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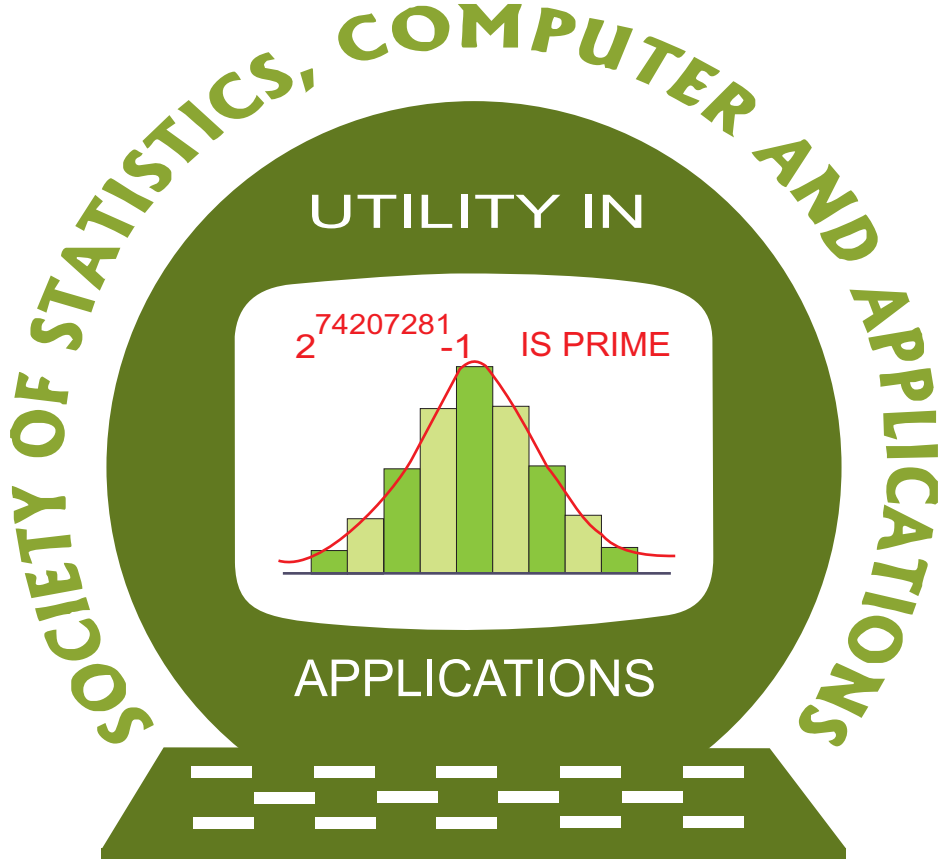

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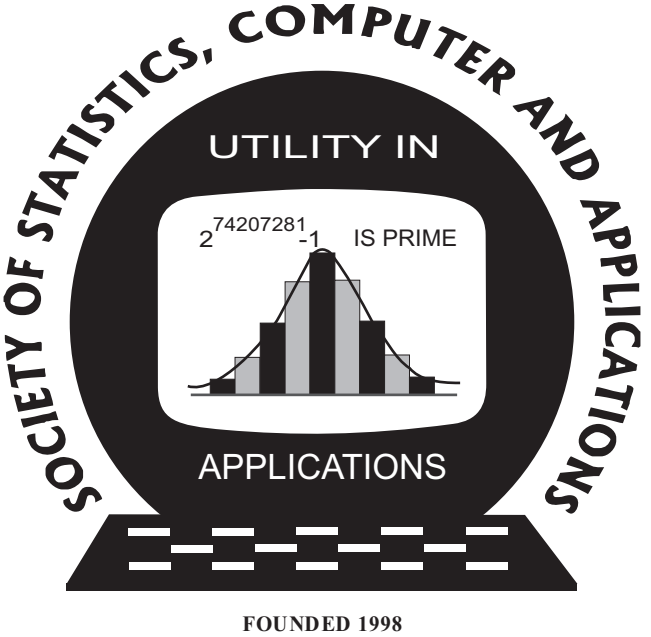

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Row-Column Partial Triallel Cross Designs

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Abstract

In the present paper we are presenting three series of row-column design for partial triallel cross which have been obtained through row- column designs of complete diallel cross method (4). These designs require only $p\,(p-1)/2$ experimental units. *i.e.,* $1/(p-2)^{th}$ crosses in comparison to complete triallel cross designs. These designs can be used to improve the quantitative traits of economic and nutritional importance in crops and animals. It has been established that the three-way hybrids are more stable than pure lines and single cross hybrids and exhibits individual as well as population buffering mechanisms because of the genetic base.

Key words: Row-column design, partial triallel cross, mating design.

1. Introduction

Mating design involving multi–allele cross $m\ (\geq 2)$ lines play very important role to study the genetic properties of a set of inbred lines in plant breeding experiments. Most commonly used mating designs are diallel or a two-way cross $(m = 2)$. Suppose there are p inbred lines and it is desired to perform a diallel cross experiment involving $v = p(p-1)/2$ crosses of the type $(i \times j) = (j \times i)$ for $i, j = 1,2,\ldots,p$, this type of mating design is called complete diallel cross (CDC) method (4) of Griffing (1956) . When we arrange these $v = p(p-1)/2$ crosses in row-column set up the mating design becomes row-column design for CDC method (4).

Triallel crosses form an important class of mating designs, which are used for studying the genetic properties of a set of inbred lines in plant breeding experiments. For p inbred lines, the number of different crosses for a complete triallel experiment is ${}^{p}C_{3} = p(p-1)(p-2)/2$ of the type $(i \times j) \times k, i \neq j \neq k = 0,1,2,\ldots,p-1$. Rawlings and Cockerham (1962) were the first to introduce mating designs for triallel crosses. Triallel cross (TC) experiments are generally conducted using a completely randomized design (CRD) or a randomized complete block (RCB) design as environmental design involving ${}^{p}C_{3}$ crosses.

Even with a moderate number of parents, say $p = 10$, in a TC experiment, the number of crosses becomes unmanageable to be accommodated in homogeneous blocks. For such situations, Hinkelmann (1965) developed partial triallel crosses (PTC) involving only a sample of all possible crosses by establishing a correspondence between PTC and generalized

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partially balanced incomplete block designs (GPBIBD). Ponnuswamy and Srinivasan (1991) and Subbarayan (1992) obtained PTC using a class of balanced incomplete block (BIB) designs. Let n denote the total number of crosses (experimental units) involved in a triallel experiment. It is desired to compare the lines with respect to their general combining abilities, the specific combining abilities being not included in the model.

Other research workers who contributed in this area are Arora and Aggarwal (1984, 1989), Ceranka *et al*. (1990). More details on TC experiments can be found in Hinkelmann (1975) and Narain (1990).

In this paper we are presenting methods of construction of three series row-column designs for PTC experiments through row-column designs of CDC experiment method (4) of Sharma and Tadesse (2017).

2. Preliminary

Let d be a row-column design with k rows and b columns for CDC method (4) involving p lines and $n = bk$. For the data obtained from d, we postulate the following model.

$$\boldsymbol{y} = \mu + \mathbf{1}_n + \boldsymbol{\Delta}_1'\boldsymbol{g} + \boldsymbol{\Delta}_2'\boldsymbol{\beta} + \boldsymbol{\Delta}_3'\boldsymbol{\gamma} + \boldsymbol{e} \tag{2.1}$$

where $\boldsymbol{y}$ is an $n \times 1$ vector of observed responses, μ is the general mean $\boldsymbol{\beta}$, $\boldsymbol{g}$ and $\boldsymbol{\gamma}$ are column vectors of p gca parameters, k row effects and b column effects, respectively, $\boldsymbol{\Delta}_1'(n \times p)$, $\boldsymbol{\Delta}_2'(n \times k)$, $\boldsymbol{\Delta}_3'(n \times b)$ are the corresponding design matrices, respectively and $\boldsymbol{e}$ denotes the vector of independent random errors having mean $\mathbf{0}$ and covariance matrix $\sigma^2\boldsymbol{I}_n$.

Let $\boldsymbol{N}_{d1} = \boldsymbol{\Delta}_1\boldsymbol{\Delta}_2'$ be the $p \times k$ incidence matrix of lines vs rows and $\boldsymbol{N}_{d2} = \boldsymbol{\Delta}_1\boldsymbol{\Delta}_3'$ be the $p \times b$ incidence matrix of treatments vs columns and $\boldsymbol{\Delta}_2\boldsymbol{\Delta}_3' = \mathbf{1}_k\mathbf{1}_b$. Let r_{dl} denote the number of times the l^{th} cross appears in the design d, $l = 1, 2, \ldots, n_c$ and similarly s_{di} denote the number of times the i^{th} line occurs in design d, $i = 1, \ldots, p$. Under (3.1), it can be shown that the reduced normal equations for estimating the gca effects of lines, after eliminating the effect of rows and columns, in design d are

$$\boldsymbol{C}_d\widehat{\boldsymbol{g}} = \boldsymbol{Q}_d \tag{2.2}$$

where

$$\boldsymbol{C}_d = \boldsymbol{G}_d - \frac{1}{b}\boldsymbol{N}_{d1}\boldsymbol{N}_{d1}' - \frac{1}{k}\boldsymbol{N}_{d2}\boldsymbol{N}_{d2}' + \frac{\boldsymbol{s}_{d1}\boldsymbol{s}_{d1}'}{\boldsymbol{s}_{d1}'\mathbf{1}}$$

and

$$\boldsymbol{Q}_d = \boldsymbol{T} + \frac{1}{b}\boldsymbol{N}_{d1}\boldsymbol{R} - \frac{1}{k}\boldsymbol{N}_{d2}\boldsymbol{C} + \frac{G}{bk}\boldsymbol{s}_{d1}$$

$\boldsymbol{C}_d$ is a $p \times p$ information matrix of the treatments and $\boldsymbol{G}_d = \boldsymbol{\Delta}_1\boldsymbol{\Delta}_1' = (g_{dii'})$, $\boldsymbol{N}_{d1} = \left(n_{dij}\right) \cdot n_{dij}$ is the number of times line i occurs in row j of d, $N_{d2} = n_{di.t}$, $n_{i.t}$ is the number of times the cross i occurs in column t. $\boldsymbol{s}_{d1}$ is the replication vector of lines in design d. $\boldsymbol{Q}$ is a $p \times 1$ vector of adjusted treatments (crosses) total. $\boldsymbol{T}$ is a $p \times 1$ vector of

treatment (line) totals, $\boldsymbol{R}$ is a $k \times 1$ vector of rows totals, $\boldsymbol{C}$ is a $b \times 1$ vector of columns totals, respectively, in design d. G is a grand total of all observations in design d.

Now we will show a connection between row- column CDC designs method (4) and PTC row- column designs through nested balanced incomplete block designs of Preece (1967).

Let us consider a nested balanced incomplete block design d with parameters $v = p, b_1, b_2, k_1, r^*, k_2 = 2$, and t. If we identify the treatments of d as lines of a CDC experiment method (4) and perform crosses among the lines appearing in the same sub block of d and considering these t sub blocks as single block, we get a block design d^* for a CDC experiment method (4) involving p lines with $p(p-1)/2$ crosses, each replicated $r = 2b_2/\{p(p-1)\}$ times in $b = b_1/t$ blocks with block size $k = t\,k_2$.

From the above design we can derive the row-column design d^{**} for CDC experiment method (4), if we consider the arrangement of $p(p-1)/2$ crosses in $b = b_1/t$ blocks and $k = t\,k_2$ rows and each cross is replicated $r = 2b_2/\{p(p-1)\}$ times in arrangement. Such a design $d^{**} \in \boldsymbol{D}_1(p, b, k)$; also, for such a design $n_{d^*ij} = 0$ or 1for $i = 1, 2, \ldots, p$, $j = 1, 2, \ldots, b$ and

$$\boldsymbol{C}_{d^{**}} = (p-1)^{-1}p(p-3)\left[\boldsymbol{I}_p - \left\{\frac{(9p^2-5p-1)}{p^2(p-3)}\right\}\boldsymbol{I}_p\boldsymbol{I}_p'\right] \tag{2.3}$$

A row-column PTC designs can be derived from d^{**} by attaching i^{th} line with each cross in j^{th} column provided i^{th} line does not appear in j^{th} column, where $i = 1, 2, \ldots, p$; $j = 1, 2, \ldots, b$. Hence we get a row-column PTC design d_1 for a PTC experiment involving p lines with $p(p-1)/2$ triallel crosses, each replicated $r = 2b_2/\{p(p-1)\}$ times, and $b = b_1/2$ blocks, each of size $k = 2k_2$. Such a design $d_1 \in D(p, b, k)$; and, for a design d_1, $n_{d^*ij} = 3$ for $i = 1, 2, \ldots, p, j = 1, 2, \ldots, b$ and

$$\boldsymbol{C}_{d1} = \frac{p(p-3)}{(p-1)}\left[\boldsymbol{I}_p - \left\{\frac{4p^2+9p-3}{p^2(p-3)}\right\}\boldsymbol{I}_p\boldsymbol{I}_p'\right] \tag{2.4}$$

The $\boldsymbol{C}_{d1}$ given by (2.4) is completely symmetric.

$$tr(\boldsymbol{C}_{d1}) = p(p-3) \tag{2.5}$$

And using d_1 each elementary contrast among gca effects is estimated with a variance

$$\left[\frac{2(p-1)}{p(p-3)}\right]\sigma^2 \tag{2.6}$$

3. Method of Construction

Series 1: Let $p = 4m + 1, m \geq 1$ be a prime or a prime power and x be a primitive element of the $GF(p)$. Consider the following m initial blocks.

$$\left\{\left(x^i, x^{i+2m}\right), \left(x^{i+m}, x^{i+3m}\right)\right\}, \quad i = 0,1,2, \ldots, m-1$$

As shown by Dey et al. (1986), these initial blocks, when developed in the sense of Bose (1939), give rise to a nested balanced incomplete block design with parameters $v = p = 4m + 1,\ k_1 = 4, b_1 = m(4m + 1), k_2 = 2$. By arranging the above m blocks into single block as given below and developing the single block over $mod(p)$.

$$\begin{bmatrix} (x^i, x^{i+2m}) \\ (x^{i+m}, x^{i+3m}) \end{bmatrix},\ i = 0,1,2, \dots, m-1$$

We obtained an optimal block design for diallel crosses with minimal number of experimental units with parameters $p = 4m + 1,\ b = 4m + 1,\ k = 2m$, and $r = 1$. This diallel cross design can be converted into row-column partial triallel cross design with parameters $p = 4m + 1,\ b = 4m + 1,\ k = 2m$, and $r = 1$ by attaching i^{th} line with the crosses in j^{th} block in which i^{th} line does not appear at all, where $i, j = 1, 2, \dots, 4m + 1$.

Example 1: Let $m = 2$. We get the following two columns.

$$\begin{bmatrix} (1,2) & (x, 2x) \\ (2x + 1, x + 2) & (2x + 2, x + 1) \end{bmatrix}$$

Now we convert the both columns in single column as given below.

$$\begin{bmatrix} (1,2) \\ (2x + 1, x + 2) \\ (x, 2x) \\ (2x + 2, x + 1) \end{bmatrix}$$

where x is a primitive element of $GF(32)$ and the elements of $GF(32)$ are $0, 1, 2, x, x + 1, x + 2,\ 2x, 2x + 1, 2x + 2$. Adding successively the non-zero elements of $GF(32)$ to the contents of the single column, the CDC design method (4) is obtained with parameters $p = 9, b = 9, k = 4$ and $r = 1$, where the lines have been relabeled 1-9, using the correspondence $0 \to 1,\quad 1 \to 2, 2 \to 3, x \to 4, x + 1 \to 5, x + 2 \to 6, 2x \to 7, 2x + 1 \to 8, 2x + 2 \to 9$:

Now attaching the $1, 2, \dots, 9$ elements, respectively, with the crosses of the 9 blocks because these elements do not appear in the respective blocks of the above design. Considering rows as row blocks, we obtain row-column design for triallel cross with parameters $p = 9, b = 9, k = 4$ and $r = 1$, which fulfill the all conditions for PTC design.

The design is given below.

Row-column partial triallel cross design

	B_1	B_2	B_3	B_4	B_5	B_6	B_7	B_8	B_9
R_1	(2 × 3)1	(1 × 3)2	(1 × 2)3	(5 × 6)4	(4 × 5)5	(4 × 5)6	(8 × 9)7	(7 × 9)8	(7 × 8)9
R_2	(6 × 8)1	(4 × 9)2	(5 × 7)3	(3 × 7)4	(3 × 7)5	(1 × 8)6	(3 × 5)7	(1 × 6)8	(2 × 4)9
R_3	(4 × 7)1	(5 × 8)2	(6 × 9)3	(2 × 8)4	(2 × 8)5	(3 × 9)6	(1 × 4)7	(2 × 5)8	(3 × 6)9
R_4	(5 × 9)1	(6 × 7)2	(4 × 8)3	(1 × 9)4	(1 × 9)5	(2 × 7)6	(2 × 6)7	(3 × 4)8	(1 × 5)9

Series 2: Let $p = 6m + 1, m \geq 1$ be a prime or a prime power and x be a primitive element of the Galois field of order p, $GF(p)$. Consider the initial blocks

$$\{(x^i, x^{i+3m}), (x^{i+m}, x^{i+4m}), (x^{i+2m}, x^{i+5m})\}, \quad i = 0,1,2, \dots, m-1$$

Dey et al. (1986) showed that these initial blocks, when developed give a solution of a nested incomplete block design with parameters $v = p = 6m + 1, b_1 = m(6m + 1), k_1 = 6, k_2 = 2, \lambda_2 = 1$.

Now arranging the above initial m blocks into single block as given below and developing $mod(p)$, will yield an optimal CDC design method (4) with parameters $p = 6m + 1, b = 6m + 1, k = 3m$, and $r = 1$.

$$\begin{bmatrix} (x^i, x^{i+3m}) \\ (x^{i+m}, x^{i+4m}) \\ (x^{i+2m}, x^{i+5m}) \end{bmatrix}, \quad i = 0,1,2, \dots, m-1$$

This design can be converted into row-column partial triallel cross design with parameters $p = 6m + 1, k = 3m, b = 6m + 1$ and $r = 1$ by the procedure described above in Series 1.

Example 2: Let $m = 2$. Then we get the following two initial blocks.

$$\begin{bmatrix} (1,12) & (2,11) \\ (4,9) & (8,5) \\ (3,10) & (6,7) \end{bmatrix}$$

Now we arrange these two blocks in a single block as given below.

$$\begin{bmatrix} (1,12) \\ (2,11) \\ (4,9) \\ (8,5) \\ (3,10) \\ (6,7) \end{bmatrix}$$

Now developing the above block $mod(13)$, we obtain optimal CDC design with parameters $p = 13, k = 6, b = 13$ and $r = 1$. Following the procedure of Example 1, we can obtain row-column design for PTC with parameters $p = 13, b = 13, k = 7$ and $r = 1$.
Series3: Let $p = 2m + 1, m \geq 2$ be a prime or a prime power, then cyclically developing the following m columns

$$(0, 2m), (1, 2m-1), (2, 2m-2), \dots, (m-1, m+1)\ mod(2m+1)$$

yields an optimal CDC design method (4) with parameters $p = 2m + 1, k = m, b = 2m + 1$. A row-column PTC design with parameters $p = 2m + 1, b = 2m + 1$, and $k = m$ can be obtained by the procedure described in Example 1.

Example 3: Let $m = 3$. Then $p = 7$ and developing the following columns $mod(7)$

$$\begin{bmatrix}(0,6)\\(1,5)\\(2,4)\end{bmatrix}$$

yields optimal CDC design with parameters $p = 7, b = 7$, and $k = 3$ and $r = 1$. A PTC design with parameters $p = 7, b = 7$, $k = 3$ and $r = 1$ can be obtained by the procedure given in Example 2.

