Uniformity of incomplete block designs

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Abstract: Incomplete block designs are a type of experimental design layout that has had widespread use in science and engineering. A balanced incomplete block design (BIB) can be characterized by the balanced arrangement of its design points. In this article, incomplete block designs will be investigated from a new perspective: the perspective of uniformity in distribution of design points. A design is of high uniformity, or low discrepancy, if its design points distribute uniformly over the entire design space. The authors use a general discrepancy measure to prove theoretically that BIBs are the most uniform ones among all binary incomplete block designs.

Keywords: balanced incomplete block design; uniformity; uniform design; discrepancy.


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1 Introduction

Block designs [1,2] are an important type of experimental design originated from agricultural experiments and have wide applications now in design of experiments in sciences and engineering. The purpose of this article is to derive a new uniformity property of this type of design. Suppose that \( n \) treatments are arranged in \( s \) blocks, such that the \( j \)th block contains \( t_j \) experimental units and the \( i \)th treatment appears \( r_i \) times in the entire design, \( i = 1, \ldots, n; j = 1, \ldots, s \). In a complete block design, each of the \( n \) treatments occurs once in every block, and thus \( t_j = n \) for all \( j \), and \( r_i = s \) for all \( i \). In an actual experiment, however, because of various constraints, it may not be possible to assign a trial to every treatment in every block. A block design in which the block size is less than the number of treatments is called an incomplete block design. An incomplete block design in which \( t_j = t \) \(<\) \( n \) and \( r_i = r \) \(<\) \( s \) for all \( i = 1, \ldots, n \) and \( j = 1, \ldots, s \) is denoted by \( IB(n, s, r, t) \). An incomplete block design is called a balanced incomplete block design, denoted by \( BIB(n, s, r, t, \lambda) \) or simply BIB, if treatment levels are binary, no treatment occurs more than once in any block, and every pair of treatments occurs in altogether exactly \( \lambda \) blocks. In a binary incomplete block design \( IB(n, s, r, t) \), the relationship \( nr = st \) is satisfied, and in a \( BIB(n, s, r, t, \lambda) \), in addition the relationship \( r(t-1) = \lambda(n-1) \) is satisfied. The balance in arrangement of a BIB has many well-known advantages. The ‘balance’ criterion can, in fact, be regarded as uniformity of spread of points over the entire experimental region. In this article, BIBs will be investigated from the perspective of uniformity of designs, and a new property of BIBs in terms of discrepancy will be proved.

In recent years, the ‘uniformity’ concept has been applied in design of experiments, especially in designs of computer experiments and fractional factorial designs [3,4], and uniform designs have been applied successfully in the industry. Readers may refer to [5–10] for an introduction, some theoretical results and examples of industrial applications of uniform designs. Some tables of uniform design are available in the web site www.math.hkbu.edu.hk/UniformDesign.

Let \( \mathcal{P} = \{x_1, \ldots, x_n\} \) be a set of \( n \) points in \([0,1]\); and let

\[
F_{\mathcal{P}}(x) = \frac{1}{n} \sum_{i=1}^{n} I(x_i \leq x) \tag{1}
\]

be the distribution function of \( \mathcal{P} \), where \( R(A) \), denotes the indicator function of the set \( A \), and the last inequality is with respect to componentwise order. The well-known \( L_2 \) discrepancy of \( \mathcal{P} \) [11] is defined as

\[
D_2(\mathcal{P}) = \left\{ \int_{[0,1]} \left| F_{\mathcal{P}}(x) - F(x) \right|^2 \, dx \right\}^{1/2},
\]

where \( F(x) \) is the distribution function of the continuous uniform distribution on \([0,1]\). This discrepancy is a measure of uniformity of the distribution of points in \( \mathcal{P} \), since the closer \( F_{\mathcal{P}}(x) \) to \( F(x) \), the smaller the value \( D_2(\mathcal{P}) \).

The \( L_2 \) discrepancy, however, has its disadvantages. For example, it relies heavily on the origin since both \( F_{\mathcal{P}}(x) \) and \( F(x) \) are defined in terms of the origin, and it is not invariant with respect to reflection, that is, for a general \( \mathcal{P} \) the value of \( D_2(\mathcal{P}) \) changes...
when the points in \( P \) are reflected about the plane \( x_k = \frac{1}{2} \) \((k = 1, \ldots, s)\). To overcome the disadvantages, [12] proposed several other discrepancies such as the centred \( L_2 \) discrepancy \( CD_2(P) \), the symmetric \( L_2 \) discrepancy \( SD_2(P) \), the unanchored \( L_2 \) discrepancy \( UD_2(P) \), and the wrap-around \( L_2 \) discrepancy \( WD_2(P) \). Readers are referred to [12–14] for the precise definitions of these discrepancies.

