and } \lambda = 2^{n-2} + 1$$

Numerical Example

Let $n = 4$. So the symmetrical factorial design is 2^4 . The incidence matrix using the above lemma is as follows

$$N = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 & 0 & 1 & 1 & 0 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 1 & 0 & 1 \end{bmatrix}_{(4 \times 12)}$$

C -matrix of the above design is obtained as

$$C = \frac{20}{12} \begin{bmatrix} 3 & -1 & -1 & -1 \\ -1 & 3 & -1 & -1 \\ -1 & -1 & 3 & -1 \\ -1 & -1 & -1 & 3 \end{bmatrix}_{(4 \times 4)} \quad (6)$$

The above matrix can be further simplified as

$$C = \frac{80}{12} \left[I_4 - \frac{1}{4} J_4 J_4^T \right] \quad (7)$$

The matrix in (6) is the C -matrix of the block design with non-zero eigenvalue $\theta = \frac{80}{12}$ with multiplicity 3. The NN^T is

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$$NN^T = \begin{bmatrix} 8 & 5 & 5 & 5 \\ 5 & 8 & 5 & 5 \\ 5 & 5 & 8 & 5 \\ 5 & 5 & 5 & 8 \end{bmatrix}_{(4 \times 4)} = 3I_v + 5E_{vv}$$

Obviously this matrix satisfies the conditions of pair-wise balanced design. Hence the resulting design is a pair-wise balanced design with parameters

$$v = 4, b = 12, r = 8 \text{ and } \underline{k} = \left(\underbrace{2, 2, \dots, 2}_{4 \text{ } C_{2\text{-times}}}; \underbrace{3, 3, \dots, 3}_{4 \text{ } C_{3\text{-times}}}; \underbrace{4, 4}_{2\text{-times}} \right)' \text{ and } \lambda = 5.$$

Pair-wise balanced design using 2^n symmetrical factorial design by deleting control and all the main effect treatments

Lemma. Let us consider a 2^n Symmetrical factorial experiment, having 2^n treatment combinations.

Let delete the control treatment as well as all main effects. In result we have $2^n - n - 1$ treatment combinations. Consider this as the blocks of the required design. This we prove with the following example. Let $n = 3$. The $2^3 = 8$ treatment combinations are

0	0	0
1	0	0
0	1	0
1	1	0
0	0	1
1	0	1
0	1	1
1	1	1

Delete control treatment. Next delete all treatment combinations whose level of one factor is one while level of other factor is zero. That is, delete all the main effects. Finally, the treatment combinations are

$$\begin{matrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \\ 1 & 1 & 1 \end{matrix}$$

Call this matrix as M which is the combinations of $(2^n - n - 1)$ treatment combinations. Call this as blocks.

Theorem. If there exist a 2^n symmetrical factorial experiment then there always exist un-equal block sizes, equi-replicated, binary pair-wise balanced design, by deleting the control treatment and all main effects with the parameters

$$v = n, b = 2^n - n - 1, r = 2^{n-1}, \underline{k} = \left(\underbrace{2, \dots, 2}_{{}^nC_2}, \underbrace{3, \dots, 3}_{{}^nC_3}, \underbrace{n-1, \dots, n-1}_{{}^nC_{n-1}}, n \right)' \text{ and } \lambda = 2^{n-2}$$

Proof: Let us consider a 2^n symmetrical factorial experiment. This has 2^n treatment combinations. Consider n factors as rows and $(2^n - n - 1)$ treatment combinations as blocks. Using the above lemma, we have the following incidence matrix of a design d .

$$N = \begin{bmatrix} 1 & 1 & 0 & 1 & \dots & \dots & 0 & 1 \\ 1 & 0 & 1 & 1 & \dots & \dots & 1 & 1 \\ 0 & 1 & 1 & 1 & \dots & \dots & 1 & 1 \\ 0 & 0 & 0 & 0 & \dots & \dots & 1 & 1 \\ 0 & 0 & 0 & 0 & \dots & \dots & 1 & 1 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \ddots & 1 & 1 \\ 0 & 0 & 0 & 0 & \dots & \dots & 1 & 1 \\ 0 & 0 & 0 & 0 & \dots & \dots & 1 & 1 \end{bmatrix} \tag{8}$$

For incidence matrix N , among nC_2 columns, element ‘1’ will occur two times and element 0 will occur $(n - 2)$ times. Similarly for nC_3 columns, element ‘1’ will occur three times and element 0 will occur $(n - 3)$ times in each column and so on i.e. for ${}^nC_{n-1}$ columns, element ‘1’ will occur $(n - 1)$ time and element 0 will occur 1 time. More over there will be one more column whose all elements

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are unity. Hence numbers of blocks are $b = {}^n C_2 + {}^n C_3 + {}^n C_{n-1} + {}^n C_n$. Since ${}^n C_0 + {}^n C_1 + {}^n C_2 + {}^n C_3 + \dots + {}^n C_n$ so $b = (2^n - n - 1)$.