Note: The m columns form a nested balanced incomplete block design with parameters

$$v = p = 2m + 1, b_1 = m, k_1 = m(2m + 1), k_2 = 2, \lambda_2 = 1$$

Block designs for CDC method (4), with $p \leq 13$, which can be obtained from NBIB designs of Morgan et al. (2001), are listed below in Table 2. Using these designs row-column partial triallel cross designs can also be constructed.

Table 1: Block design for complete diallel crosses method (4) with $p \leq 13$ generated by using NBIB designs of Morgan, Preece and Rees (2001)

S. No.	p	b	k	Source
1	7	7	6	MPR 2
2	9	18	4	MPR5w
3	9	9	8	MPR8
4	11	11	5	MPR 14
5	13	39	4	MPR 20w
6	13	26	6	MPR21
7	13	13	12	MP23

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A Combinatorial Arrangement of Six Elements

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Abstract

A combinatorial arrangement of 15 unordered pairs of six elements in 6 x 6 square with empty diagonals and off-diagonal cells having three disjoint unordered pairs, such that in each row and in each column all the 15 unordered pairs occur once only, is presented. This arrangement is called triangular Room square of order six.

Key words: 6 × 6 squares with empty diagonals, triangular designs, Room squares

1. Introduction

Combinatorial arrangements have drawn the attention of mathematicians as long back as Kirkman's School Girl Problem (1850), see Dey (2010), pp.47. Some relevant definitions in the context of the paper follow as:

Block design

An equi-replicate, equi-block size, incomplete block design is an arrangement of v elements into b blocks such that: each block contains k ($<v$) distinct elements and each element occurs in r blocks.

Triangular design

Let there be $v = n(n–1)/2$ elements($n \geq 5$) which are arranged in an $n \times n$ array such that the positions on the principal diagonal are left blank, the $n(n–1)/2$ positions above the principal diagonal are filled with the v elements and the positions below the principal diagonal are also filled with the same v elements in such a manner that the resultant arrangement is symmetric about the principal diagonal. Then, two treatments are called first associates if they belong to the same row or same column of the array, otherwise they are second associates.

Alternatively, a triangular association scheme may be defined as : Let X be a set of n elements, 1,2, . . . , n. Then by $v = n(n–1)/2$ elements are denoted by pairs $(i, j) = (j, i)$, $i \neq j$, $i, j \in X$. Any two elements are first associates if there is an element in common between the pairs,

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otherwise they are second associates. Triangular designs are special class of two associate class partially balanced incomplete block designs.

Resolvable block designs

A block design with parameters v, b, r, k is said to be resolvable, if its blocks can be partitioned into r sets of blocks, each set containing $b|r$ blocks, such that every set contains each treatment precisely once only (see, Dey 2010).

Doubly resolvable designs

Following Stinson (1980) and elsewhere the definition is as follows: Let $R = R_1, R_2, \ldots, R_r$ and $T = T_1, T_2, \ldots, T_r$ be two resolutions of one and the same design. These two resolutions are orthogonal if $|R_i \cap T_j| \leq 1$, $1 \leq i, j \leq r$. When a design has at least two orthogonal resolutions it is called doubly resolvable. Let D be *a* doubly resolvable design with orthogonal resolution classes $R = R_1, R_2, \ldots, R_r$ and $T = T_1, T_2, \ldots, T_r$. Now, form an $r \times r$ array **A**, where the rows are indexed by the elements of R and columns by the elements of T.

The (i, j)-th cell of **A** contains $R_i \cap T_j$. Here, any cell will either be empty or contain a block of D. Obviously this array **A** is row-wise as well as column-wise resolvable.

Here, a combinatorial arrangement of 15 unordered pairs of six elements in 6×6 square with empty diagonals and off-diagonal cells having three disjoint unordered pairs, such that in each row and in each column all the15 unordered pairs occur once only, is presented. This arrangement is called triangular Room square of order six. The results obtained here might be of interest for possible applications in cryptography [see, Chaudhary and Seberry (1998), Zhelezova (2011), Topolova and Zhelezova (2014)]. For terminologies, definitions see Raghavarao and Padgett (2005), Dey (2010).

2. The Arrangement

Given below is an arrangement of 15 unordered pairs of six elements in a 6×6 square with empty diagonals and off-diagonal cells having three disjoint unordered pairs, such that in each row and in each column all the 15 unordered pairs occur once only.

Table.1: 6 × 6 square with empty diagonals

-	(12,34,56)	(15,24,36)	(16,23,45)	(14,26,35)	(13,25,46)
(12,34,56)	-	(13,26,45)	(14,25,36)	(15,23,46)	(16,24,35)
(14,25,36)	(16,23,45)	-	(12,35,46)	(13,24,56)	(15,26,34)
(13,26,45)	(15,24,36)	(12,35,46)	-	(16,25,34)	(14,23,56)
(16,24,35)	(13,25,46)	(14,23,56)	(15,26,34)	-	(12,36,45)
(15,23,46)	(14,26,35)	(16,25,34)	(13,24,56)	(12,36,45)	-

Further by the transformation: 12→1, 13→2, 14→3, 15→4, 16→5, 23→6, 24→7, 25→8, 26→9, 34→10, 35 →11, 36→12, 45→13, 46→14, 56→15, the above arrangement may alternatively be viewed as a doubly resolvable, triangular design with empty diagonals. The parameters of this triangular design are: v =15, r = 6, k = 3, b = 30, n_1 = 8, n_2 = 6, $\lambda_1 = 0$, $\lambda_2 = 2$.

The triangular designs are partially balanced incomplete block designs based on two associate triangular association schemes. For details, see Clatworthy (1973), Dey (2010), Raghavarao and Padgett (2005). Tables of triangular designs may be found in Clatworthy (1973).

A doubly resolvable BIBD (v, 2, 1) is a Room square. There is extensive literature on this topic. A doubly resolvable BIBD (v, k, λ) is a Generalised Room square and vice-versa (Stinson, 2004). Doubly resolvable, BIBD and Group divisible designs are studied by Vanstone (1980). The arrangement obtained above may be known as triangular Room square (TRS) of order six. Analogously, Room Squares based on BIB designs and Group divisible designs may be denoted as BIBRS and GDRS respectively. A special feature of the above triangular Rooms square is that the (i, j)-th cell entry $R_i \cap T_i$ is zero, while $R_i \cap T_j$ is 1.

This triangular design is reported in Clatworthy (1973) as duplicate of T16. A resolvable solution of this triangular design was reported in Sinha (1973). It is not known if the resolvable solution of triangular design T3 given in Sinha and Dey (1982) also has a similar arrangement in 6×6 squares with empty principal diagonal.

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Ratio Type HT Estimators for Negative Adaptive Cluster Double Sampling

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Abstract

When the population is rare and clustered, the traditional sampling design gives the poor estimate of population total/ mean. In this situation, the negative adaptive cluster double sampling (NACDS) design is useful to gather the information. It is assumed that auxiliary information is negatively correlated with study of interest variable and auxiliary information is abundant. Hence, information of interest variable is rare and clustered. Traditional, ratio estimator performs poor. Hence, exponential ratio type Horvitz Thompson (HT) estimator and log ratio type HT estimator is proposed. The performance of these two estimators are compared by using sample survey.

Key words: NACDS; HT Estimator; Ratio Type Estimators; NACS.

1. Introduction

While conducting a sample survey, a number of difficult sampling problems are encountered. One of them is the problem in estimating the population mean/total when it is rare or geographically uneven. If the population of interest is hidden or elusive then it becomes difficult to identify it for sampling. The researcher may find the conventional sampling design such as simple random sampling (SRS), stratified sampling etc. as inadequate for producing data from the sampling units while studying such type of population. If conventional sampling designs are applied to population that are rare and clustered then usually very few units possessing the characteristic of interest are selected in the sample. Even a very large conventional sample would be inadequate in such cases. Due to these reasons researchers have thought about the unconventional sampling designs.

According to Thompson and Seber (1996), designs that can redirect sampling effort during a survey in response to observed values are known as adaptive sampling designs. These designs use

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information gathered during the survey to select the succeeding sampling units. This distinguishes adaptive sampling from conventional sampling designs.

Neyman (1938) introduced two-phase sampling (double sampling). Horvitz and Thompson (1952) provided a general method of dealing with sampling without replacement from a finite universe when variable probabilities of selection are used for the elements remaining prior to each draw. They proposed an unbiased linear estimator of the population total of the variable of interest. An unbiased estimator of the sampling variance of this estimator is also obtained. The above estimator of population total is applicable to one-stage design. The authors presented an extension of this method for two-stage design. But this has a serious disadvantage of the possibility of having negative variance. Murthy (1957) has shown that corresponding to any ordered estimator there exists a more efficient unordered estimator.

Cassel et al. (1977) reviewed adaptive designs under the term informative designs. Thompson and Ramsey (1983) analyzed the situations of adaptive sampling designs. Seber(1986) described the potential importance of adaptive designs for the estimation of animal abundance. Thompson (1987) described the examples analyzed by him and Ramsey (1981). In this paper, they proved a theorem for a non-adaptive design in which the entire sample is selected ahead of time, will be optimum if and only if there is some possible selection of second phase units which is best for every possible outcome of the first phase observations. Särndal and Swensson (1987) have discussed estimation in the case of two-phase sampling and in the case of non-response. In this paper, general results were given for two- phase sampling with emphasis on regression estimation and on the problem of variance estimation. The concept of inclusion probability proportional to size sampling plans excluding adjacent units separated by at most a distance of $m \geq 1$ units is introduced by Mandal (2008).

Thompson (1990, 1991) presented designs in which, whenever the observed value of a selected unit satisfies a condition of interest, additional units are added to the sample from the neighbourhood of that unit. In these designs, the selection procedure depends on observed values of the variable of interest. Latpate et al. (2018 a) evaluated the sample size for adaptive cluster sampling. Medina and Thompson (2004) presented a multi-phase variant of ACS. They combined the ideas of double sampling and ACS. They called this new design as adaptive cluster double sampling. In this design the authors assumed the availability of an inexpensive and easy to measure auxiliary variable.

Latpate and Kshirsagar (2019) proposed negative adaptive cluster sampling (NACS) design. In this design, the variable of interest is negatively correlated with auxiliary variable. The adaptive procedure is used by using auxiliary variable. The condition of adaptation is on the auxiliary variable. The population is rare and clustered for interest variable. Because of negative correlation between interest and auxiliary variable, there is abundance of auxiliary information. It is easy to measure and less costly as compared to interest variable. The networks are formed for the rare occurrence of the auxiliary variable. It means the selected network has abundant information of interest variable. There is substantial expected sample size and cost reduction for the interest variable. Also, the auxiliary information is used at estimation and design stage. They have proposed the modified ratio and regression estimator. Latpate and Kshirsagar (2020) presented the two-stage negative adaptive cluster sampling design. This design is a combination of two-stage cluster sam-

pling and NACS. Also, the modified ratio and regression estimator is proposed. In this design, auxiliary information is used at design and estimation stage.

Latpate and Kshirsagar (2018 b) presented the negative adaptive cluster double sampling (NACDS) design. It is a combination of NACS and double sampling. In this design,they assume that the auxiliary information is easily available and less expensive. The nature of underlined population is rare and patchy. To exploit the auxiliary information at design and estimation stage, auxiliary information must be abundantly available, easy to measure and less costly. The procedure of NACDS is as follows. Let $U = \{u_1, u_2, ..., u_N\}$ be a finite population of N units. Let Y and X be the interest and auxiliary variable respectively. They are known to be highly negatively correlated. Let X_i and $Y_i, i = 1, 2, ..., N$ be the values of X and Y respectively associated with the unit u_i. It is assumed that the information on auxiliary variable can be obtained from all the units selected in the sample. The goal is to estimate the population total of Y, given by $\tau_Y = \sum_{i=1}^{N} Y_i$.

An initial sample of size n units is drawn from the population by using SRSWOR. We denote this initial sample drawn as S_0. From S_0, obtain an adaptive cluster sample S_1 by using the following procedure: Denote the condition of interest with respect to X values by C_X. According to the negative correlation the condition is reversed for adaptation. Now following the procedure given by Thompson (1990), we add the neighbors of the units in S_0 that satisfy the condition C_X. The units to the right, left, above and below a unit are called as the neighbors of that unit. If any of these neighbors satisfy C_X then their neighbors are also added to the sample. This is continued till the neighbors not satisfying C_X are obtained. The units added to the sample S_0 adaptively which satisfy the condition C_X constitute a network. The units added to the sample S_0 adaptively which do not satisfy the condition C_X are called as the edge units. The set of units in a network along with its edge units is called as a cluster. The set of units included in all such clusters is called as an adaptive cluster sample. We denote it by S_1. Thus, indirectly we are assuming that the condition C_X for the additional sampling and a set of neighboring units for each $u_i \in U$ have been defined. Let K denote the number of distinct clusters formed by S_0. Mark the corresponding K clusters in the Y population and drop down the edge units to get K networks. This completes the first phase of the design. From each of these selected networks draw a sample by using SRSWOR. The sizes of these samples may be different. Suppose m_i denotes the number of units selected from the i^{th} selected network. Collection of all these units selected be denoted by S_2. This completes the second phase of sampling design. Now, note the values of X and Y for all the units included in S_2. This data is used to estimate the population parameter. In this design, the X value associated with every unit in the adaptive cluster sample S_1 has to be measured. Hence, the procedure does not control the number of observations on the auxiliary variable, but only the number of observations on the survey variable.

Bahl and Tuteja (1991) proposed the ratio and product type exponential estimators. Using this approach, I proposed the ratio and exponential ratio type HT estimator and log ratio type HT estimators. These estimators are useful to handle the problem of rare/clustered population. Särandal et al.(1992) proposed ratio type estimator. But, this estimator is less precise. These two estimators are compared by using monte carlo simulation method. The sample survey is presented for the comparison purpose. The proposed estimators are presented in section 2. Section 3, the sample survey is conducted by using NACDS. The results and discussion are added in section 4. The concluding remarks are incorporated in section 5.

2. The Proposed Estimators

The first phase sample S_I of size n_0 from population U is drawn by using simple random sampling without replacement and units are added by using Thompson [1990] procedure. The first order inclusion probabilities are as follows:

π_i : probability that unit i is included in $S_I = \sum_{i \in S_I} P(S_I)$
π_{ij} : probability that units i and j is included in $S_I = \sum_{i,j \in S_I} P(S_I)$
with $\pi_{ii} = \pi_i$ and $\pi_i > 0$ for all i and $\pi_{ij} > 0$ for all $i \neq j$.

Again, the second phase sample S_{II} of size n_1 from S_I is drawn by using simple random sampling without replacement. The second order conditional inclusion probabilities are as follows:

$\pi_{i|S_I}$: probability that i^{th} unit is included in S_{II} given $S_I = \sum_{i \in S_{II}} P(S_{II}|S_I)$
$\pi_{ij|S_I}$: probability that i^{th} and j^{th} units is included in S_{II} given $S_I = \sum_{i,j \in S_{II}} P(S_{II}|S_I)$
with $\pi_{ii|S_I} = \pi_{i|S_I}$ and for any S_I, $\pi_{i|S_I} > 0$ for all i and $\pi_{ij|S_I} > 0$ for all $i \neq j$.

The π^* estimator can be expressed as follows (Särandal et al.[1992]).

$$\pi_i^* = \begin{cases} \pi_i & ;if \quad i \in S_I \\ \pi_i \pi_{i|S_I} & ;if \quad i \in S_I \quad and \quad i \in S_{II} \end{cases}$$

and

$$\pi_{ij}^* = \begin{cases} \pi_{ij}\pi_{ij|S_I} & ;if \quad i,j \in S_I \quad and \quad i,j \in S_{II} \\ \pi_{ij}\pi_{i|S_I} & ;if \quad i,j \in S_I \quad and \quad i \in S_{II} \\ \pi_{ij}\pi_{j|S_I} & ;if \quad i,j \in S_I \quad and \quad j \in S_{II} \\ \pi_{ij} & ;if \quad i,j \in S_I \end{cases}$$

The HT estimator for the interest variable Y is,

$(\hat{\tau}_{IIy})_{HT} = \sum_{i \in S_{II}} y_i^*/\pi_i^*$
where, y_i^* the sum of the selected units at the second stage of the networks which includes the i^{th} unit. The HT estimator for the auxiliary variable X at second phase and first phase respectively are,

$(\hat{\tau}_{IIx})_{HT} = \sum_{i \in S_{II}} x_i^*/\pi_i^*$.
where, x_i^* the sum of the selected units at the second stage of the networks which includes the i^{th} unit.

$(\hat{\tau}_{Ix})_{HT} = \sum_{i \in S_I} x_i^*/\pi_i^*$ where, x_i^* the sum of the selected first stage of the networks which includes the i^{th} unit. We assume the large sample approximation to obtain the MSE.
$e_y = \frac{(\hat{\tau}_{IIy})_{HT} - \tau_y}{\tau_y}$
$e_x = \frac{(\hat{\tau}_{IIx})_{HT} - \tau_x}{\tau_x}$
$e_{x'} = \frac{(\hat{\tau}_{Ix})_{HT} - \tau_x}{\tau_x}$
We get
$E(e_y) = E_I(E_{II}(e_y|S_I)) = 0$, $E(e_x) = E_I(E_{II}(e_x|S_I)) = 0$, $E(e_{x'}) = E_I(E_{II}(e_{x'}|S_I)) = 0$;