The objective of this article is to characterize the BIB by a minimum discrepancy criterion. Using a general discrepancy measure, the authors show that the BIB is the most uniform one among all binary incomplete block designs with the same parameters \( n, s, r \) and \( t \).

In the Section 2, the authors shall extend the definition of discrepancy from the cube \([0,1]^s\) to any measurable set \( X \) in \( \mathbb{R}^s \), and use a reproducing kernel in Hilbert space to define a discrepancy which can be used to measure the uniformity of binary incomplete block designs. This discrepancy can be applied no matter whether \( X \) is continuous or discrete, and it includes several other known discrepancies as special cases. In Section 3, the BIB will be characterized in term of this discrepancy; more precisely, it will be shown that the lower bound of the discrepancy is attained by the BIB.

### 2 Discrepancy measure of block designs

Let \( X \) be a measurable set in \( \mathbb{R}^s \). A function \( K(x, w) \) is a reproducing kernel for a Hilbert space if it is symmetric in its arguments and nonnegative definite, that is,

\[
K(x, w) = K(w, x), \quad \text{for any } x, w \in X
\]  

(2)

and

\[
\sum_{i,j=1}^N a_i a_j K(x_i, x_j) \geq 0, \quad \text{for any } a_i, a_j \in \mathbb{R}, x_i, x_j \in X, \ N = 1, 2, \ldots
\]  

(3)

For the detailed theory and discussions of reproducing kernels, readers may refer to Ref. [15,16]. Let \( F_x \) denote the distribution function of \( X \), \( P = \{z_1, \ldots, z_n\} \subseteq X \) be a set of points, and \( F_P \) denote the distribution function of \( P \) as defined by (1). For a reproducing kernel \( K(x, w) \), a discrepancy of \( P \) [17] is defined by

\[
D(P; K) = \left\{ \int_{X^s} K(x, w) \, d[F_x(x) - F_p(x)] \, d[F_x(w) - F_p(w)] \right\}^{1/2}
\]

\[
= \left\{ \int_{X^s} K(x, w) dF_x(x) dF_x(w) - \frac{2}{n^2} \sum_{z \in P} K(z, z') \int_{X^s} K(x, z) dF_x(x) + \frac{1}{n^2} \sum_{z \in P} K(z, z') \right\}^{1/2}
\]

A small value of \( D(P; K) \) indicates that the distribution of \( P \) is close to the uniform distribution on \( X \). The discrepancy \( D(P; K) \) includes several other discrepancies as special cases. When \( X = [0,1]^s \), \( F_x(x) = x_1 \cdots x_s \) and \( K(x, w) = \prod_{i=1}^s [1 - \max(x_i, w_i)] \), the discrepancy \( D(P; K) \) reduces to the \( L_2 \) discrepancy \( D_2(P) \) [17]. For other specific
forms of $K(x, w)$, the discrepancy $D(P, K)$ reduces to respectively the centred
$L_2$ discrepancy $CD_2(P)$, the symmetric $L_2$ discrepancy $SD_2(P)$, the unanchored $L_2$
discrepancy $UD_2(P)$, and the wrap-around $L_2$ discrepancy $WD_2(P)$ [18].

Let $Z = (z_{ij})_{n \times s}$ be the incidence matrix of a binary incomplete block design, where
$z_{ij}$ is 1 if the $i$th treatment appears in the $j$th block, and is 0 otherwise. Regard the $s$
blocks as $s$ factors each having two levels, 0 and 1, and regard each allocation of
treatments to these $s$ blocks as a point with elements 0 and 1, where 1 means that the
treatment appears in the corresponding block and 0 means it does not. Then the $n$ points
of a binary incomplete block design correspond to the $n$ rows of the incidence matrix $Z$.

Let $X_d = \{0, 1\}^s$ denote the collection of all possible level combinations of the $s$ blocks.

Note that

\begin{equation}
\sum_{j=1}^{s} z_{ij} = r, \quad \text{for all } i = 1, \ldots, n, \quad (4)
\end{equation}

\begin{equation}
\sum_{i=1}^{n} z_{ij} = t, \quad \text{for all } j = 1, \ldots, s. \quad (5)
\end{equation}