Again each row of N contains $2^{n-1} - 1$ times '1' and n times "zero", so the number of replication is $r = 2^{n-1} - 1$. Since we have considered rows as treatments and hence we have $v = n$ treatments. Similarly columns as blocks and hence $b = 2^n - n - 1$ blocks. Hence

$$\underline{k} = \left(\underbrace{2, \dots, 2}_{{}^n C_2}; \underbrace{3, \dots, 3}_{{}^n C_3}; \underbrace{n-1, \dots, n-1}_{{}^n C_{n-1}}; n \right)'$$

For the design having the incidence matrix N given in equation (8), the NN^T is defined as

$$NN^T = \begin{bmatrix} 2^{n-1} - 1 & 2^{n-2} & \dots & 2^{n-2} \\ 2^{n-2} & 2^{n-1} - 1 & \dots & 2^{n-2} \\ \vdots & \vdots & \ddots & \vdots \\ 2^{n-2} & 2^{n-2} & \dots & 2^{n-1} - 1 \end{bmatrix} \quad (9)$$

In the above matrix all the off diagonal elements are same and it can further be expressed as

$$(2^{n-1} - 2^{n-2})I_v + 2^{n-2}E_{vv} \quad (10)$$

Hence it proves that the resulting design is a unequal block sizes, equi-replicated and binary pair-wise balanced designs with parameters

$$v = n, b = 2^n - n - 1, r = 2^{n-1} - 1, \underline{k} = \left(\underbrace{2, \dots, 2}_{{}^n C_2}; \underbrace{3, \dots, 3}_{{}^n C_3}; \underbrace{n-1, \dots, n-1}_{{}^n C_{n-1}}; n \right)'$$
 and $\lambda = 2^{n-2}$

Numerical Example

In a 2^4 factorial design, after deleting the control treatment and all main effects, the incidence matrix is given as

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

Here $v = n = 4$.

The C -matrix is given by

$$C = \begin{bmatrix} 17/4 & -17/12 & -17/12 & -17/12 \\ -17/12 & 17/4 & -17/12 & -17/12 \\ -17/12 & -17/12 & 17/4 & -17/12 \\ -17/12 & -17/12 & -17/12 & 17/4 \end{bmatrix}$$

The non-zero eigenvalues of the above C -matrix is $17/3$ with multiplicity 3.

The NN^T is

$$NN^T = \begin{bmatrix} 7 & 4 & 4 & 4 \\ 4 & 7 & 4 & 4 \\ 4 & 4 & 7 & 4 \\ 4 & 4 & 4 & 7 \end{bmatrix} = 3I_v + 4E_{vv}$$

Hence the resulting design is a pair-wise balanced design with parameters

$$v = 4, b = 11, r = 7 \text{ and } \underline{k} = \left(\underbrace{2 \ 2 \ 2 \ 2 \ 2 \ 2}_{{}^4C_2} \underbrace{3 \ 3 \ 3 \ 3}_{{}^4C_3} \underbrace{4}_{{}^4C_4} \right)' \text{ having } \lambda = 4$$

Optimal Pair-wise balanced design

A-Optimality: Let d belongs $D(v, b, r, k, \lambda)$ with C_d matrix, where $C_d = R_d - N_d K^{-1} N_d^T$. Design d will be A-Optimal if it maximizes $tr(C_d)$. That is, $tr(C_d) = tr(R_d - N_d K^{-1} N_d^T) = tr(R_d) - tr(N_d K^{-1} N_d^T)$.

For a design d , it can be shown that the sum of the variances of the estimates of all elementary treatment contrast is proportional to the sum of the reciprocals of the non-zero eigenvalues of C .

Let $\theta_1, \theta_2, \theta_3, \dots, \theta_{(v-1)}$ are non-zero eigenvalues. For this design there will be only one non-zero eigenvalues with multiplicities $(v - 1)$ of C_d matrix. That is, $\theta_1 = \theta_2 = \theta_3 = \dots = \theta_{(v-1)} = \theta$ as C -matrix is positive semi-definite. Finally we can say that the design is A-Optimal if

$$\sum_{i=1}^{(v-1)} \frac{1}{\theta_i} \geq \frac{(v-1)^2}{tr(C_d)} \tag{11}$$

D-Optimality: Let $\theta_1, \theta_2, \theta_3, \dots, \theta_{(v-1)}$ are non-zero eigenvalues with multiplicities $(v - 1)$ of C_d matrix of design d . A design is D-Optimal if

$$\prod_{i=1}^{(v-1)} \frac{1}{\theta_i} \leq \prod_{i=1}^{(v-1)} \left(\frac{\sum_{i=1}^{(v-1)} \frac{1}{\theta_i}}{(v-1)} \right) \tag{12}$$

E-Optimality: Let $\theta_1, \theta_2, \theta_3, \dots, \theta_{(v-1)}$ are non-zero eigenvalues with multiplicities $(v - 1)$ of C_d matrix of design d . A design is E-Optimal if

$$Min(\theta_i) \leq \frac{tr(C_d)}{(v-1)} \tag{13}$$

Example: Consider the pair-wise balanced design obtained in the numerical example with parameters $v = 4, b = 12, r = 8, \underline{k} = (2,2,2,2,2,2,3,3,3,3,4,4)$. The trace of C -matrix of pair-wise balanced design comes out as 20 and non-zero eigenvalue of C -matrix is $\theta = \frac{80}{12}$ with multiplicity 3. Here the inequality (11) holds true which is required condition to be A-Optimal

of pair-wise balanced design with equal replication and unequal block sizes and hence pair-wise balanced designs is an A -Optimal.

Again the inequalities in (12) and (13) holds true and hence the pair-wise balanced design is D -Optimal as well as E -Optimal. Since the constructed pair-wise balanced design is A -Optimal, D -Optimal as well as E -Optimal and hence the constructed pair-wise balanced design is the universal optimal.

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