$V(e_y) = V_I(E_{II}(\frac{(\hat{\tau}_{IIy})_{HT}-\tau_y}{\tau_y}|S_I)) + E_I(V_{II}(\frac{(\hat{\tau}_{IIy})_{HT}-\tau_y}{\tau_y}|S_I))$
$= V_I\big(\frac{(\hat{\tau}_{Iy})_{HT}-\tau_y}{\tau_y}\big) + \frac{1}{2\tau_y^2}E_I\big(\sum\sum_{i\neq j\in S_I}(\pi_{i|S_I}\pi_{j|S_I}-\pi_{ij|S_I})(\frac{y_i}{\pi_i^*}-\frac{y_j}{\pi_j^*})^2\big)$
$= \frac{1}{2\tau_y^2}\big[\sum\sum_{i\neq j\in U}(\pi_i\pi_j-\pi_{ij})(\frac{y_i}{\pi_i}-\frac{y_j}{\pi_j})^2 + E_I\big(\sum\sum_{i\neq j\in S_I}(\pi_{i|S_I}\pi_{j|S_I}-\pi_{ij|S_I})(\frac{y_i}{\pi_i^*}-\frac{y_j}{\pi_j^*})^2\big)\big]$
$V(e_x) = V_I(E_{II}(\frac{(\hat{\tau}_{IIx})_{HT}-\tau_x}{\tau_x}|S_I)) + E_I(V_{II}(\frac{(\hat{\tau}_{IIx})_{HT}-\tau_x}{\tau_x}|S_I))$
$= V_I\big(\frac{(\hat{\tau}_{Ix})_{HT}-\tau_x}{\tau_x}\big) + \frac{1}{2\tau_x^2}E_I\big(\sum\sum_{i\neq j\in S_I}(\pi_{i|S_I}\pi_{j|S_I}-\pi_{ij|S_I})(\frac{x_i}{\pi_i^*}-\frac{x_j}{\pi_j^*})^2\big)$
$= \frac{1}{2\tau_x^2}\big[\sum\sum_{i\neq j\in U}(\pi_i\pi_j-\pi_{ij})(\frac{x_i}{\pi_i}-\frac{x_j}{\pi_j})^2 + E_I\big(\sum\sum_{i\neq j\in S_I}(\pi_{i|S_I}\pi_{j|S_I}-\pi_{ij|S_I})(\frac{x_i}{\pi_i^*}-\frac{x_j}{\pi_j^*})^2\big)\big]$
$V(e_{x'}) = V_I(E_{II}(\frac{(\hat{\tau}_{Ix})_{HT}-\tau_x}{\tau_x}|S_I)) + E_I(V_{II}(\frac{(\hat{\tau}_{Ix})_{HT}-\tau_x}{\tau_x}|S_I))$
$= V_I\big(\frac{(\hat{\tau}_{Ix})_{HT}-\tau_x}{\tau_x}\big)$
$= \frac{1}{2\tau_x^2}\big[\sum\sum_{i\neq j\in U}(\pi_i\pi_j-\pi_{ij})(\frac{x_i}{\pi_i}-\frac{x_j}{\pi_j})^2\big]$
$Cov(e_x,e_y) = Cov_I(E_{II}(\frac{(\hat{\tau}_{IIy})_{HT}-\tau_y}{\tau_y}|S_I), E_{II}(\frac{(\hat{\tau}_{IIx})_{HT}-\tau_x}{\tau_x}|S_I))+$
$E_I(Cov_{II}(\frac{(\hat{\tau}_{IIy})_{HT}-\tau_y}{\tau_y}, \frac{(\hat{\tau}_{IIx})_{HT}-\tau_x}{\tau_x}|S_I))$
$= Cov_I\big(\frac{(\hat{\tau}_{Iy})_{HT}-\tau_y}{\tau_y}, \frac{(\hat{\tau}_{Ix})_{HT}-\tau_x}{\tau_x}\big) + \frac{1}{2\tau_x\tau_y}E_I\big(\sum\sum_{i\neq j\in S_I}(\pi_{i|S_I}\pi_{j|S_I}-\pi_{ij|S_I})(\frac{x_i}{\pi_i^*}-\frac{y_j}{\pi_j^*})^2\big)$
$= \frac{1}{2\tau_x\tau_y}\big[\sum\sum_{i\neq j\in U}(\pi_i\pi_j-\pi_{ij})(\frac{x_i}{\pi_i}-\frac{y_j}{\pi_j})^2 + E_I\big(\sum\sum_{i\neq j\in S_I}(\pi_{i|S_I}\pi_{j|S_I}-\pi_{ij|S_I})(\frac{x_i}{\pi_i^*}-\frac{y_j}{\pi_j^*})^2\big)\big]$
$Cov(e_{x'},e_x) = Cov_I(E_{II}(\frac{(\hat{\tau}_{Ix})_{HT}-\tau_x}{\tau_x}|S_I), E_{II}(\frac{(\hat{\tau}_{IIx})_{HT}-\tau_x}{\tau_x}|S_I))+$
$E_I(Cov_{II}(\frac{(\hat{\tau}_{Ix})_{HT}-\tau_x}{\tau_x}, \frac{(\hat{\tau}_{IIx})_{HT}-\tau_x}{\tau_x}|S_I))$
$= Cov_I\big(\frac{(\hat{\tau}_{Ix})_{HT}-\tau_x}{\tau_x}, \frac{(\hat{\tau}_{Ix})_{HT}-\tau_x}{\tau_x}\big)$
$= \frac{1}{2\tau_x^2}\big[\sum\sum_{i\neq j\in U}(\pi_i\pi_j-\pi_{ij})(\frac{x_i}{\pi_i}-\frac{x_j}{\pi_j})^2$
$Cov(e_{x'},e_y) = Cov_I(E_{II}(\frac{(\hat{\tau}_{Ix})_{HT}-\tau_x}{\tau_x}|S_I), E_{II}(\frac{(\hat{\tau}_{IIy})_{HT}-\tau_y}{\tau_y}|S_I))+$
$E_I(Cov_{II}(\frac{(\hat{\tau}_{Ix})_{HT}-\tau_x}{\tau_x}, \frac{(\hat{\tau}_{IIy})_{HT}-\tau_y}{\tau_y}|S_I))$
$= Cov_I\big(\frac{(\hat{\tau}_{Ix})_{HT}-\tau_x}{\tau_x}, \frac{(\hat{\tau}_{Iy})_{HT}-\tau_y}{\tau_y}\big)$
$= \frac{1}{2\tau_x\tau_y}\big[\sum\sum_{i\neq j\in U}(\pi_i\pi_j-\pi_{ij})(\frac{x_i}{\pi_i}-\frac{y_j}{\pi_j})^2$

(i). Exponential Ratio Type HT Estimator: The exponential ratio type HT estimator for NACDS is as follows.
$\hat{\tau}_{RADE} = (\hat{\tau}_{IIy})_{HT}\ exp\big[\frac{(\hat{\tau}_{Ix})_{HT}-(\hat{\tau}_{IIx})_{HT}}{(\hat{\tau}_{Ix})_{HT}+(\hat{\tau}_{IIx})_{HT}}\big]$

Using the large sample approximation and neglecting the higher order terms we get. $\hat{\tau}_{RADE} = \tau_y\ \big[1+e_y+\frac{1}{2}(e_{x'}-e_x)+\frac{1}{2}(e_ye_{x'}-e_ye_x)-\frac{1}{8}e_{x'}^2+\frac{3}{8}e_x^2-\frac{1}{4}e_{x'}e_x\big]$
$\hat{\tau}_{RADE}$ is a biased estimator.The bias of $\hat{\tau}_{RADE}$ is as follows.
$Bias(\hat{\tau}_{RADE}) = \tau_y\big(\frac{3}{16\tau_x^2}\big[E_I\big(\sum\sum_{i\neq j\in S_I}(\pi_{i|S_I}\pi_{j|S_I}-\pi_{ij|S_I})(\frac{x_i}{\pi_i^*}-\frac{x_j}{\pi_j^*})^2\big)\big]$
$-\frac{1}{4\tau_x\tau_y}\big[E_I\big(\sum\sum_{i\neq j\in S_I}(\pi_{i|S_I}\pi_{j|S_I}-\pi_{ij|S_I})(\frac{x_i}{\pi_i^*}-\frac{y_j}{\pi_j^*})^2\big)\big]\big)$

The mean square error of $\hat{\tau}_{RADE}$ can be expressed as follows.
$MSE(\hat{\tau}_{RADE}) = \tau_y^2\ Var\big[e_y+\frac{1}{2}(e_{x'}-e_x)\big]$
$= \tau_y^2\ E\big[e_y^2+\frac{1}{4}e_{x'}^2-\frac{1}{2}e_{x'}e_x+\frac{1}{4}e_x^2+e_ye_{x'}-e_ye_x\big]$
$MSE(\hat{\tau}_{RADE}) = \tau_y^2\ \big[\frac{1}{2\tau_y^2}\big[\sum\sum_{i\neq j\in U}(\pi_i\pi_j-\pi_{ij})(\frac{y_i}{\pi_i}-\frac{y_j}{\pi_j})^2+E_I\big(\sum\sum_{i\neq j\in S_I}(\pi_{i|S_I}\pi_{j|S_I}-\pi_{ij|S_I})(\frac{y_i}{\pi_i^*}-\frac{y_j}{\pi_j^*})^2\big)\big]\ +\ \frac{1}{8\tau_x^2}\big[\sum\sum_{i\neq j\in U}(\pi_i\pi_j-\pi_{ij})(\frac{x_i}{\pi_i}-\frac{x_j}{\pi_j})^2\big]\ -\ \frac{1}{4\tau_x^2}\big[\sum\sum_{i\neq j\in U}(\pi_i\pi_j-\pi_{ij})(\frac{x_i}{\pi_i}-\frac{x_j}{\pi_j})^2\big]\ +$

$\frac{1}{8\tau_x^2}\big[\sum\sum_{i\neq j\in U}(\pi_i\pi_j-\pi_{ij})(\frac{x_i}{\pi_i}-\frac{x_j}{\pi_j})^2+E_I\big(\sum\sum_{i\neq j\in S_I}(\pi_{i|S_I}\pi_{j|S_I}-\pi_{ij|S_I})(\frac{x_i}{\pi_i^*}-\frac{x_j}{\pi_j^*})^2\big)\big]+$
$\frac{1}{2\tau_x\tau_y}\big[\sum\sum_{i\neq j\in U}(\pi_i\pi_j-\pi_{ij})(\frac{x_i}{\pi_i}-\frac{y_j}{\pi_j})^2\big]-\frac{1}{2\tau_x\tau_y}\big[\sum\sum_{i\neq j\in U}(\pi_i\pi_j-\pi_{ij})(\frac{x_i}{\pi_i}-\frac{y_j}{\pi_j})^2+$
$E_I\big(\sum\sum_{i\neq j\in S_I}(\pi_{i|S_I}\pi_{j|S_I}-\pi_{ij|S_I})(\frac{x_i}{\pi_i^*}-\frac{y_j}{\pi_j^*})^2\big)\big]\big]$

After Simplification, the MSE of $\hat{\tau}_{RADE}$ is,

$MSE(\hat{\tau}_{RADE})=\tau_y^2\ \big[\frac{1}{2\tau_y^2}\big[\sum\sum_{i\neq j\in U}(\pi_i\pi_j-\pi_{ij})(\frac{y_i}{\pi_i}-\frac{y_j}{\pi_j})^2+E_I\big(\sum\sum_{i\neq j\in S_I}(\pi_{i|S_I}\pi_{j|S_I}-\pi_{ij|S_I})(\frac{y_i}{\pi_i^*}-\frac{y_j}{\pi_j^*})^2\big)\big]+\frac{1}{8\tau_x^2}\big[E_I\big(\sum\sum_{i\neq j\in S_I}(\pi_{i|S_I}\pi_{j|S_I}-\pi_{ij|S_I})(\frac{x_i}{\pi_i^*}-\frac{x_j}{\pi_j^*})^2\big)\big]-\frac{1}{2\tau_x\tau_y}\big[E_I\big(\sum\sum_{i\neq j\in S_I}(\pi_{i|S_I}\pi_{j|S_I}-\pi_{ij|S_I})(\frac{x_i}{\pi_i^*}-\frac{y_j}{\pi_j^*})^2\big)\big]\big]$ (1)

(ii). Log Ratio Type HT Estimator: The log ratio type HT estimator for NACDS is as follows.

$\hat{\tau}_{RADL}=(\hat{\tau}_{IIy})_{HT}\big(1+log\big[\frac{(\hat{\tau}_{IIx})_{HT}}{(\hat{\tau}_{Ix})_{HT}}\big]\big)$

Using the large sample approximation and neglecting the higher order terms we get. $\hat{\tau}_{RADL}=\tau_y(1+e_y-e_{x'}+e_x+e_{x'}^2-e_xe_{x'}-e_{x'}e_y+e_xe_y)$

$\hat{\tau}_{RADL}$ is a biased estimator. The bias of $\hat{\tau}_{RADL}$ is as follows.

$Bias(\hat{\tau}_{RADL})=\tau_y\big(\frac{1}{2\tau_x^2}\big[\sum\sum_{i\neq j\in U}(\pi_i\pi_j-\pi_{ij})(\frac{x_i}{\pi_i}-\frac{x_j}{\pi_j})^2\big]+\frac{1}{2\tau_x\tau_y}\big[E_I\big(\sum\sum_{i\neq j\in S_I}(\pi_{i|S_I}\pi_{j|S_I}-\pi_{ij|S_I})(\frac{x_i}{\pi_i^*}-\frac{y_j}{\pi_j^*})^2\big)\big]\big)$

The mean square error of $\hat{\tau}_{RADL}$ is as follows.

$$\begin{aligned}MSE(\hat{\tau}_{RADL})&=V\big(\tau_y(1+e_y+e_{x'}-e_x)\big)\\&=\tau_y^2\big[V(e_y)+V(e_{x'})+V(e_x)-2Cov(e_x,e_{x'})-2Cov(e_y,e_{x'})+2Cov(e_y,e_x)\big]\end{aligned}$$

$MSE(\hat{\tau}_{RADL})=\tau_y^2\big[\frac{1}{2\tau_y^2}\big[\sum\sum_{i\neq j\in U}(\pi_i\pi_j-\pi_{ij})(\frac{y_i}{\pi_i}-\frac{y_j}{\pi_j})^2+E_I\big(\sum\sum_{i\neq j\in S_I}(\pi_{i|S_I}\pi_{j|S_I}-\pi_{ij|S_I})(\frac{y_i}{\pi_i^*}-\frac{y_j}{\pi_j^*})^2\big)\big]+\frac{1}{2\tau_x^2}\big[\sum\sum_{i\neq j\in U}(\pi_i\pi_j-\pi_{ij})(\frac{x_i}{\pi_i}-\frac{x_j}{\pi_j})^2\big]+\frac{1}{2\tau_x^2}\big[\sum\sum_{i\neq j\in U}(\pi_i\pi_j-\pi_{ij})(\frac{x_i}{\pi_i}-\frac{x_j}{\pi_j})^2+E_I\big(\sum\sum_{i\neq j\in S_I}(\pi_{i|S_I}\pi_{j|S_I}-\pi_{ij|S_I})(\frac{x_i}{\pi_i^*}-\frac{x_j}{\pi_j^*})^2\big)\big]-\frac{1}{\tau_x^2}\big[\sum\sum_{i\neq j\in U}(\pi_i\pi_j-\pi_{ij})(\frac{x_i}{\pi_i}-\frac{x_j}{\pi_j})^2-\frac{1}{\tau_x\tau_y}\big[\sum\sum_{i\neq j\in U}(\pi_i\pi_j-\pi_{ij})(\frac{x_i}{\pi_i}-\frac{y_j}{\pi_j})^2+\frac{1}{\tau_x\tau_y}\big[\sum\sum_{i\neq j\in U}(\pi_i\pi_j-\pi_{ij})(\frac{x_i}{\pi_i}-\frac{y_j}{\pi_j})^2+$
$E_I\big(\sum\sum_{i\neq j\in S_I}(\pi_{i|S_I}\pi_{j|S_I}-\pi_{ij|S_I})(\frac{x_i}{\pi_i^*}-\frac{y_j}{\pi_j^*})^2\big)\big]\big]$

After Simplification, the MSE of $\hat{\tau}_{RADL}$ is,

$MSE(\hat{\tau}_{RADL})=\tau_y^2\big[\frac{1}{2\tau_y^2}\big[\sum\sum_{i\neq j\in U}(\pi_i\pi_j-\pi_{ij})(\frac{y_i}{\pi_i}-\frac{y_j}{\pi_j})^2+E_I\big(\sum\sum_{i\neq j\in S_I}(\pi_{i|S_I}\pi_{j|S_I}-\pi_{ij|S_I})(\frac{y_i}{\pi_i^*}-\frac{y_j}{\pi_j^*})^2\big)\big]+\frac{1}{2\tau_x^2}\big[E_I\big(\sum\sum_{i\neq j\in S_I}(\pi_{i|S_I}\pi_{j|S_I}-\pi_{ij|S_I})(\frac{x_i}{\pi_i^*}-\frac{x_j}{\pi_j^*})^2\big)\big]+$
$\frac{1}{\tau_x\tau_y}\big[E_I\big(\sum\sum_{i\neq j\in S_I}(\pi_{i|S_I}\pi_{j|S_I}-\pi_{ij|S_I})(\frac{x_i}{\pi_i^*}-\frac{y_j}{\pi_j^*})^2\big)\big]\big]$ (2)

3. Sample Survey

A sample survey was conducted by using NACDS. The area of 400 acres in the Tamhini Ghat, Maharashtra, India was divided into 400 plots each of size 1 acre. A random sample of 12

plots was drawn from this area by using SRSWOR. The percentage of silica content of the soil (X) was measured on these selected plots. Silica is abundant in the soil from Tamhini Ghat to Mumbai. But, there are intermediate patches of laterite where the occurrence of evergreen plants is more. We considered the condition C_X = $\{X \leq 20\}$ = $\{Percentage of silica \leq 20\}$. Further the plots in the sample satisfying C_X were located. Then the clusters were formed around these plots by using the procedure given by Thompson (1990). Each plot with $\{X > 20\}$ and selected in the initial sample formed a cluster of size one. Here the clusters were formed by using auxiliary information and the domain knowledge of silica content and evergreen plants. The two variables, percentage of silica content X and number of evergreen plants Y are negatively correlated. After forming such clusters in the X population, the edge units of clusters of size more than one were dropped to get networks. The networks are formed by using percent of silica content. The corresponding networks of number of evergreen plants are located. Figures 1 and 2 illustrate this methodology.

These plots formed the first phase sample S_1. Let K denote the number of distinct networks represented in this sample. A random sample of m_i (say), $(i = 1, 2, \cdots, K)$ units was drawn from the i^{th} network among these K networks by using SRSWOR. The collection of all so selected units formed the second phase sample S_2. In our study there were 12 networks formed in S_1. We took $m_1 = m_2 = m_3 = 2, m_4 = 3, m_5 = 4, m_6 = 2, m_7 = 2, m_8 = 2, m_9 = m_{10} = 4, m_{11} = 3$ and $m_{12} = 0$.

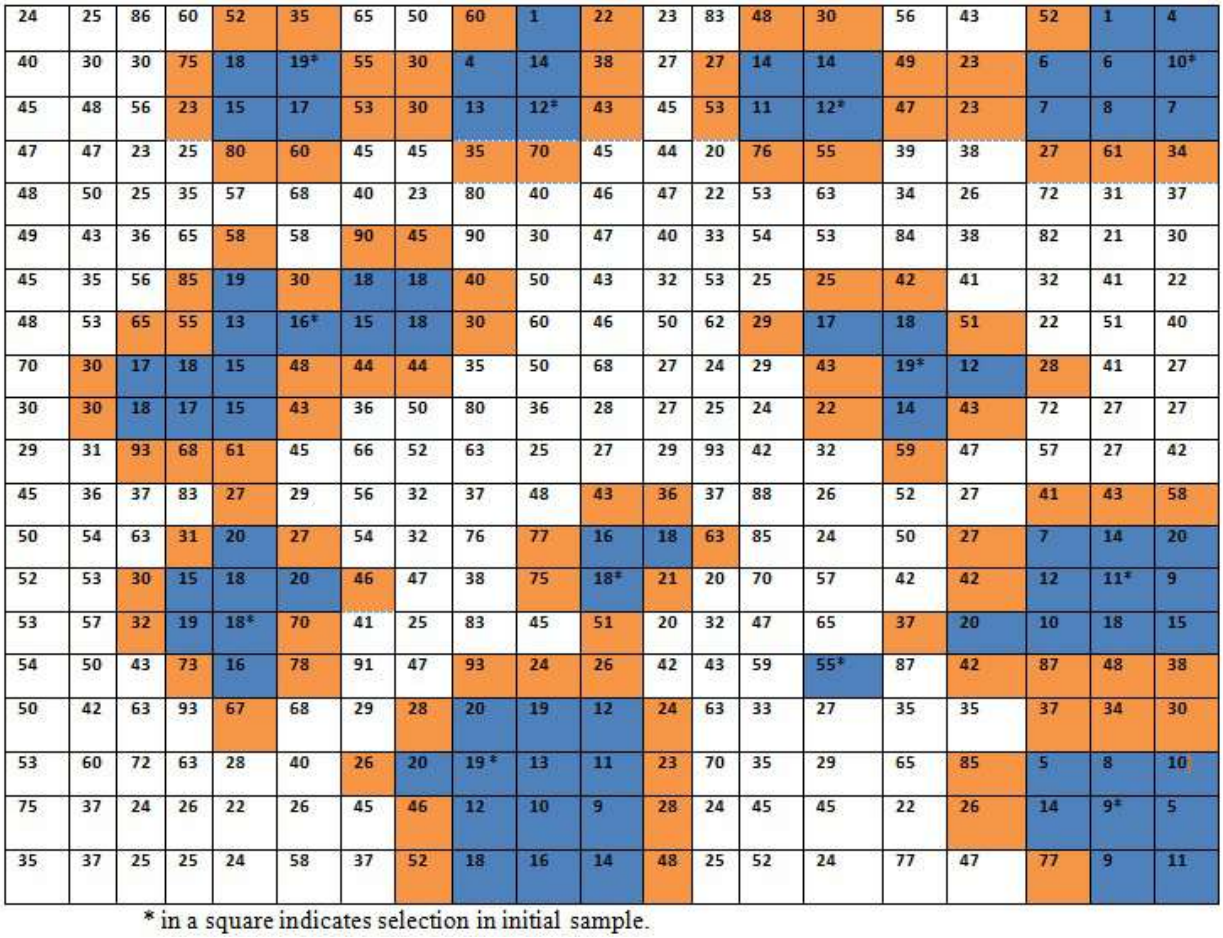
This set of units formed S_2. Values of the variables X and Y corresponding to the plots included in the second phase sample were recorded together to form a bivariate data. Using this data, the total number of evergreen plants in that area was estimated by using the proposed estimators.