Allocations of $n$ treatments to $s$ blocks can be carried out by selecting $n$ points in the
discrete domain $X_d$ under the above constraints (4) and (5). Let $F_{x_d}$ be the uniform
distribution function defined on the discrete set $X_d$. For a function $K^*(x, w)$ defined for
$x, w = 0,1$ such that

\begin{equation}
K^*(0, 0) = K^*(1, 1) = a > K^*(0, 1) = K^*(0, 1) = b > 0, \quad (6)
\end{equation}

define the reproducing kernel

\begin{equation}
K_d(x, w) = \prod_{k=1}^{n} K^*(x^k, w^k), \quad \text{for any } x, w \in X_d, \quad (7)
\end{equation}

and use the corresponding discrete discrepancy $D(Z; K_d)$ as a measure of uniformity of
a binary incomplete block design with incidence matrix $Z$. The condition $a > b > 0$
guarantees that all eigen values of the matrix $[K(x_i, x_j)]_{i,j=1,\ldots,n}$ are positive so that
this matrix is positive definite and condition (3) is satisfied. Let $n_{yi}^0$ be the number of
$(l, h)$-pairs in points $z_i$ and $z_j$ ($i \neq j$) for $l, h = 0, 1$, so that $n_{yi}^{01}$ is the number of blocks in
which the pair of treatments $i$ and $j$ appears together. Then for the incidence matrix of a
binary incomplete block design, we have $n_{yi}^{10} = n_{yi}^{01} = 0$, and

\begin{equation}
n_{yi}^{11} + n_{yi}^{10} = n_{yi}^{01} + n_{yi}^{00} = r, \quad (8)
\end{equation}

\begin{equation}
n_{yi}^{11} + n_{yi}^{10} = n_{yi}^{01} + n_{yi}^{00} = s. \quad (9)
\end{equation}
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From (6)–(9) we obtain

\[ K_d(z_i, z_j) = \prod_{z'_i = z'_j} K^*(z'_i, z'_j) \prod_{z'_i \neq z'_j} K^*(z'_i, z'_j) \]

\[ = a^{n-i} b^{n-j} \left( \frac{b}{a} \right)^{2r} \left( \frac{a}{b} \right)^{2s} \]

It is not difficult to prove that

\[ \int_{x_i} K_d(x, w) dF_X(x) dF_X(w) = \left( \frac{a + b}{2} \right)^{2r} \left( \frac{b}{a} \right) \sum_{i,j \neq j} K_d(x, z) dF_X(x). \]

Thus, we obtain the following Theorem 1.

**Theorem 1** Let Z be the incidence matrix of a binary incomplete block design IB(n, s, r, t). For the kernel defined by (6) and (7), the square discrete discrepancy of Z is

\[ D^2(Z, K_d) = - \left( \frac{a + b}{2} \right)^{2r} + \frac{a^n}{n} - \frac{a^r}{a^r} \left( \frac{b}{a} \right)^{2s} \sum_{i,j \neq j} \left( \frac{a}{b} \right)^{2s}. \] 

(10)

3 Uniformity of BIB

**Theorem 2** Let Z be the incidence matrix of a binary incomplete block design IB(n, s, r, t). Then

\[ D^2(Z, K_d) \geq - \left( \frac{a + b}{2} \right)^{2r} + \frac{a^n}{n} - \frac{a^r}{a^r} \left( \frac{b}{a} \right)^{2s} \sum_{i,j \neq j} \left( \frac{a}{b} \right)^{2s} \]

(11)

where \( \lambda = r(t - 1)/(n - 1) \), and the lower bound of \( D^2(Z, K_d) \) given by the right hand side of (11) can be achieved if and only if \( \lambda \) is a positive integer and every pair of treatments appears in altogether \( \lambda \) blocks, i.e. the design is a BIB(n, s, r, t, \( \lambda \)).

**Proof.** For a binary incomplete block design IB(n, s, r, t), it is obvious that for each fixed \( i = 1, \ldots, n \), we have

\[ \sum_{j \neq j} n_{ij}^1 = r(t - 1). \]

Since geometric mean does not exceed arithmetic mean, we have

\[ \frac{\sum_{i,j \neq j} \left( \frac{a}{b} \right)^{2s}}{n(n - 1)} \geq \left( \prod_{i,j \neq j} \left( \frac{a}{b} \right)^{2s} \right)^{1/n(n - 1)} = \left( \frac{a}{b} \right)^{\frac{2s}{n(n - 1)}}, \]

and the last but one equality holds if and only if all the \( n_{ij}^1 \)'s for \( i \neq j \) are equal to the positive integer \( \lambda = r(t - 1)/(n - 1) \), i.e., every pair of treatments appears altogether in \( \lambda \) blocks, which means that the design is a BIB(n, s, r, t, \( \lambda \)). Thus (11) follows and the proof of the theorem is completed.
Theorem 2 shows that for a BIB\((n, s, r, t, \lambda)\), the lower bound of \(D^2(Z; K_d)\) is attained, and thus BIB\((n, s, r, t, \lambda)\)’s are the most uniform ones among all IB\((n, s, r, t)\)’s. Note that this conclusion holds for a wide range of discrepancies in which the kernel satisfies (6) and (7).

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