4. Results and Discussion

For the computational efficiency in estimation, r number of repetitions were performed; where r varied as 5000, 10000 and 20000. We considered the initial sample sizes as 5, 10, 15, 20 and 25 for each repetition.

The estimated population total over r repetitions is given by:
$\hat{\tau}_Y = \frac{\sum_{i=1}^{r} \hat{\tau}_{Y_i}}{r}$
where $\hat{\tau}_{Y_i}$ denotes the estimated value of an estimator of the population total of the variable Y for the i^{th} repetition.

The estimated mean square error of the estimator of population total of the variable Y is given by:
$\widehat{MSE}(\hat{\tau}_Y) = \frac{\sum_{i=1}^{r} (\hat{\tau}_{Y_i} - \tau_Y)^2}{r}$



* in a square indicates selection in initial sample.

Figure 1: Silica (SiO_2) percentage on the different plots in the region.

Table 1: Estimated Values of Population Total of interest variable and its SE.

No. of Repetitions	Initial Sample Size	Exp Ratio Estimator		Ratio Estimator		Log Ratio Estimator	
r	n	$\hat{\tau}_{RADE}$	$\hat{SE}(\hat{\tau}_{RADE})$	$(\hat{\tau}_y)_{Ratio}$	$\hat{SE}(\hat{\tau}_y)_{Ratio}$	$\hat{\tau}_{RADL}$	$\hat{SE}(\hat{\tau}_{RADL})$
5000	5	9073.83	9594.65	9555.85	10461.68	8875.46	9212.46
	10	9094.24	6558.31	9206.55	6778.47	9044.51	6443.12
	15	9099.11	5200.63	9230.12	5373.81	9048.99	5085.60
	20	9075.71	4401.83	9106.03	4595.43	9031.09	4330.44
	25	9060.59	3878.48	9144.12	3992.87	8994.69	3800.33
10000	5	9429.05	9738.40	9458.85	10383.6	9053.38	9375.20
	10	9018.30	6452.53	9223.40	6738.29	8900.90	6384.41
	15	9055.01	5186.37	9114.49	5328.22	8936.08	5076.77
	20	9096.61	4416.34	9173.93	4577.09	9012.60	4317.32
	25	9082.23	3830.18	9110.27	3964.64	9014.61	3758.87
20000	5	9189.86	9676.48	9421.81	10328.04	8812.90	9277.79
	10	9071.97	6507.64	9224.23	6724.55	8962.86	6347.45
	15	9047.53	5197.31	9097.89	5313.16	8945.107	5112.01
	20	9108.18	4406.09	9047.11	4529.84	9025.19	4316.37
	25	9078.90	3868.39	9047.08	3947.24	9006.03	3781.37

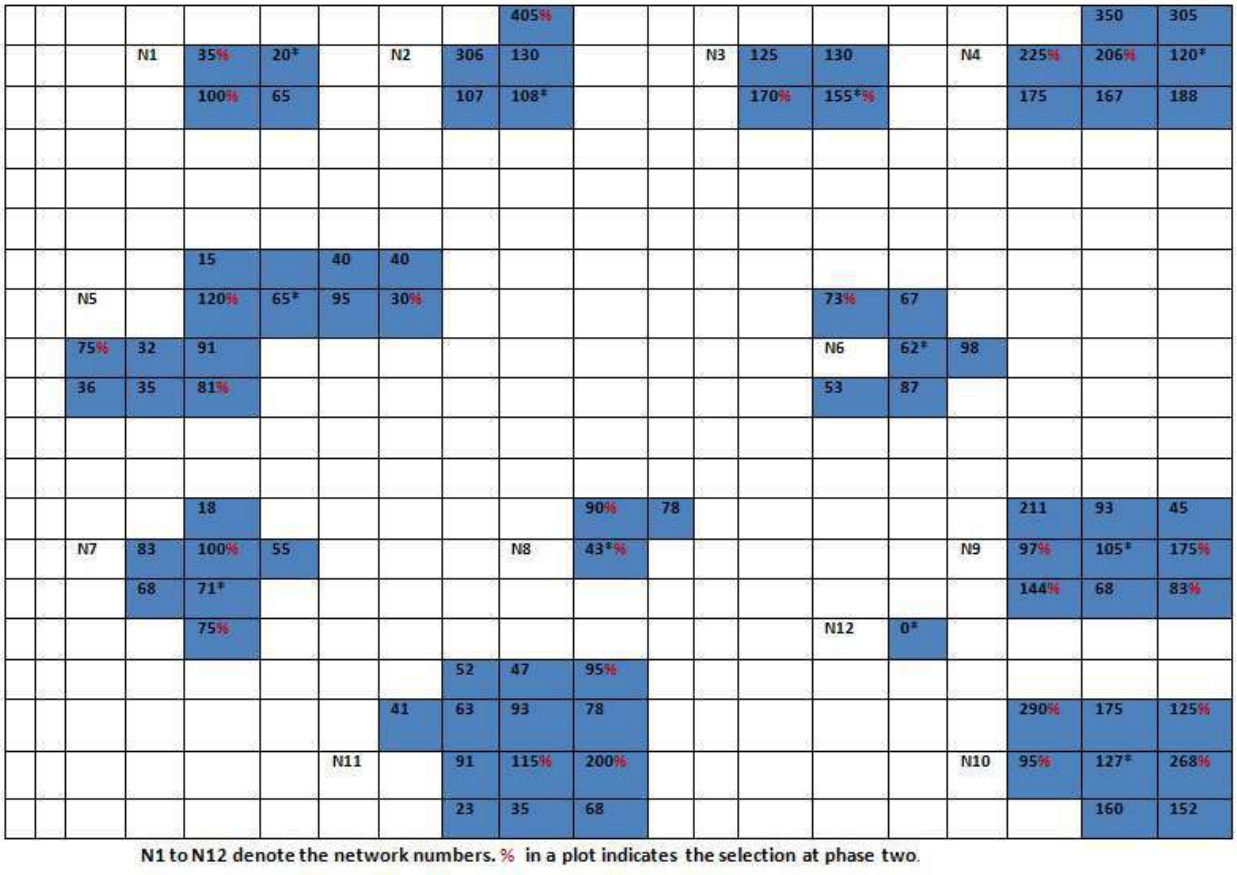


Figure 2: Number of evergreen plants observed on the plots in the population.

The estimated values are presented in Table 1. It showed that, as the initial sample size increases, the standard error decreases. The proposed exponential ratio type HT estimator performs better as compared to ratio estimator proposed by Särandal et al.(1992). The log ratio type HT estimator is more efficient as compared to ratio estimator proposed by Särandal et al.(1992) and exponential ratio type HT estimator. Even though, exponential ratio type HT estimator and log ratio type HT estimator are biased with minimum MSE. Log ratio type HT estimator is negatively biased and exponential ratio type HT estimator is positively biased estimator.

Remark: If there is positive correlation between X and Y. Then, exponential ratio type HT estimator is more efficient as compared to ratio estimator proposed by Särandal et al.(1992) and log ratio type HT estimator.

Theoretically, it clearly shows that equation 1 and 2 of MSE. The covariance term is added in equation 1 and subtracted in equation 2.

5. Conclusions

The auxiliary variable and interest variable are negatively correlated. The auxiliary information is used at design and estimation stage. Using auxiliary information in NACDS, the network of interest information is identified and random samples are selected from these selected networks. The inclusion probabilities are evaluated. The proposed log ratio type HT estimator is efficient as compared to traditional ratio estimator and proposed exponential ratio type HT estimator. When, we employ this methodology for positively correlated variables. The exponential ratio type HT estimator is efficient as compared to log ratio type HT estimator and traditional ratio estimator. This is the important features of these estimators. These estimators can be useful for estimation of population total for the sample surveys in ecology, environmental science, health science and forestry.

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On A New Bivariate One Parameter Archimedean Copula Function and Its Application to Modeling Dependence in Climate and Life Sciences

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Abstract

Copulas provide models to describe the dependence structure between two or more random variables. This study focuses on a special class of copulas namely Archimedean copulas which have some nice mathematical properties. The easiness of generating of Archimedean copula by a generator function and defining a bivariate Archimedean copula by a univariate function are appealing properties which make Archimedean copulas popular to work with them. In this study, a new generator function is proposed to generate a new one parameter bivariate Archimedean copula. The new copula parameter is estimated and the tail dependence properties are presented. In application part of the study, Archimedean copulas are considered to model the dependence structure of the studied data sets. The studied data sets refer to α amylase levels in saliva experiment and the climate change parameters. Simulations to the studies are performed to generate data from the copula-based methodology which is implemented to estimate prediction models. Results are presented.

Key words: Archimedean copulas; dependency; generator function; climate change; radiative forcing; methane; saliva experiment

1. Introduction

Copula is a multivariate function of distribution functions which are themselves random variables. Since copulas connect the marginal distributions to their joint distribution function, they can be considered a dependence model for random variables. Abe Sklar first introduced copula as a term in his article Sklar (1959). For a brief introduction to copulas Belgorodski (2010), Frees and Valdez (1998), Genest and Favre (2007), Joe (1997), Matteis De(2001), Nelsen (2006), Sklar (1959), Sklar (1973) can be recommended. Applications of copula in finance and insurance field can be found in Belgorodski (2010), Frees and Valdez (1998), Embrechts et.al. (2002), Cherubini et.al. (2004). Modelling time to event data, competing risks problems and related subjects in survival analysis are discussed in Clayton (1978), Shih and Louis (1995), Wang and Wells (2000). Traditionally, measuring and summarizing dependencies of random variables have centered on correlation measures. However, several shortcomings of the well-known correlation measures such as Pearson correlation, Kendall's tau in modeling dependencies are studied and presented in Embrechts et.al. (2002). In this manner copulas are considered as alternative measures because of the flexibility they possess, Embrechts et.al. (2002). For example, copula functions allow for

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describing dependence structure of random variables independently of their marginal, and also allow for asymmetric dependence unlike linear correlation coefficient.

Throughout the study, we focus on modeling dependencies with Archimedean copulas in bivariate context. The dependence structure between two random variables is completely described by known bivariate distributions. Although there are many bivariate distributions in literature, researchers need different models which are able to capture different types of dependence structures. Archimedean copulas can be generated by a generator function which have some particular properties. More detailed information about Archimedean copulas and corresponding generator functions can be found in Frees and Valdez (1998), Genest and McKay (1986), Genest and Rivest (1993), Hennesey and Lapan (2005), Hutchinson and Lai (1990), Nelsen (2006), Smith (2003).

In this study, bivariate Archimedean copula along with their properties and relationship between copula parameter and Kendall's tau are discussed in Section (2). In sub-section (2.1), a new generator function is proposed to generate a new one parameter bivariate Archimedean copula. The properties of the proposed generator function are presented and a new one parameter bivariate Archimedean copula is generated. The method of moments based on Kendall's tau is applied to estimate the parameter of the proposed Archimedean copula. In sub-section (2.2), the algorithm to simulate data from the Archimedean copula is described. The tail behavior of the proposed copula is studied and represented by the scatterplot in sub-section (2.3). The method for fitting copula to the data and comparing copula fits are given in sub-section (2.4). In section (3), copula-based methodology is considered to estimate linear prediction models for two data sets. Three well-known Archimedean copula Clayton, Clayton (1978), Gumbel, Gumbel (1960), Frank, Frank (1979) and the proposed Archimedean copula are employed and the prediction models are estimated by simulating data from the copulas. The minimum distance measure is used to specify an appropriate Archimedean copula which gives best possible fit to the data.

2. Archimedean Copulas

The bivariate cumulative distribution function H of any pair (X,Y) of random variables may be written in the form [22], [23].

$$H(x,y) = C(u,v), \quad u,v \in (0,1) \tag{1}$$

where u and v denote the marginal distributions $F(x)$ and $G(y)$ of X and Y, respectively. Here, C is the copula function with $C:[0,1]^2 \to [0,1]$ So the equation in (1) can be rewritten

$$H(x,y) = C(F(x),G(y)), \quad F(x),G(y) \in (0,1). \tag{2}$$

It should be noted that, if the marginals are continuous, there is a unique copula representation, Sklar (1973). C copula function has the following properties:

1. C is symmetric, $C(u,v) = C(v,u), \ \forall u, \ v \in (0, 1)$.
2. C is associative $C(C(u,v),w) = C(u,C(v,w)) \ \ \forall u, \ v, \ w \in (0, 1)$
3. If a is a constant, $a\varphi$ is also a generator of C
4. $C(u,1) = u$ and $C(1,v) = v, \ \forall u, \ v \in (0, 1)$.

Archimedean copulas can be generated by a function that is called generator function. Generator function is defined as follows:

Definition 1: Let Φ be a class of functions $\varphi:[0,1]\to[0,\infty]$ is satisfying that

(i) $\varphi(1)=0$

(ii) $\varphi(0)=\infty$

(iii) $\varphi'(t)<0\ ,\ 0<t<1$

(iv) $\varphi''(t)>0\ ,\ 0<t<1.$

Thus, φ is a continuous, strictly decreasing and convex function and always has an inverse, φ^{-1}. By using a defined generator function, a bivariate Archimedean copula can be constructed in the way which is given below:

$$C(x,y)=\varphi^{-1}\{\varphi(F(x))+\varphi(G(y))\}. \tag{3}$$

If $\varphi(0)<\infty$ the generator function is called non-strict and is also capable of generating an Archimedean copula.

The pseudo-inverse of non-strict generator function exists and it is defined by

$$\varphi^{[-1]}(t)=\begin{cases}\varphi^{-1}(t), & 0\le t\le\varphi^{-1}(t)\\ 0, & \varphi^{-1}(0)\le t\le\infty\end{cases} \tag{4}$$

Note that, an Archimedean copula that is generated by a non-strict generator function takes the form

$$C(u,\ v)\ =\ \max(C(u,\ v),\ 0). \tag{5}$$

For Archimedean copulas, Kendal's tau can be written in copula form as follows

$$\tau=\iint_{I} C(u,\ v)dC(u,\ v)-1=4E\left[C(U,\ V)\right]-1. \tag{6}$$

This relationship is useful to estimate copula parameter. The method of moments based on Kendall's tau can be used to estimate copula parameter. The properties of this method and the estimator are studied and presented in Genest and MacKay (1986), Genest and Rivest (1993), Kojadinovic and Yan (2010).

One of the appealing properties of Archimedean copulas is that a bivariate Archimedean copula can be uniquely determined by a univariate function. This univariate function, $K(t)$, is called Kendall distribution function and defined as:

$$\Pr(C(U,V)\le t)=K(t)=t-\frac{\varphi(t)}{\varphi'(t)},\ \ 0<t<1 \tag{7}$$

Here, $K(t)$ is the distribution function of an Archimedean copula and the expression in (6) can be re-expressed as follows:

$$\tau=4\int_0^1\frac{\varphi(t)}{\varphi'(t)}dt+1 \tag{8}$$

In the following sub-section 2.1, a new generator function is proposed to generate a new bivariate Archimedean copula and the properties of the new Archimedean copula are studied.

2.1. Bivariate Archimedean copula

Considering that different generator functions generate different Archimedean copulas and recalling the Definition 1, new generator function can be defined.

The proposed new generator function, $\varphi:[0,1]\to[0,\infty]$ is defined

$$\varphi(t)=e^{\theta(1-t)}-1, \quad \theta>0, \ 0<t<1 \tag{9}$$

The properties in Definition 1 are checked for the proposed function as follows:

(i) $\varphi(1)=0 \Rightarrow \varphi(1)=(e^0-1)=0$

(ii) $\varphi(0)<\infty \Rightarrow \lim_{t\to 0^+}(e^{\theta(1-t)}-1)=(e^{\theta}-1)<\infty$

(iii) $\varphi'(t)=-\theta e^{-\theta(t-1)}<0, \quad 0<t<1$

(iv) $\varphi''(t)=\theta^2 e^{-\theta(t-1)}>0, \ 0<t<1$

It can be seen that, because of $\varphi(0)<\infty$, the proposed function in (9) is a non-strict generator function. It can be used to generate an Archimedean copula. Its pseudo-inverse, $\varphi^{[-1]}:(0,\infty)\to(0,1)$ is defined as follows

$$\varphi^{[-1]}(t)=\begin{cases}1-\dfrac{1}{\theta}\ln(1+t), & 0\le t\le\varphi(0)\\ 0, & \varphi(0)\le t\le\infty\end{cases} \tag{10}$$

Definition 2: Let φ be a generator function that is defined in (6). Then $C:[0,1]\times[0,1]\to[0,1]$ is a bivariate Archimedean copula that is generated by φ and has the form

$$C(u,v)=\begin{cases}1-\dfrac{1}{\theta}\ln(e^{\theta(1-u)}+e^{\theta(1-v)}-1), & \varphi(u)+\varphi(v)\le\varphi(0)\\ 0, & ow.\end{cases} \tag{11}$$

The copula presented in (11) is indexed by a parameter θ that is called copula parameter. Recalling (7) and (8), the distribution function and the parameter estimation of the new bivariate Archimedean copula are given, respectively.

$$K(t)=t-\frac{e^{\theta(1-t)}-1}{-\theta e^{-\theta(t-1)}} \tag{12}$$

$$\tau=4\int_0^1\frac{e^{\theta(1-t)}-1}{-\theta e^{-\theta(t-1)}}dt+1 \tag{13}$$

By solving the integral (13),

$$\tau=4\left(\frac{1-e^{-\theta}-\theta}{\theta^2}\right)+1 \tag{14}$$

is obtained. Figure 1 illustrate the relationship between the parameter of the proposed copula and Kendall's tau.

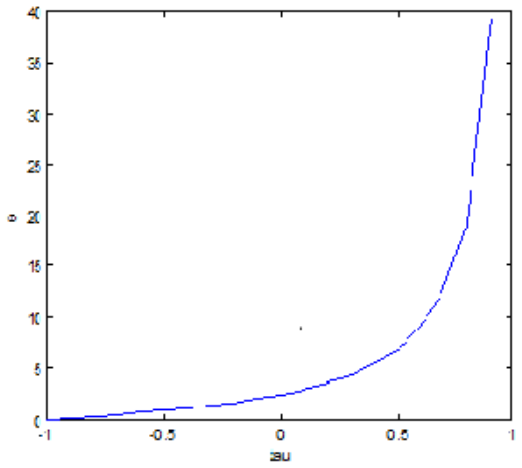

Figure 1: New Copula Parameter and Kendall's τ

The corresponding generator and distribution functions of the studied Archimedean copulas in this study are presented in Table 1. Figure 2 shows the graphs of the distribution functions of the studied Archimedean copulas. The bivariate Archimedean copulas along with the relationship between their parameters and Kendall's tau are presented in Table 2. The plots of the studied copulas are illustrated in Figure 3.

Table 1: Distribution Functions of Archimedean Copulas

Family	$\varphi(t)$	$\varphi(t)$	$K(t)=t-\frac{\varphi(t)}{\varphi'(t)}$
Gumbel	$(-\ln t)^{\theta}$	$-\frac{\theta}{t}(-\ln t)^{\theta-1}$	$t-\frac{(t\ln t)}{\theta}$
Clayton	$\frac{1}{\theta}\left(t^{-\theta}-1\right)$	$-t^{-\theta-1}$	$t-\frac{\left(t^{\theta+1}-t\right)}{\theta}$
Frank	$-\ln(\frac{e^{-\theta t}-1}{e^{-\theta}-1})$	$\frac{\theta}{1-e^{-\theta t}}$	$t-\frac{1}{\theta}\ln(\frac{e^{-\theta t}-1}{e^{-\theta}-1})\left(1-e^{-\theta t}\right)$
NewCop.	$e^{\theta(1-t)}-1$	$-\theta e^{-\theta(t-1)}$	$t-\frac{e^{\theta(1-t)}-1}{-\theta e^{-\theta(t-1)}}$

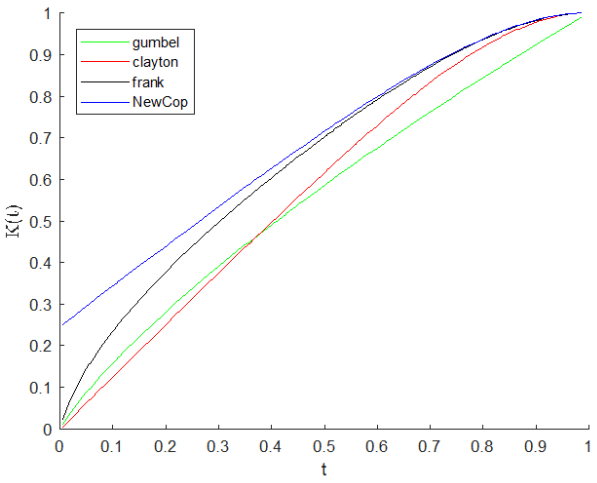

Figure 2: Distribution Functions of Archimedean Copulas

Table 2: Bivariate Archimedean Copulas and the Relationship with Kendall's τ

Family	Bivariate Copula	Dependence Parameter	Kendall's τ
Gumbel	$e^{-((-\ln u)^{\theta}+(-\ln v)^{\theta})^{1/\theta}}$	$\theta \geq 1$	$(\theta-1)/\theta$
Clayton	$((u)^{-\theta}+(v)^{-\theta}-1)^{-1/\theta}$	$\theta > 1$	$\theta/(\theta+2)$
Frank	$\left(-\frac{1}{\theta}\right)\ln\left\{\frac{\left(1-e^{-\theta}\right)-\left(1-e^{-\theta u}\right)\left(1-e^{-\theta v}\right)}{\left(1-e^{-\theta}\right)}\right\}$	$-\infty < \theta < \infty$	$1-\frac{4}{\theta}[D_1(\theta)]$
NewCop	$1-\frac{1}{\theta}\ln(e^{\theta(1-u)}+e^{\theta(1-v)}-1)$	$\theta > 0$	$4\left(\frac{1-e^{-\theta}-\theta}{\theta^2}\right)+1$

Here, $D_n(\theta)=\frac{n}{\theta^n}\int_0^{\theta} t^n/e^t-1dt,\ \ n>0$ is a Debye function.

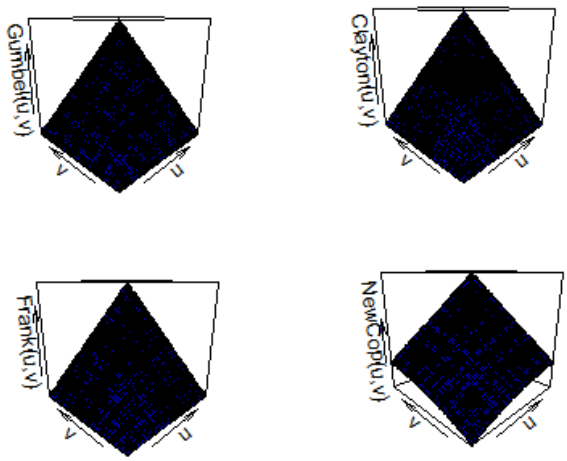

Figure 3: Plots of Archimedean Copulas

The sub-section 2.2 provides a method to simulate data from Archimedean copulas.

2.2. Generating random numbers from bivariate Archimedean copula

Generating random numbers from copulas is important for simulation studies, modelling, selecting random samples, etc. In this study generated random numbers are used to plot a scatter plot, which is a graphical tool to detect the tail dependence. The following steps are listed to generate random numbers from a bivariate copula.

Let (U,V) be a random pair from a bivariate Archimedean copula, $\varphi(t)$ is the generator function and $K(t)$ defined by (8) is the distribution function of copula. A pair of data (x_i, y_i) from a bivariate Archimedean copula can be generated by using the following procedure:

(i) Generate two independent random variables, p and p from Uniform $(0,1)$

(ii) $t=K^{-1}(q)$

(iii) $u=\varphi^{-1}[p\varphi(t)]$ and $v=\varphi^{-1}[(1-p)\varphi(t)]$

(iv) $x=F^{-1}(u)$ and $y=F^{-1}(v)$

Repeating the above steps (i) to (iv), n times n pairs of data (x_i, y_i), $i=1,2,...,n$ can be generated.

Since the inverse of the distribution function of the proposed Archimedean copula, $K(t)$ which is defined in (12) doesn't have the closed form, Newton-Raphson numerical root finding method is applied to solve the following equation.

$$\left[t-\frac{\varphi(t)}{\varphi'(t)}\right]-q=0 \tag{15}$$

$$\left[t-\frac{e^{\theta(1-t)}-1}{-\theta e^{-\theta(t-1)}}\right]-q=0\,. \tag{16}$$

To understand the concept of the clustering of extreme event, tail dependence property of copulas is discussed in the following sub-section 2.3.

2.3. Tail dependence properties of bivariate Archimedean copula

The concept of tail dependence refers to clustering of extreme events. Modelling dependence of events, such as economic systems, natural hazards contexts generally exhibit tail dependence. It becomes very important to obtain accurate results especially in tail ends. The definition of tail dependence is the limiting probability that a random variable exceeds a certain threshold, given that another random variable already exceeds that threshold.

More formally definitions of the upper and lower tail dependence of a bivariate copula $C(u,v)$ are given as follows, respectively in (17) and (18).

$$\lambda_U=\Pr\left[F(x)>u\,|\,G(y)>u\right]=\lim_{u\to 1^-}\frac{1-2u+C(u,u)}{1-u} \tag{17}$$

$$\lambda_L=\Pr\left[F(x)<u\,|\,G(y)<u\right]=\lim_{u\to 0^+}\frac{C(u,u)}{u}\ . \tag{18}$$

If the above limits exist, $\lambda_U(\lambda_L)=0$ shows that the copula has no upper (lower) tail dependence. In case of, $\lambda_U(\lambda_L)\neq 0$ there is upper (lower) tail dependence. The upper and lower tails of the new copula in (8) are examined, respectively.

$$\lambda_U=\lim_{u\to 1^-}\frac{2-2u-\frac{1}{\theta}\ln(e^{\theta(1-u)}-e^{\theta(1-v)}-1)}{1-u}\to 2 \tag{19}$$

$$\lambda_L=\lim_{u\to 0^+}\frac{1-\frac{1}{\theta}\ln(e^{\theta(1-u)}-e^{\theta(1-v)}-1)}{u}\to\infty\ . \tag{20}$$

The tail dependence coefficients of studied bivariate Archimedean copulas are listed in Table 3 and Figure 4 demonstrates the tail dependence of the considered copulas. The scatter plots visualize that Gumbel copula has an upper tail, Clayton copula has a lower tail, Frank copula has no tail and the proposed Archimedean copula has both lower and upper tail dependencies.

Table 3: Tail Dependence Coefficients of Considered Archimedean Copulas

Family	λ_L	λ_U
Gumbel	0	$2-2^{1/\theta}$
Clayton	$2^{-1/\theta}$	0
Frank	0	0
New Cop.	∞	2

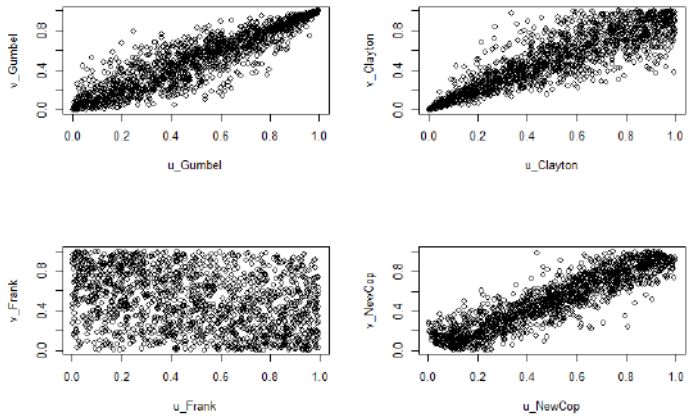

Figure 4: Scatter Plots of Considered Archimedean Copulas

In the following sub-section (2.4), we describe the method of fitting copula.

2.4. Fitting copula to data

Genest and Rivest (1993) suggested a nonparametric approach to select the appropriate bivariate Archimedean copula which gives the best fit to the data. The estimation procedure consists of mainly two steps. First one is to estimate the marginal distributions and the second one is to specify the copula function. Marginal distributions can be estimated by empirical or parametric ways. The procedure which is followed in this study is summarized as follows:

Let $(X_1, Y_1), \ldots, (X_n, Y_n)$ be a random sample from a bivariate population (X, Y) with distribution functions $F(x)$ and $G(y)$, respectively.

(i) Estimate the copula parameter.

(ii) Obtain the empirical estimate of distribution of copula function, say $K_n(t)$. First, define the pseudo-observations,

$$T_i = \sum_{i=1}^{n} \frac{I\left(X_j \le X_i \,\&\, Y_j \le Y_i\right)}{n+1},\ i = 1,\ldots,n \text{ and then calculate}$$

$$K_n(t) = \frac{\sum_{i=1}^{n} I(T_i \le t)}{n+1},\ i = 1,\ldots,n$$

(iii) Construct parametric estimate of $K_\varphi(t) = t - \dfrac{\phi(t)}{\phi'(t)}$

(iv) Compare the distance between $K_n(t)$ and $K_\varphi(t)$

Comparing $K_n(t)$ and $K_\varphi(t)$ can be done in several ways. For instance, by considering information criteria such as Akaike Information Criterion, Bayesian Information Criterion and log likelihood. In this study, we follow Frees and Valdez (1998) and use the following minimum distance measure.

$$MD = \int \left[K_n(t) - K_\varphi(t)\right]^2 dK_n(t). \qquad (21)$$

In the following Section 3, we illustrate the applications of copulas with the help of two examples.

3. Application

In this section, we apply the new copula along with other well-known Archimedean copulas namely Clayton, Gumbel and Frank to fit the linear prediction models to the data from two examples described below. We follow the copula-based methodology as described and studied in Kumar and Shoukri (2008, 2007, 2011). Using the copulas, new data sets which have the similar dependence structure and sample sizes as in the actual data sets are simulated choosing the 50, 150, 250 and 350 runs. For each data set, linear prediction models are estimated and the %95 confidence intervals of model parameters are computed. The estimated prediction models from the fitted copulas are compared using the mean absolute prediction error (MAPE) measure.

3.1. Copula applications for α-amylase levels in saliva experiment

This example refers to the study of saliva content which is an enzyme called amylase and which hydrolyses starch into maltose. The experimental data on α-amylase levels in saliva are considered. The data set can be found in Brunner et al. (2004). The α-amylase levels in saliva are measured on different times and in a day. In this study, we have considered the data set which consists of the 14 measurements of α amylase levels in saliva taken on Thursday at 12 a.m. (independent variable, X) and 9 p.m. (dependent variable, Y).

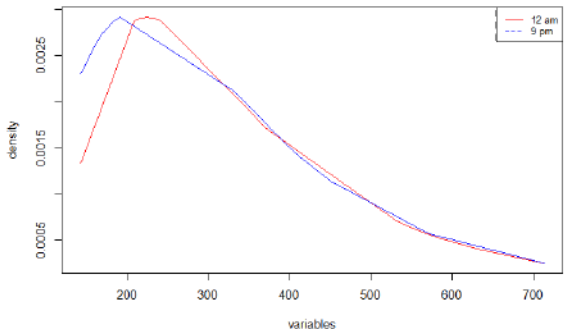

Figure 5: Marginal Fitting to Amylase Levels

To specify the dependence structure between the amylase levels in saliva at two time points, *i.e.*, between Y and X, their marginal distributions are estimated as the Log Normal (mean = 5.6210, sd = 0.6988) for X and the Log Normal (mean = 5.6525, sd = 0.5487) for Y, see Figure 5. Kendall's Tau between two amylase levels is estimated as τ = 0.64835. The copula parameters are estimated based on the Kendall's Tau and the minimum distance measure (MD) are given in Table 4. Fitted copulas are then plotted and compared in Figure 6.

Table 4: Estimated Copula Parameters and Minimum Distance Measure for Amylase Levels

	Clayton	Gumbel	Frank	New Cop
$\hat{\theta}$	3.6875	2.8438	9.3816	10.2671
MD	0.0785	0.0312	0.0281	0.0208*

It may be noted from Table 4 that the minimum distance measure (MD) for the proposed new copula is 0.0208 and thus, new copula is the best fit compared to the Frank,

Gumbel and Clayton copulas to represent the dependence structure between two amylase levels. New data sets (X,Y) of size 14 are simulated using the new copula 50, 150, 250 and 350 times. For each data set, linear prediction models are estimated along with the intercept and slope, standard error and the % 95 confidence interval of slope. Results are listed in Table 5.

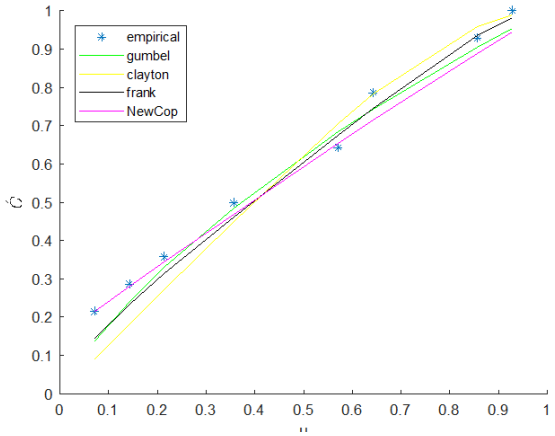

Figure 6: Copula Fitting for Amylase Levels

Table 5: Estimated prediction models and confidence intervals for amylase levels

	Intercept	Slope (b)	Std.Error (b)	CI Lower	CI Upper	CI Width
Data Model	73.3113	0.7443	0.1011	0.5462	0.9424	0.3962
New Copula Simulations						
50	66.0857	0.7942	0.1460	0.5080	1.0803	0.5723
150	67.3012	0.7741	0.1191	0.5406	1.0076	0.4670
250	68.5123	0.7625	0.0787	0.6082	0.9167	0.3085
350	66.4007	0.7278	0.0701	0.5904	0.8652	0.2748

In Table 5, it is noted that the estimated models from the actual data set and also from the simulated data sets have the intercept and slope estimates in close agreement with each other. For instance, the estimates of intercept, slope and the %95 confidence interval width of the slope in actual data set are 73.3113, 0,7443 and 0.3962, respectively, while these values for the new data set using 350 simulations run are 66.4007, 0.7278 and 0.2748, respectively. With regard to the comparison of the prediction errors, it is noted from Table 6 that the mean absolute prediction errors (MAPE) for actual data set and the new data sets with 50, 150, 250 and 350 simulation runs are 18.2229, 19.8664, 18.2299, 18.1937 and 16.0277, respectively.

However, as expected, when the number of simulation runs increases, the estimated models have smaller standard errors and narrow confidence intervals of slope estimation, and mean absolute prediction errors. Thus, having the smallest confidence interval width of the model parameters and also, the prediction errors, the proposed new copula-based prediction model may be recommended to study the relationship between two amylase levels.

Table 6: Mean Absolute Prediction Errors (MAPE) of Estimated Models of Amylase Levels

	MAPE
Data Model	18.2299
New Cop Sim.	
50	19.8664
150	18.2299
250	18.1937
350	16.0277

3.2. Copula applications for climate change indicators

The second example is about the climate change indictors [Source: Earth System Research Laboratory, Global Monitoring Division, https://www.esrl.noaa.gov/gmd/aggi]. Radiative Forcing (RF) is one of the climate change indicator which measures heating effect caused by greenhouse gases in the atmosphere. RF is calculated in watts per square meter, which represents the size of the energy imbalance in the atmosphere. Since RF (denoted by Y) is directly associated with the methane (CH4, one the of greenhouse gases), denoted by X, the prediction model of RF and CH4 will be useful to study their cause-and-effect relationship.

We fitted the marginal distributions of RF and CH4 from the given data set as Log Normal (mean = 0.9449, sd = 0.1032) and Log Normal (mean = –0.7279, sd = 0.0261), respectively, as seen in Figure 7. Kendall's tau is estimated as $\tau = 0.9600$ and used to estimate copula parameters. Following the copula fitting procedure in sub-section (2.2), copula parameter estimates and MD measures are given in Table 7 and copulas plotted in Figure 8 for the comparison purpose. From Table 7, the Gumbel copula has mean distance value MD = 0.0110, followed by MD = 0.0128 for the new copula. Thus, for this data set, Gumbel copula gives the best fit followed by the new copula to model the dependence structure between Radiative Forcing and CH4.

Using the Gumbel copula and the new copula, simulation studies are performed to generate data sets by having the number of simulation runs as 50, 150, 250 and 350 and the sample sizes 28. The prediction models are estimated and the results are listed in Table 8.

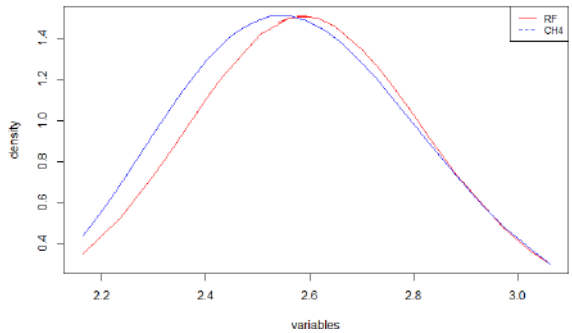

Figure 7: Marginal Distributions for RF and CH4

Table 7: Estimated Copula Parameters and Minimum Distance Measure for RF and CH4 Levels

	Clayton	Gumbel	Frank	New Cop
$\hat{\theta}$	48.0384	25.0198	98.4040	99.0667
MD	0.0138	0.0110*	0.0162	0.0128

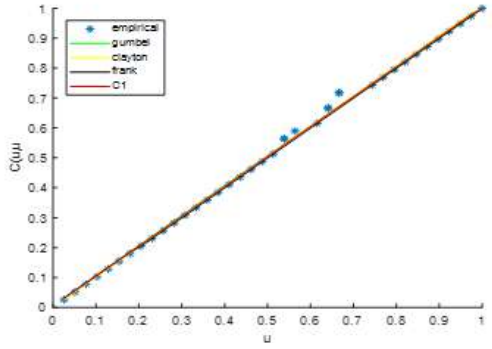

Figure 8: Copula Fitting for RF and CH4

Table 8: Estimated Prediction Models and Confidence Intervals for RF and CH4

	Intercept	Slope (b)	Std.Error (b)	CI Lower	CI Upper	CI Width
DataModel	–7.3891	20.6498	0.8597	18.8826	22.4170	3.5344
50	–7.4207	20.7121	0.3404	20.0449	21.3793	1.3340
150	–7.4957	20.8635	0.3304	20.2207	21.5160	1.5150
250	–7.5152	20.9089	0.3244	20.2730	21.5447	1.2717
350	–7.5095	20.8964	0.3353	20.2392	21.5536	1.3144
NewCop Simulation						
50	–7.2123	20.2801	0.5471	19.2084	21.3529	2.1444
150	–7.4755	20.8260	0.5189	19.2084	21.8430	2.0340
250	–7.4574	20.7879	0.4946	19.8185	21.7574	1.9389
350	–7.4567	20.7873	0.4929	19.8213	21.7534	1.9322

Table 9: Mean Absolute Prediction Errors (MAPE) of Estimated Models of RF and CH4

	MAPE	
Data Model	0.01924	
	Gumbel Sim.	New Cop Sim.
50	0.01911	0.01941
150	0.01906	0.01908
250	0.01904	0.01909
350	0.01903	0.01924

From Table 8, we note that the estimated model parameters from the actual data set and also from the simulated data sets are in close agreement with each other. For instance, the estimates of intercept, slope and the %95 confidence interval width of the slope in the actual data set are –7.3891, 20.6498 and 3.5344, respectively, while these values using the Gumbel copula and 350 simulations run are –7.5095, 20.8964 and 1.3144, respectively. With regard to the comparison of the prediction errors, it is noted from Table 9 that the mean absolute prediction error (MAPE) for the actual data set is 0.01924, while for the 50, 150, 250 and 350 simulation runs, MAPE values are, respectively, 0.01911, 0.01906, 0.01904 and 0.01903 for the Gumbel copula and 0.01941, 0.01908, 0.01909 and 0.01924 for the new copula. Thus, the Gumbel copula followed by the proposed new copula may be recommended to model the dependence structure between the Radiative Forcing and CH4 and also to make predictions of the Radiative Forcing (heating effect) resulting from the levels of CH4.

4. Conclusion

In multivariate data sets, studying the dependence or specifying the pattern between random variables is commonly of main interest. Copulas have been used to model different types of dependence patterns between the random variables. Main advantage of working with copulas is that any kind of marginal distributions can be employed in simulating data sets. Therefore, copula-based methodology is an appropriate approach for modelling especially skewed data. Archimedean copulas are preferable in most applications due to their appealing mathematical properties and simple simulation algorithms. In observational studies, researchers may face different kinds of dependence structures and known models may be insufficient to represent the dependency between random pairs. Thus, to generate new and applicable models can be a solution. For this purpose, in this study, we have proposed a new generator function and discussed its properties. Based on this new generator function, a new bivariate Archimedean copula is constructed. Tail dependency of the new copula is examined. Copula based methodology is applied to prediction modeling in two applications, namely, to study α- amylase levels in saliva and to study effect of Methane, one of greenhouse gases on the Radiative Forcing (heating effect) in climate change. The results indicate that the new copula performs well compared to commonly used Archimedean copulas and can be applied in the copula based prediction models.

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Robust Nonparametric Covariance Technique

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Abstract

Outlier detection and robust estimation are the integral part of data mining and has attracted much attention recently. Generally, the data contain abnormal or extreme values either due to the characteristics of the individual or due to the errors in tabulation, data entry etc. The presence of outliers may badly affect the data modeling and analysis. Analysis of semi-parametric regression with design matrix as the parameter component and covariate as the nonparametric component is considered in this paper. The regression estimate and the cross validation technique can behave very badly in the presence of outliers in the data or when the errors are heavy-tailed. The cross-validation technique to estimate the optimum smoothing parameter will also be affected badly by the presence of outliers. A robust method, which is not influenced by the presence of outliers in the data, is proposed to fit the semi-parametric regression with design matrix as the parameter component and covariate as the nonparametric component. Robust M- kernel weighted local linear regression smoother is used to fit the regression function. The cross-validation technique to estimate the optimum smoothing parameter will also be affected badly by the presence of outliers. A robust cross-validation technique is proposed to estimate the smoothing parameter. The proposed method is useful to compare the treatments after eliminating the covariate effect. The method is illustrated through simulated and field data.

Key words: Nonparametric, robust inference, covariance.

1. Introduction

The fundamental objective of statistical data analysis is to obtain data systematically and to make inferences or appropriate decisions based on the data. Presence of outliers or extreme values in the experimental data is a major concern for data analysis. Outlier is an observation that appears to be inconsistent with the remainder of the observations in the data set. Agricultural field experimental data may contain abnormal or extreme values due to various reasons such as genetical variations (super trees/very low yielders), loss of yield due to pest/ disease infestation, errors in tabulation, data entry etc. These extreme values or outliers, generally increase the experimental error in data analysis. Detection of outliers and the possible remedies are very important in data analysis. These outliers are nuisance for the data analysts. A robust method is proposed for the analysis of semi-parametric regression model in the presence of outliers.

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2. Model Settings and Estimators

The semi-parametric or the non-parametric covariance model considered for the study is of the form

$$\mathbf{Y}=\mathbf{X}\boldsymbol{\beta}+\phi(\mathbf{U})+\boldsymbol{\varepsilon} \tag{1}$$

where, $\mathbf{Y}$ is the observation vector, $\mathbf{m}=\mathbf{X}\boldsymbol{\beta}+\phi(\mathbf{U})$, is the regression function, $\mathbf{X}$ is the design matrix, $\boldsymbol{\beta}$ is the vector of treatment effect, $\phi(\mathbf{U})$ is the non-parametric function representing the relationship between $\mathbf{Y}-\mathbf{X}\boldsymbol{\beta}$ and the covariate $\mathbf{U}$ which is assumed to be a smooth function and $\boldsymbol{\varepsilon}$ is the error term assumed to be *iid* with mean vector $\mathbf{0}$ and covariance matrix $\sigma^2\mathbf{I}$. Backfitting algorithm (Buja *et al.*, 1989) is used to estimate the treatment vector and covariate effect in the regression model and estimates are given by

$$\hat{\boldsymbol{\beta}}=[\mathbf{X}^T(\mathbf{I}-\mathbf{S})\mathbf{X}]^{-1}\mathbf{X}^T(\mathbf{I}-\mathbf{S})\mathbf{Y},\quad \hat{\boldsymbol{\phi}}=\mathbf{S}\left(\mathbf{Y}-\mathbf{X}\hat{\boldsymbol{\beta}}\right)\ \text{and}\ \ \hat{\mathbf{m}}=\mathbf{X}\hat{\boldsymbol{\beta}}+\hat{\boldsymbol{\phi}}$$

where, $\mathbf{S}$ is the smoothing matrix derived using local linear regression (Ruppert and Wand, 1994). Let $\mathbf{S}_i$ be the ith row of the smoother matrix, then

$$\mathbf{S}=[\mathbf{S}_1\ \ldots\ \mathbf{S}_n]^T$$
$$\mathbf{S}_i^T=\mathbf{e}_1^T\left(\mathbf{Z}_{u_i}^T\mathbf{W}_{u_i}\mathbf{Z}_{u_i}\right)^{-1}\mathbf{Z}_{u_i}^T\mathbf{W}_{u_i}$$

where,

$$\mathbf{Z}_{u_i}=\begin{bmatrix}1 & (u_1-u_i)\\ \vdots & \vdots\\ 1 & (u_n-u_i)\end{bmatrix},\quad \mathbf{e}_1{}^T=[1\ 0\ 0]$$

and $\mathbf{W}_{u_i}=diag\left\{K\left(\frac{u_1-u_i}{h}\right),\ldots,K\left(\frac{u_n-u_i}{h}\right)\right\}$for some kernel functions K and bandwidth h. The properties of the estimates are provided by Jose and Ismail (2001) and Rupert and Wand (1994). Cross validation (leave-one-out) technique is generally used to estimate the optimum bandwidth h. The cross validation score is given by

$$CV(h)=\frac{1}{n}\sum_{i=1}^{n}\left[y_i-\hat{m}_{(-i)h}\right]^2$$

where, y_i, i=1,…,n are the observations and $\hat{m}_{(-i)h}$is the leave-one-out estimate (estimated value of m_i without using the i^{th} observation) with h as bandwidth. The optimum bandwidth is the value of h which minimizes the cross validation score $CV(h)$. The estimate, $\hat{\boldsymbol{\beta}}$ is asymptotically unbiased and its asymptotic variance is $\sigma^2(\mathbf{X}^T\mathbf{X})^{-1}$ which is same as the fully parametric model (Opsomer and Ruppert, 1999). Cleveland and Devlin (1988) and Hastie and Tibshirani (1990) discussed the estimation of error variance in linear regression smoothers. An approximate estimate of the error variance is given by

$$\hat{\sigma}^2=\frac{1}{[n-p-2trace(\mathbf{S})+trace(\mathbf{S}^T\mathbf{S})]}\left[\mathbf{Y}-\mathbf{X}\hat{\boldsymbol{\beta}}-\hat{\boldsymbol{\phi}}\right]^T\left[\mathbf{Y}-\mathbf{X}\hat{\boldsymbol{\beta}}-\hat{\boldsymbol{\phi}}\right]$$

The variance of $\widehat{\boldsymbol{\beta}}$ is estimated by

$$\widehat{V}\left(\widehat{\boldsymbol{\beta}}\right) = diag(\mathbf{P}\mathbf{P}^T)\hat{\sigma}^2$$

where, $\mathbf{P} = (\mathbf{X}^T(\mathbf{I}-\mathbf{S})\mathbf{X})^{-1}\mathbf{X}^T(\mathbf{I}-\mathbf{S})$. The significance of the covariate effect $\boldsymbol{\phi}$ can be tested using the lack of fit statistic or by comparing the mean residual sum of squares (Hart, 1997; Jose, *et al.*, 2009). Under the null hypothesis that the covariate effect $\phi(\mathbf{U}) = \mathbf{0}$, the mean residual sum of squares obtained by fitting the model (1) is given by

$$\hat{\sigma}_0^2 = \mathbf{Y}^T[\mathbf{I} - \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}]^T[\mathbf{I} - \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}]\mathbf{Y}/(n-p-1)$$

The lack of fit statistic is given by

$$R = \frac{\hat{\sigma}_0^2}{\hat{\sigma}^2}$$

The statistic R asymptotically follows an F distribution with (n-p-1), [n-p-2*trace*($\mathbf{S}$)+ *trace*($\mathbf{S}^T\mathbf{S}$)] degrees of freedom and it can be used for testing the significance of the covariate effect.

3. Analysis of Data in the Presence of Outliers

The regression estimate and the cross validation technique can behave very badly in the presence of outliers in the data or when the errors are heavy-tailed (Leung, D., 2005). One remedy is to remove the influential observations from the data. Another approach is to use robust smoother, which is not as vulnerable as the usual smoothing technique. A robust M-type estimate $\hat{m}$ of the regression function can be obtained by minimizing the objective function

$$\sum_{i=1}^{n} \rho\left[\frac{y_i - \hat{m}_i}{s}\right] \tag{2}$$

where, $\rho(.)$ is an even function with bounded first derivative $\psi(.)$ and a unique minimum at zero. The derivative $\psi(x) = \frac{d\rho(x)}{dx}$ is called the influence function and $w(x) = \frac{\psi(x)}{x}$ is the corresponding weight function. Several M-type estimators have been discussed in literature using different types of influence functions (Huber, 1981; Rey, 1983; Hampel *et al.*, 1986; Tukey, 1977). Tuckey's biweight robust function is very popular and it is considered in this paper. The ρ, ψ and w functions corresponding to the Tuckey's robust estimator is given by

$$\rho(x) = \begin{cases} \frac{c^2}{6}\left[1 - \left(1 - \left(\frac{x}{c}\right)^2\right)\right]^3 & |x| \le c \\ \frac{c^2}{6} & |x| > c \end{cases}$$

$$\psi(x) = \begin{cases} x\left[\left(1 - \left(\frac{x}{c}\right)^2\right)\right]^2 & |x| \le c \\ 0 & |x| > c \end{cases}$$

$$w(x) = \begin{cases} \left[\left(1 - \left(\frac{x}{c}\right)^2\right)\right]^2 & |x| \le c \\ 0 & |x| > c \end{cases}$$

The turning constant c is picked to give reasonably high efficiency. When the errors are normal and x is the standardized residual, then c=4.685 produce 95% efficiency.

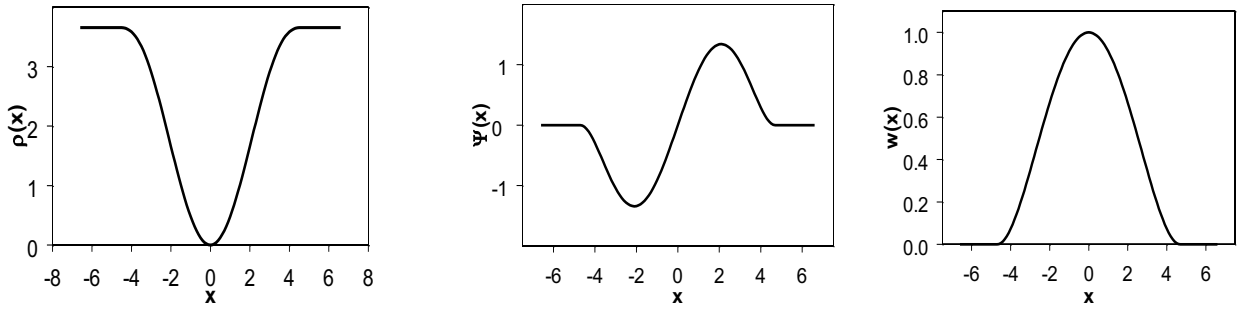

Figure 1: ρ, ψ and w functions of Tuckey's biweight robust estimate

Iterated reweighted least squares technique is used to solve the minimization problem in eq. (2) to obtain the robust estimate of the regression function. The estimate of the regression function in the k^{th} iteration is given by

$$\widehat{\mathbf{m}}_{(k)} = \mathbf{X}\widehat{\boldsymbol{\beta}}_{(k)} + \widehat{\boldsymbol{\Phi}}_{(k)}$$

$$\widehat{\boldsymbol{\beta}}_{(k)} = \left[\mathbf{X}^T\left(\mathbf{I} - \mathbf{S}_{(k)}\right)\mathbf{X}\right]^{-1}\mathbf{X}^T\left(\mathbf{I} - \mathbf{S}_{(k)}\right)\boldsymbol{Y}$$

$$\widehat{\boldsymbol{\Phi}}_{(\mathbf{k})} = \mathbf{S}_{(k)}\left(\mathbf{Y} - \mathbf{X}\widehat{\boldsymbol{\beta}}_{(k)}\right)$$

where, $\mathbf{S}_{(k)}$ is the smoothing matrix in the k^{th} iteration derived using robust local linear regression. Let $\mathbf{S}_{i(k)}$be the i^{th} row of the smoothing matrix in the k^{th} iteration, then

$$\mathbf{S}_{(k)} = \left[\mathbf{S}_{1(k)} \dots \mathbf{S}_{n(k)}\right]^T$$

$$\mathbf{S}_{i(k)}^T = \boldsymbol{e}_1^T\left(\mathbf{Z}_{u_i}^T\mathbf{W}_{u_i(k)}^*\mathbf{Z}_{u_i}\right)^{-1}\boldsymbol{Z}_{u_i}^T\boldsymbol{W}_{u_i(k)}^*$$

$$\mathbf{W}_{u_i(k)}^* = diag\left\{w_i^*\left(r_{1(k-1)}\right), \dots, w_i^*\left(r_{n(k-1)}\right)\right\}$$

$$w_i^*\left(r_{j(k-1)}\right) = \frac{K\left(\frac{u_i - u_j}{h}\right)w\left(r_{j(k-1)}\right)}{\sum_{l=1}^{n} K\left(\frac{u_i - u_l}{h}\right)w\left(r_{l(k-1)}\right)}, \qquad j = 1, \dots, n$$

where $w\left(r_{j(k-1)}\right)$is the value of the robustness weight function corresponding to y_j in the k^{th} iteration and $r_{(k-1)j} = \frac{[y_j - \widehat{m}_{j(k-1)}]}{s_{(k-1)}}$ is the standardized residual of the j^{th} datum in the $(k\text{-}1)^{\text{th}}$ iteration with $\widehat{m}_{j(k-1)}$ as the estimated value and $r_{(0)i}$=0 for i=1,…,n. The Median of Absolute Deviation from median (*MAD*) is used for computing a robust estimate for the scale factor s and

$$s_{(k-1)} = \frac{\underset{i}{median}\left|e_{(k-1)i} - \underset{j}{median}(e_{(k-1)j})\right|}{0.6745}$$

where $e_{(k-1)i} = y_i - \hat{m}_{i(k-1)}$

The estimate of the regression function in the k^{th} iteration is written as

$$\hat{\mathbf{m}}_{(k)} = \mathbf{X}\hat{\boldsymbol{\beta}}_{(k)} + \mathbf{S}_{(k)}\left(\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}}_{(k)}\right)$$

Iteration is continued till there is no significant improvement in the estimated values and the final estimate of the regression function is written as

$$\hat{\mathbf{m}}^* = \mathbf{X}\hat{\boldsymbol{\beta}}^* + \mathbf{S}^*(\mathbf{Y} - \mathbf{X}\hat{\boldsymbol{\beta}}^*)$$
$$\hat{\boldsymbol{\beta}}^* = [\mathbf{X}^T(\mathbf{I} - \mathbf{S}^*)\mathbf{X}]^{-1}\mathbf{X}^T(\mathbf{I} - \mathbf{S}^*)\mathbf{Y}$$
$$V(\hat{\boldsymbol{\beta}}^*) = diag(\mathbf{P}^*\mathbf{P}^{*T})\hat{\sigma}^{*2}$$

Where $\mathbf{S}^*$ is the smoothing matrix of the final iteration, $\hat{\mathbf{m}}^*$, $\hat{\boldsymbol{\beta}}^*$ and $\hat{\sigma}^*$ are the final estimates of the regression function, treatment vector and scale factor respectively and

$$\mathbf{P}^* = (\mathbf{X}^T(\mathbf{I}\text{-}\mathbf{S}^*)\mathbf{X})^{-1}\mathbf{X}^T(\mathbf{I}\text{-}\mathbf{S}^*)$$

Optimum bandwidth: Let $w_i^{\#}$ be the final robustness weight assigned to y_i and $\hat{m}_{i(h)}^{\#}$ be the estimated value of m_i with bandwidth h. The Mean Squared Error (*MSE*) of the estimated value corresponding to the bandwidth h is given by

$$MSE(h) = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - \hat{m}_{i(h)}^{\#}\right)^2$$

The cross validation score $CV(h)$ does not work well for the robust smoothers because the *CV* function itself is strongly influenced by the outliers (Wang and Scott, 1994). The cross validation score is the sum of squares of the prediction errors of the smoother at each of the design points. When there are outliers, the prediction errors corresponding to the outliers will be uncharacteristically extreme and these extreme prediction errors will inflate the $CV(h)$. Therefore, similar to robust smoothing technique, the influence of extreme prediction errors should be minimized. A robust cross validation score $RCV(h)$ is defined as

$$RCV(h) = \frac{\sum_{i=1}^{n} w_i^{\#}\left(y_i - \hat{m}_{(-i)(h)}^{\#}\right)^2}{\sum_{i=1}^{n} w_i^{\#}}$$

where, $w_i^{\#}$ is the final robustness weight defined earlier, $\hat{m}_{(-i)(h)}^{\#}$ is the robust estimate of y_i with h as bandwidth and without using the i^{th} observation y_i. The value of h which minimizes the robust cross validation score $RCV(h)$ will be the optimum bandwidth. In the computation of $RCV(h)$, the effect of outliers is controlled by taking weighted sum of squares of the prediction errors of the smoother at each of the design points with the robustness weight $w_i^{\#}$.

4. Simulation Study

A simulation study was conducted to evaluate the performance of the proposed method. The semi-parametric regression model considered for the simulation study is given by

$$\mathbf{Y}=\mathbf{X}\boldsymbol{\beta}+\phi(\mathbf{U})+\boldsymbol{\varepsilon} \tag{3}$$

where $\mathbf{Y}$ is the n x 1 observation vector, $\mathbf{m}=\mathbf{X}\boldsymbol{\beta}+\phi(\mathbf{U})$, is the regression function, $\mathbf{X}$ is the nxk design matrix, $\boldsymbol{\beta}$ is the k x 1 treatment effect vector which is taken as $\boldsymbol{\beta}^T$=[-2 -2 0 4], $\phi(u)=1+2sin(\pi u)$ and the random error vector $\boldsymbol{\varepsilon}$ follows $N(\mathbf{0}, \sigma^2\mathbf{I})$ and uϵ[0,1]. Based on the above, 100 sets of data are simulated for different values of n (100, 200, 400) and σ (1.0, 2.0) with 0%, 4% and 8% outliers. To generate data with specific percentage of outliers, the required number of random numbers between 0 to n are generated and the value of the regression function m corresponding to the data points are replaced with $m+6\sigma$. The Epanechnikov kernel function $K(u)=0.75(1-u^2)$ is employed in the study. The treatment effect vector $\boldsymbol{\beta}^T=[\beta_1\ \beta_2\ \beta_3\ \beta_4]$, the nonparametric function ϕ and the error variance σ^2 are estimated using the method given in Section 2. Tuckey's biweight function with the turning point c=4.685 is used as the robustness function. The Average Mean Squared Errors (*AMSE*) of the estimated values of σ, $\boldsymbol{\beta}$, $\boldsymbol{\phi}$ and $\mathbf{m}$ with the true values of 100 sets of simulated data for different values of n (100, 200, 400) and σ (1.0, 2.0) are given in Table 2. The *AMSE* of the estimated parameters are calculated as follows:

$$AMSE \text{ of } \hat{\sigma}=\frac{1}{100}\sum_{i=1}^{100}\left(\sigma-\hat{\sigma}_{(i)}\right)^2,$$

$$AMSE \text{ of } \hat{\boldsymbol{\beta}}=\sum_{j=1}^{4}\frac{1}{100}\sum_{i=1}^{100}\left(\beta_j-\hat{\beta}_{j(i)}\right)^2$$

$$AMSE \text{ of } \hat{\boldsymbol{\phi}}=\frac{1}{100}\sum_{i=1}^{100}\frac{1}{n}\sum_{j=1}^{n}\left[\phi(u_j)-\hat{\phi}_{(i)}(u_j)\right]^2,$$

$$AMSE \text{ of } \hat{\mathbf{m}}=\frac{1}{100}\sum_{i=1}^{100}\frac{1}{n}\sum_{j=1}^{n}\left[m-\hat{m}_{(i)}(u_j)\right]^2$$

where, $\hat{\sigma}_{(i)}$, $\hat{\beta}_{j(i)}$, $\hat{\phi}_{(i)}$ and $\hat{m}_{(i)}$ are the estimated values of σ, β_j, ϕ and the regression function m corresponding to the i^{th} simulated data set. The bias of the point estimates of $\hat{\sigma}, \hat{\beta}_j$, j=1,…,4 are calculated as follows

$$\text{Bias of } \hat{\sigma}=\frac{1}{100}\sum_{i=1}^{100}\left(\sigma-\hat{\sigma}_{(i)}\right)$$

$$\text{Bias of } \hat{\beta}_j=\frac{1}{100}\sum_{i=1}^{100}\left(\beta_j-\hat{\beta}_{j(i)}\right),\ j=1,\ldots,4$$

The *AMSE* of the estimates are converging to zero as n increases or in other words, the estimated values are converging to the true values as n increases. Note that the bias of the point estimates $\hat{\sigma}, \hat{\beta}_j, j=1,\ldots,4$ are also negligible as n increases (Table 2). This indicates the consistency of the estimates. The *MSE* varies with change in the choice of bandwidths. The optimum bandwidth (bandwidth corresponds to the minimum *MSE*) depends on the curvature of the function. The optimum bandwidth for estimating the parameters of the model was obtained based on the robust cross validation technique given in Section 2.

The comparison of Average Mean Squared Errors (*AMSE*) of the estimated values of σ, $\boldsymbol{\beta}$, $\boldsymbol{\phi}$ and **m** with the true values of 100 sets of simulated data for different values of *n* (100, 200, 400) and σ(1.0, 2.0) showed that in the presence of outliers (4% and 8%) the robust method performs much better than the non-robust method. In the absence of outliers the performance of both the robust and non-robust methods is almost the same. The value of *AMSE* decreases as *n* increases or in other words the estimates converges to the true value.

5. Application

The proposed method is used to analyze the yield data (both weight of nuts and number of nuts) of arecanut recorded in an experiment to evaluate the effects of organic and inorganic fertigation in arecanut + cocoa systems conducted at Central Plantation Crops Research Institute, Vittal, India. The experiment consists of 6 levels of nutrition (denoted as $\beta_1, \ldots, \beta_6$) applied randomly to 12 year old arecanut palms to evaluate their effect on the yield of arecanut. Treatments were applied to a total of 253 arecanut palms. Pre-treatment yield was taken as the covariate to control the error due to palm to palm variation. The yield obtained after a gap of two year from the start of the experiment was taken as the response variable. The estimated treatment effects and its standard errors using the linear covariance technique, nonparametric covariance technique as well as the robust nonparametric covariance technique with pre-treatment yield as covariate for both weight of nuts and number of nuts are given in Table 3 and 4 respectively. Even though, there is not much difference in the estimated value of the treatment effects employing different methods, the standard error of the estimates are comparatively lower in the case of the proposed robust technique. Since the outliers are present in both the extremes (high and low) and the number of observations is also high, the difference in treatment effects estimated using robust and other methods are very less. The estimated value of σ corresponding to the linear, nonparametric and robust nonparametric covariance technique for weight of nuts and number of nuts are also given in Table 3 and 4 respectively. The standard errors of the estimates and the estimated value of σ are less in the proposed robust method than that of the linear and nonparametric covariance technique.

6. Conclusion

Linear covariance technique is generally used for analysing the designed experiments having covariates, assuming a linear relationship between response and covariate. A more flexible semi-parametric model is used when the relationship is not linear or unknown. The experimental data particularly, those from field experiments generally contains some extreme values or outliers due to large plant to plant variations and their presence very badly affect the analysis and generate distorted results. In the present study, a robust method is proposed to analyse the semi-parametric regression model in the presence of outliers. The proposed method is useful when the data contains extreme values or outliers and there is no advance information about the relationship between the response variable and covariate.

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Appendix

Table 1: Optimum bandwidth ad *AMSE* of the estimates in the simulation study

σ	Outliers (%)	n	h	$AMSE(\hat{\boldsymbol{\beta}})$		$AMSE(\hat{\boldsymbol{\phi}})$		$AMSE(\hat{\mathbf{m}})$		$AMSE(\hat{\sigma})$	
				SP	Robust SP	SP	Robust SP	SP	Robust SP	SP	Robust SP
1	0	100	0.30	0.1486	0.1471	0.0796	0.0541	0.0731	0.0664	0.0064	0.0182
		200	0.20	0.0720	0.0740	0.0309	0.0256	0.0398	0.0389	0.0030	0.0078
		400	0.15	0.0315	0.0341	0.0167	0.0148	0.0215	0.0218	0.0011	0.0033
	4	100	0.30	0.3712	0.1741	0.0946	0.0608	0.1835	0.0810	0.3194	0.0143
		200	0.25	0.1656	0.0849	0.0522	0.0308	0.1041	0.0408	0.3089	0.0080
		400	0.15	0.0774	0.0384	0.0459	0.0162	0.0944	0.0241	0.2948	0.0038
	8	100	0.25	0.5138	0.1793	0.2440	0.0594	0.4018	0.0846	0.8825	0.0180
		200	0.25	0.2285	0.0985	0.1704	0.0285	0.2723	0.0439	0.8511	0.0133
		400	0.25	0.1250	0.0548	0.1440	0.0179	0.2222	0.0231	0.8331	0.0121
2	0	100	0.30	0.5399	0.5672	0.1913	0.1591	0.2631	0.2588	0.0188	0.0644
		200	0.30	0.3009	0.3142	0.1144	0.0887	0.1451	0.1452	0.0101	0.0415
		400	0.25	0.1463	0.1530	0.0543	0.0401	0.0689	0.0674	0.0043	0.0125
	4	100	0.30	1.4690	0.6348	0.3745	0.1797	0.7428	0.2981	1.2803	0.0432
		200	0.30	0.5670	0.2865	0.2134	0.0931	0.3958	0.1386	1.2292	0.0281
		400	0.20	0.3239	0.1418	0.2455	0.0509	0.3576	0.0810	1.1912	0.0224
	8	100	0.30	1.7699	0.6486	1.0668	0.1936	1.6062	0.3138	3.3692	0.0716
		200	0.30	0.9476	0.3266	0.6910	0.0900	1.0818	0.1394	3.3647	0.0584
		400	0.25	0.4338	0.1461	0.7617	0.0442	0.9799	0.0709	3.3693	0.0576

SP: Semi- parametric

Table 2: Bias of the robust point estimates in the simulation study

σ	Outliers (%)	n	h	Bias of				
				$\hat{\beta}_1$	$\hat{\beta}_2$	$\hat{\beta}_3$	$\hat{\beta}_4$	$\hat{\sigma}$
1	0	100	0.30	–0.0184	–0.0187	0.0201	0.0169	–0.0610
		200	0.20	–0.0182	–0.0157	0.0155	0.0185	–0.0282
		400	0.15	0.0026	–0.0053	0.0127	–0.0100	–0.0187
	4	100	0.30	–0.0232	0.0100	–0.0010	0.0143	0.0440
		200	0.25	–0.0161	0.0112	–0.0002	0.0051	0.0346
		400	0.15	0.0033	0.0019	–0.0004	–0.0048	0.0294
	8	100	0.30	–0.0002	0.0166	–0.0077	–0.0088	0.0851
		200	0.25	–0.0008	0.0093	–0.0084	0.0000	0.0789
		400	0.20	0.0010	0.0039	–0.0058	0.0010	0.0745
2	0	100	0.30	–0.0060	–0.0079	0.0055	0.0085	–0.1037
		200	0.25	–0.0090	0.0234	–0.0156	0.0013	–0.0586
		400	0.20	–0.0030	0.0040	–0.0060	0.0051	–0.0398
	4	100	0.30	0.0222	–0.0271	–0.0120	0.0168	–0.0558
		200	0.25	0.0131	–0.0135	–0.0110	0.0114	0.0490
		400	0.20	–0.0060	0.0184	–0.0088	–0.0037	0.0445
	8	100	0.30	–0.0132	0.0294	–0.0131	–0.0031	0.1248
		200	0.30	–0.0143	0.0292	–0.0061	–0.0089	0.1160
		400	0.25	–0.0117	0.0202	–0.0106	0.0020	0.1119

Table 3: Estimated values with standard errors (weight of nuts) of the field data

Parameter	Linear		Semi-parametric		Robust Semi-parametric	
	Estimate	SE	Estimate	SE	Estimate	SE
$\mu + \beta_1$	9.969	0.683	9.924	0.622	9.925	0.548
$\mu + \beta_2$	9.414	0.683	9.570	0.626	9.573	0.552
$\mu + \beta_3$	10.029	0.638	9.949	0.594	9.950	0.524
$\mu + \beta_4$	9.883	0.675	9.994	0.617	9.991	0.543
$\mu + \beta_5$	9.922	0.691	9.918	0.636	9.916	0.560
$\mu + \beta_6$	10.767	0.630	10.758	0.587	10.758	0.517
σ	4.317		4.312	-	3.803	-

μ: Overall mean

Table 4: Estimated values with standard errors (number of nuts) of the field data

Parameter	Linear		Semi-parametric		Robust Semi-parametric	
	Estimate	SE	Estimate	SE	Estimate	SE
$\mu + \beta_1$	328.80	22.71	331.96	20.71	330.80	16.83
$\mu + \beta_2$	307.84	22. 70	308.87	20.70	308.85	16.83
$\mu + \beta_3$	331.13	21.12	334.87	19.62	336.45	15.95
$\mu + \beta_4$	332.86	22.40	336.57	20.45	337.32	16.63
$\mu + \beta_5$	324.32	22.91	315.21	21.27	313.69	17.29
$\mu + \beta_6$	370.57	20.87	374.34	19.35	374.71	15.72
σ	143.06		142.96		116.16	

μ: Overall mean

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Privacy Protection in Optional Randomized Response Surveys for Quantitative Characteristics

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Abstract

A survey regarding sensitive or stigmatizing issues often bears a challenge as most respondents either deny answering direct queries or hide true response. Warner (1965) designed an ingenious device by a dint of a probabilistic procedure for estimating qualitative sensitive population proportion, called randomized response (RR) device and the novel technique is well known as randomized response technique (RRT). Greenberg et al. (1971) used the RR technique in quantitative attributes. An issue often raised with RRT is that some are more willing to answer directly rather than compulsory RR as the perception of sensitivity may not be same for all. Considering this fact, Chaudhuri and Mukerjee (1985) developed the optional randomized response technique (ORRT) which was restricted to Simple Random Sampling (SRS) design only. Later Chaudhuri and Saha (2005), Pal (2008) extended their work for unequal probability sampling. We discuss here about the privacy protection measure dealing with quantitative sensitive issues like alcohol consumption, earning through gambling, income etc. The literature is an extension of Chaudhuri and Christofides (2013) aiming at to develop how privacy is protected while applying ORRT into quantitative sensitive issues. In this paper we theoretically develop few well known RRTs for quantitative case in ORRT context first and unbiased estimators with its variance estimators are obtained. Protections of privacy of the proposed techniques are measured theoretically.

Key words: Protection of privacy, randomized response, sensitive issues, quantitative characteristics, unequal probability.

1. Introduction

Enumeration related to sensitive issues like alcohol consumption, drug addiction etc is usually impossible by direct survey method because the respondents may fear oppression if they disclose their actual status. Randomized response technique (RRT) refers to a widely used method for estimating population proportion or others which is related to a sensitive characteristic avoiding the direct queries. Warner (1965) developed the novel RRT technique. Erikson (1973) presented the estimation of total stigmatizing real variable like amount earns through gambling, alcohol consumption etc. Chaudhuri and Mukherjee (1985, 1988) illustrated optional randomized response technique (ORRT) while respondents were selected by SRS with replacement only. Later Arnab (2004) and Chaudhuri and Saha (2005) extended the theory in unequal probability design. Chaudhuri (2011), Chaudhuri and Christofides (2013) provide extensive developments in RRT, also in ORRT along with protection of privacy measures. For further references and recent developments, please refer to a monograph edited by Chaudhuri, Christofides, Rao (2016). Full ORRT and partial ORRT are

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two classifications in ORRT. In the first one, overall sample of respondents are classified into two parts to gather direct response (DR)'s from one part and randomized response (RR) from another part. The final estimator was constructed by combining two linear unbiased estimators based on DR and RR separately. Arnab (2018) and many others had contributed in this full ORRT approach. In partial ORRT, DR option is offered along with a RR device to the respondents and respondents are requested to report the response directly if he/she does not feel the survey question sensitive otherwise it will be answered by using RR device without divulging the option so exercised.

The purpose of this paper is to extend some well-known quantitative RR technique in partial ORRT along with the study of their privacy protection capacity as the motivation of RRT is to gather information maintaining the respondents' confidentiality. Section 2 is designed for the extension of Chaudhuri's device I and device II (2011) and Eichhorn and Hayre (1983) in partial ORRT. In section 3, we briefly discuss the protection of privacy for different partial ORRT. In section 4, we provide the measures of jeopardy related to the proposed ORR models as discussed in section 2.

2. Proposed ORR Models for Quantitative Characteristics

Initially the basic purpose of RR was to gather reliable information on qualitative sensitive variables. Greenberg et al. (1971) first developed the RR technique for quantitative stigmatizing characteristics. Eriksson (1973) also extended the well-known unrelated question model in quantitative response concept. Taking the initial idea of masking true sensitive values by a random number from known distribution, Eichhorn and Hayre (1983) developed scrambled response model. Chaudhuri (2011) and Chaudhuri and Mukerjee (1988) in their books have mentioned two different randomized devices (Device I and Device II) along with the estimation of total amount and the variance relating to such sensitive issues. Following the idea of the above, we try to develop ORRT in quantitative measures which are as well as sensitive also.

Consider a finite population of units $U = (1, 2, 3, ..., N)$ and let Y be the quantitative stigmatizing variable having the values $y_1, y_2, ...y_i, ..., y_N$. A sample s of size n is chosen from the population according to a general sampling scheme P. The sampled persons are approached with a request to provide ORR responses for estimating the population total $Y = \sum_{i=1}^{N} y_i$ based on the sample s.

2.1. ORR using Eichhorn and Hayre (1983)

Pollock and Bek (1976) envisaged the data masking procedure to answer the sensitive question hiding his/her actual value by adding a random value from known distribution with the true value. The development of Eichhorn and Hayre (1983) method known as "Scrambled Response method" is actually in-depth analysis of Pollock and Bek (1976). In this part of this literature, we use the scramble response method to develop optional randomized response (ORR) model. Pal (2008) already worked on this by capturing two responses for each respondent giving an opportunity to report the second response as the earlier one with known probability p or by using other random variables with known probability $1 - p$. Our proposed ORR method is a modification on Pal (2008).

Let y_i be the true sensitive value of the i^{th} respondent $(i = 1,2,....,N)$. Let X denote a discrete random variable with known mean θ_1 and variance σ_1^2. Also, let Ψ be another discrete random variate independent to X, with known mean 0 and variance σ_2^2. Considering the fact that someone may wish to answer directly of the sensitive question, we give them a choice of direct response (y_i) or by randomized value (I_i) instead of compulsory RR. The procedure is known as ORRT as discussed in the introduction section. Here $I_i = \frac{y_i x_i}{\theta_1} + \psi_i$ while x_i and ψ_i are the values of the random variable X and Ψ respectively for i^{th} individual and $i = 1,2,..., N$.

Mathematically the response of i^{th} person may be written as,

$z_i = y_i$ with unknown probability $c_i \in [0,1]$

$= \frac{y_i x_i}{\theta_1} + \psi_i$ with unkonwn probability $1 - c_i$

Denoting E_R as expectation due to RR device and V_R as variance due to RR device, we get $E_R(z_i) = c_i y_i + (1 - c_i)\{\frac{y_i \theta_1}{\theta_1} + 0\} = y_i$ and

$V_R(z_i) = E_R(z_i^2) - E_R{}^2(z_i)$

$= c_i y_i^2 + (1 - c_i)\{\frac{y_i^2}{\theta_1^2}(\sigma_1^2 + \theta_1^2) + \sigma_2^2 + 2\frac{y_i \theta_1}{\theta_1}.0\} - y_i^2$

$= (1 - c_i)(\frac{y_i^2 \sigma_1^2}{\theta_1^2} + \sigma_2^2)$ which is unknown to us as y_i is unknown.

So, to estimate the variance, the whole process is repeated independently one more time to get another response z_i'. Technique of interpenetrating network of subsampling pioneered by Mahalanobis (1946) is used here to provide the final RR based estimator of y_i, which becomes $r_i = \frac{z_i + z_i'}{2}$ with variance estimator $v_i^* = \frac{1}{4}(z_i - z_i')^2$.

2.2. ORR using Chaudhuri' s device I

In ***device I***, the person labeled "i" is directed to give out his/her true response regarding the sensitive issues directly or by the offered two randomized devices. That process is repeated two times independently with the same RR device but with different RR parameters. In one RR device, first box contains T (>1) cards identical in shape, size, color and height bearing real numbers $a_1, a_2, a_3, ...a_T$ with mean $\mu_a = \frac{1}{T}\sum_i a_i = 1$ and the second box contains M (>1) identical cards with real numbers $b_1, b_2, b_3, ..., b_M$. In another RR device, T' cards $a_1', a_2' ....a_{T'}'$ bearing real numbers with mean 1 are placed in first box and M' cards $b_1', b_2', ...b_{M'}'$ bearing real numbers but the mean $\mu_{b'} = \frac{1}{M'}\sum_i b_i' \neq \mu_b = \frac{1}{M}\sum_i b_i$ are placed in the second box. The sampled person i is instructed to draw independently one card from each

box for both the RR devices and report the number $z_i = a_j y_i + b_k \ \ (j = 1,2,...,T \ \ k = 1,2,...,M)$ and $z_i' = a_j' y_i + b_k' \ \ (j = 1,2,...,T' \ \ k = 1,2,...M')$without disclosing the numbers drawn from the boxes and y_i is defined for the amount related to the sensitive quantitative variable Y.

In our proposed method, the optional randomized response for i^{th} person is

$z_i = y_i$ with unknown probability $c_i \in [0,1]$

$= a_j y_i + b_k$ with unknown probability $1 - c_i$

$z_i' = y_i$ with unknown probability c_i

$= a_j' y_i + b_k'$ with unknown probability $1 - c_i$

Writing, $E_R(z_i) = c_i y_i + (1 - c_i)(\mu_a y_i + u_b)$ and $E_R(z_i') = c_i y_i + (1 - c_i)(\mu_{a'} y_i + u_{b'})$. It follows $r_{1i} = \dfrac{\mu_{b'} z_i - \mu_b z_i'}{\mu_{b'} - \mu_b}$; $\mu_{b'} \neq \mu_b$ such that $E_R(r_{1i}) = y_i$.

To estimate the variance, the process is repeated independently one more time (as described in 2.1.) and the responses for the i^{th} person are (g_i, g_i') with corresponding estimator of y_i is $r_{2i} = \dfrac{\mu_{b'} g_i - \mu_b g_i'}{\mu_{b'} - \mu_b}$; $\mu_{b'} \neq \mu_b$. So the final RR based estimator of y_i is $r_i^* = \dfrac{r_{1i} + r_{2i}}{2}$ with the variance estimator $v_i^* = \dfrac{1}{4}(r_{1i} - r_{2i})^2$ such that $E_R(r_i^*) = y_i$.

2.3. ORR using Chaudhuri's device II

In ***device II***, a box with full of different kind of cards is given to the sampled person. The cards are marked as "corrected" with proportion k and others bearing with numbers $x_1, x_2, ..., x_M$ in proportion $q_1, q_2, ..., q_M$ such that $\sum_{i=1}^{M} q_i = 1 - k$. The sampled person is directed to draw a card randomly and report the true sensitive value $(i.e.\ y_i)$ if he gets a card marked as "corrected" otherwise report the number $x_j \ \ (j = 1,2,...,M)$ printed over the cards. The procedure is extended to ORRT by giving a choice of direct response or RR *device II* to the sampled person whichever he is willing too.

So the optional randomized response of i^{th} person is:-

$z_i = y_i$ with unknown probability $c_i \in [0,1]$

$= y_i$ with known proportion of cards (k) marked as "corrected" and unknown probability $(1 - c_i)$

$= x_j$ with unknown probability $q_j(1 - c_i)$

It follows that, $E_R(z_i) = c_i y_i + (1 - c_i)(k y_i + \sum_{j=1}^{M} q_j x_j)$. The whole process is repeated independently one more time with different set of cards in different proportion and the response is recorded as z_i'. Clearly, $E(z_i') = c_i y_i + (1 - c_i)(k' y_i + \sum_{j=1}^{M} q_j' x_j')$.

So, $E_R((1-k')z_i-(1-k)z_i')=(k-k')y_i+(1-c_i)[(1-k')\sum_{j=1}^{M}q_jx_j-(1-k)\sum_{j=1}^{M}q_j'x_j'].$

The sensitive attribute y_i is estimable if $(1-k')\sum_{j=1}^{M}q_jx_j-(1-k)\sum_{j=1}^{M}q_j'x_j'=0$.

i.e. $E_R[\frac{(1-k')z_i-(1-k)z_i'}{(k-k')}]=y_i$ if $\frac{1-k'}{1-k}=\frac{\sum_{j=1}^{M}q_j'x_j'}{\sum_{j=1}^{M}q_jx_j}$.

The final RR based estimator with the variance estimator can be obtained similarly as discussed in sections 2.1. and 2.2. in this article.

3. Privacy Protection Measures

The objective of performing RR survey is to produce a good estimator from statisticians' point of view for sensitive traits. As the respondents' actual state of nature is covered by RR device, it is necessary to know whether the procedure assures all the respondents that they could not definitely be classified in A or A^ci.e. protection of privacy measure. Undoubtedly, greater the protection; increase the participation but it has to be noted that no universally accepted measure is mentioned there. Privacy measure have been studied earlier by many researchers like Lanke (1975, 1976), Leysieffer and Warner (1976), Anderson (1975 a, b, c). Leysieffer and Warner (1976) suggested a jeopardy measure by quantifying the probability of an observation belonging to the sensitive trait A and its complement A^c, while giving his/ her response as R , termed as *revealing probabilities.* Lanke (1976) considered the quantity $g(A)=\max\{P(A\mid R=1),P(A\mid R=0)\}$ for comparison implying smaller the value of $g(A)$ is more protective than other. To evaluate how effectively the scrambling response model works, Eichhorn and Hayre (1983) proposed a privacy measure based on the ratio of the upper limit and lower limit of $100(1-\alpha)$confidence interval for the mean of the scrambling variable X . For a given α , larger the ratio implies greater the protection.

In order to evaluate how privacy is protected for quantitative sensitive variable is also investigated by Chaudhuri and Christofides (2013). Considering the prior unknown probability for the value y_i of i^{th} person as $L(y_i)=L_i$, by Bayes' theorem the posterior probability of y_i for the given value of z_i turns out to be,

$$L(y_i\mid z_i)=\frac{L_iP(z_i\mid y_i)}{P(z_i)} \tag{1}$$

where $P(z_i\mid y_i)$ denotes the conditional probability of reported RR value for the i^{th} person while true response is y_i. The degree of privacy protection measure is maximum, if the value of the measure approaches to one.

Taking a cue from the above approach, the idea of measuring protection of privacy for quantitative ORR model has been developed here.

4. Measures of Jeopardy

Suppose that y be the real stigmatizing quantitative variable for a set of finite population $U=(1,2,...,i,...,N)$ having values $y_1,y_2,....y_i,...y_N$ and the total be defined as $Y=\sum_{i=1}^{N}y_i$. In order

to estimate Y, a sample s is selected with probability $p(s)$ from the population U and respective ORR technique is performed to record their responses for further analysis.

4.1. Using Eichhorn and Hayre (1983) method

To check how well the response is protected in case of ORR survey while scrambled response method is used for RR value, responses are gathered by following the step by step guidance as described in the section 2.1. The conditional probability of the i^{th} person can be calculated by the following function

$$P(z_i \mid y_i) = c_i + (1-c_i)(\sum_{x_j} P(X = x_j)P(\Psi = z_i - \frac{y_i x_j}{\theta_1})),$$

as the respondent disclose the true response with probability c_i (at this point $z_i = y_i$) otherwise provide the randomized response with probability $1-c_i$ following Eichhorn and Hayre (1983) suggestion (as described briefly in section 2.2) which is equal to z_i if the randomized value of the variate X is x_i along with another variate (Ψ) value ψ_i.

Also, the probability that the i^{th} respondent gives the response z_i is defined as $P(z_i) = c_i + (1-c_i)(\sum_{x_j} P(X = x_j)P(\Psi = z_i - \frac{y_i x_j}{\theta_1}))$, this is exactly equal to the above given conditional probability.

So from equation (1), we get $L_i(y_i \mid z_i) = L_i$ *i.e.* posterior probability = prior probability. Clearly privacy is well protected for each individual by this method.

4.2. Using Chaudhuri's device I

For this model, the conditional probability of the given response z_i, while the actual response is y_i, denoted by $P(z_i \mid y_i)$, is evaluated as $P(z_i \mid y_i) = c_i + \frac{1}{TM}(1-c_i) = P(z_i)$. This indicates the posterior probability exactly equal to the prior probability L_i, *i.e.* the i^{th} respondent's privacy are well protected, as well as all the respondents.

4.3. Using Chaudhuri's device II

To check whether their response is well protected or not while device II is suggested for ORR survey, we calculate the posterior probability $L_i(y_i \mid z_i)$ by Bayes' theorem as defined in section 3 by following Chaudhuri and Christofides (2013). Here,

$$L_i(y_i \mid z_i) = \frac{L_i(c_i + k(1-c_i))}{L_i(c_i + k(1-c_i)) + (1-L_i)(1-c_i)(1-k)} = [1 + \frac{1-L_i}{L_i}\frac{\theta_i}{1-\theta_i}]^{-1}$$

considering $\theta_i = (1-c_i)(1-k)$.

Thus, $L_i(y_i \mid z_i)$ approaches to L_i if and only if $\theta_i \to \frac{1}{2}$. We can't say anything else as θ_i is unknown to us.

5. Concluding Remarks

Main purpose of this article is to demonstrate the accuracy level of privacy protection while studying quantitative and sensitive characteristics by optional RR survey. Few of the well-known quantitative RR models are illustrated in ORR context to investigate their degree of protection in privacy. Their performance levels are pointed out in Section 4. The posterior and prior coincide in our proposed quantitative ORR model if the randomized device is either Eichhorn and Hayre (1983) or Chaudhuri 's ***device I***.

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Construction of Optimal Foldover Designs with the General Minimum Lower-Order Confounding

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Abstract

Fractional factorial designs are widely used in industry and agriculture. Foldover fractional factorial designs can de-alias effects of interest so that the effects can be estimated without ambiguities. We consider optimal foldover designs using general minimum lower-order confounding criterion. A catalogue of 16- and 32-run optimal foldover designs is constructed and tabulated for practical use. A comparison is made between the general minimum lower-order confounding optimal foldover designs and other optimal foldover designs obtained using minimum aberration and clear effect criteria.

Key words: Foldover; Alias; Optimal designs; Aliased effect number pattern.

1. Introduction

Fractional factorial designs have been widely used in industry and agriculture. One problem an experimenter is likely to face by employing a fractional factorial design is that some effects may be aliased with others. This creates ambiguities about the analysis and estimation of the factors. Hence, sometimes there is the need for additional runs to clarify these ambiguities. Foldover is a follow-up method that is often used to solve the problem.

Foldover designs have been in the literature for many years. Some textbook, such as, Box et al. (2005) and Wu and Hamada (2009) studied foldover techniques. Montgomery and Runger (1996) considered the foldover plans that reverse the signs of one or two factors. They pointed out that for a resolution IV initial design, when changing the signs of a factor of interest, the combined foldover design can de-alias all the two-factor interactions that contain the factor; Li and Lin (2003) searched optimal foldover plans using minimum aberration optimality criterion

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and provided catalogues of optimal foldover designs. However, Wang et al. (2010) pointed out that some optimal foldover designs in Li and Lin (2003) may not be optimal under the clear effect optimality criterion. Uniformity criteria were also used to construct optimal foldover designs. Ou et al. (2011) provided some lower bounds of centered L_2-discrepancy, the symmetric L_2-discrepancy and the wrap-around L_2-discrepancy on combined foldover designs that can be used to evaluate the optimal foldover plans for two-level fractional factorial designs. The lower bounds were further improved by Ou et al. (2017). Qin et al. (2013) extended the results in Ou et al. (2011) to a set of asymmetric fractional factorials and obtained a new lower bound of centred L_2-discrepancy of combined designs, which can be used as a benchmark for searching optimal foldover plans. Recently, Li and Lin (2016) proposed to further improve foldover designs by allowing column permutations. Yang and Li (2019) investigated under what circumstances can a foldover design be improved by doing column permutations and provided some theoretical results. For more work related to optimal foldover designs, see Li and Mee (2002), Li and Jacroux (2007), and Ai et al. (2010).

Optimal designs have been studied extensively in the literature recently. The most popular optimality criterion for fractional factorial designs is minimum aberration (MA). However, Minimum aberration criterion is used to choose designs in cases where there is very small or lack of knowledge about the likely important effects. Recently, Zhang et al. (2008) proposed the general minimum lower-order confounding (GMC) criterion to select optimal designs. This criterion reveals the basic information of all effects aliased with other effects at varying severity degrees in a design. In particular, when an experimenter has a prior knowledge about which factors are more important, the GMC optimal designs are better than other optimal designs. It has been proved that the GMC criterion chooses optimal designs in a more elaborate and explicit manner than the existing ones, such as minimum aberration, clear effects, and maximum capacity criteria. A lot of research has been done for constructing general minimum lower-order confounding designs. In particular, Zhang and Cheng (2010), Cheng and Zhang (2010), and Li et al. (2011) provided construction theory for two-level unblocked GMC designs, and Zhang and Mukerjee (2009) and Zhao et al. (2013) constructed two-level blocked GMC designs.

Some optimality criteria, such as minimum aberration and clear effects criteria, have been used to finding optimal foldover designs. Most of the optimal foldover designs in the literature are obtained from the minimum aberration designs tabulated in Chen et al. (1993). Zhang et al. (2008) obtained a catalogue of optimal GMC designs which are more useful comparing to MA designs when experimenters have prior knowledge about the important factors. The objective of this research is to find the optimal foldover plans using the general minimum lower-order confounding criterion from the GMC designs tabulated in Zhang et al. (2008). We then compare our results to the optimal foldover designs under the minimum aberration and clear effects criteria.

In section 2, we introduce aliased effect number pattern and general minimum lower-order confounding criterion. Minimum aberration and clear effects criteria will also be introduced. Some relationships between these criteria are mentioned as well as their limitations and drawbacks. The relationships of aliased effect number patterns between initial designs and combined foldover designs are presented in section 3. In section 4, we present optimal foldover designs obtained using general minimum lower-order confounding criterion, minimum aberration, and clear effects criteria. The comparison between those optimal foldover designs are made.

2. GMC Criterion, Foldover Designs and Other Optimality Criteria

Let n be the number of factors of a design and p be the number of generators. For a given 2^{n-p} design, we can find how ith-order effects and jth-order effects of the design are aliased with each other. When ith-order effects is aliased with k jth-order effects, we say that the *degree* of ith-order effects being aliased with jth-order effects is k. The number of ith-order effects that are aliased with jth-order effects at degree k is denoted by ${}_i^{\#}C_j^{(k)}$, which tells us how severe ith-order effects are aliased with jth-order effects. At the same time, it also tells how many ith-order effects are aliased with jth-order effects. It reveals the general aliasing that exists among effects. All the ${}_i^{\#}C_j^{(k)}$'s in a design forms a set

$$\{{}_i^{\#}C_j^{(k)}, i = 0, 1, 2, ..., n, j = 0, 1, 2, ...n, k = 0, 1, 2, ..., \binom{n}{j}\}.$$

The smaller the degree at which an ith-order effect is aliased with other effects, the less difficult it becomes in estimating the effect. Moreover, since the total number of i-th order effects of a design is $\binom{n}{i}$, the smaller the ${}_i^{\#}C_j^{(0)}$, that is, the smaller the number of i-th order effects that are not aliased j-th order effects, the more the severity of the confounding between ith-order effects and jth-order effects. On the other way, when the value of ${}_i^{\#}C_j^{(0)}$ is greater, the less severity of ith-order effects are aliased with jth-order effects.

Since for different k, ${}_i^{\#}C_j^{(k)}$s are not equally important. As the degree k increases, the severity of aliasing increases. Thus Zhang et al. (2008) arranged ${}_i^{\#}C_j^{(k)}$s as

$${}_i^{\#}C_j = ({}_i^{\#}C_j^{(0)}, {}_i^{\#}C_j^{(1)}, ..., {}_i^{\#}C_j^{(v)}), \tag{1}$$

where $v = \binom{n}{j}$. Equation (1) gives the total number of ith-order effects aliased with jth-order effects at various degrees starting from the least to the greatest in terms of severity.

Example 1. Consider the design with generators $4 = 12$ and $5 = 13$. The defining relation is I=124=135=2345. Since all the main effects are aliased with two-factor interactions, ${}_1^{\#}C_2^0$=0. Note that the number of main effects that are aliased with one and two two-factor interactions are 4 and 1, respectively, hence ${}_1^{\#}C_2^1$=4 and ${}_1^{\#}C_2^2$=1. Moreover, there are no main effects that are aliased with three or more two-factor interactions, hence ${}_1^{\#}C_2^k$=0 for $k \geq 3$. Therefore ${}_1^{\#}C_2 = (0, 4, 1)$

Similarly, there are four two-factor interactions that are not aliased with other two-factor interactions, we get ${}_2^{\#}C_2^0$=4; there are six two-factor interactions that are aliased with only one two-factor interactions, hence ${}_2^{\#}C_2^1$=6; there are no two-factor interactions that are aliased with other two or more two-factor interactions, hence ${}_2^{\#}C_2^k$=0 for $k \geq 2$. Therefore ${}_2^{\#}C_2 = (4, 6)$. One can find other ${}_i^{\#}C_j s$ similarly.

Zhang et al. (2008) defined the *aliased effect number pattern* (AENP) as

$$^{\#}C = ({}_1^{\#}C_1, {}_0^{\#}C_2, {}_1^{\#}C_2, {}_2^{\#}C_1, {}_2^{\#}C_2, {}_0^{\#}C_3, {}_1^{\#}C_3, {}_2^{\#}C_3, {}_3^{\#}C_1, {}_3^{\#}C_2, {}_3^{\#}C_3, {}_0^{\#}C_4, {}_1^{\#}C_4, ...) \tag{2}$$

The elements in $^{\#}C$ are placed in using a rule: If $max(i, j) < max(q, r)$, then ${}_i^{\#}C_j$ is placed before ${}_q^{\#}C_r$; if $max(i, j) = max(q, r)$ and $i < q$, then ${}_i^{\#}C_j$ is placed before ${}_q^{\#}C_r$; if $max(i, j) = max(q, r)$, $i = q$ and $j < r$, then ${}_i^{\#}C_j$ is placed before ${}_q^{\#}C_r$.

Suppose $^{\#}C(d_1)$ and $^{\#}C(d_2)$ are the aliased effect number patterns of two designs d_1 and d_2, respectively, and $^{\#}C_m$ is the mth component of $^{\#}C$. Let $^{\#}C_m$ be the first component for which $^{\#}C_m(d_1)$ and $^{\#}C_m(d_2)$ differ. If $^{\#}C_m(d_1) > {}^{\#}C_m(d_2)$ we say that d_1 has less general lower order confounding relative to d_2. A design is said to be a *general minimum lower-order confounding* (GMLOC or GMC) design, if it has minimum general lower order confounding relative to other designs.

A foldover design is obtained by reversing the signs of one or more factors of the initial design. The combination of the initial design and the foldover design is called a *combined foldover design*. The set of factors whose signs are revised in a foldover design is referred to as a *foldover plan*. For each initial design, there are many foldover plans. Li and Lin (2003) showed that any foldover plan is equivalent to a *core foldover plan*, which contains only generated factors. Thus, we only need to consider core foldover plans when studying combined foldover designs.

Eexample 2. Consider the combined foldover designs obtained from the initial design discussed in Example 1. The generated factors are 4 and 5. Thus, there are three core foldover plans 4, 5 and 45, where 45 indicates that the signs of both factors 4 and 5 are switched. The resulting three combined foldover designs are denoted as d_1, d_2 and d_3, respectively. The defining relations of d_1, d_2 and d_3 are $I = 135$, $I = 124$, and $I = 2345$, respectively. The AENPs of the three combined foldover designs first differ at $^{\#}_1C^1_2(d_1) = {}^{\#}_1C^1_2(d_2) = 2$ and $^{\#}_1C^1_2(d_3) = 5$. Since $^{\#}_1C^1_2(d_3)$ is larger than both $^{\#}_1C^1_2(d_1)$ and $^{\#}_1C^1_2(d_2)$, we obtain that 45 is the optimal foldover plan and the corresponding combined foldover design is the optimal combined foldover design.

Zhang et al. (2008) discussed the relationships between the GMC criterion and other criteria, such as minimum aberration and clear effects criteria. The minimum aberration criterion was introduced by Fries and Hunter (1980) and it has remained one of the popular criteria in choosing optimal designs when experimenters do not have information about the important effects. Define the length of a word as the number of factors in the word. The minimum aberration criterion depends on the *word length pattern* which is defined as $(A_1, A_2, A_3...)$, where $A_i, i = 1, 2, ...$, represent the number of length-i words in the defining relation of the design. For instance, for the design in Example 1, the word length pattern is (0, 0, 2, 1, 0...). The minimum aberration design can be obtained by sequentially minimizing the component of the word length pattern. Zhang et al. (2008) pointed out that the WLP is only related to $^{\#}_iC^1_0$, $i = 1, 2, ...$, and AENP is a more refined pattern than the WLP for judging designs.

Clear effects are effects that are not aliased with main effects and two-factor interactions. One of the drawbacks of the minimum aberration criterion is that, sometimes it is unable to maximize the number of some clear lower-order effects especially two-factor interactions. One of the criteria that takes care of this situation is the *clear effects criterion*. The optimal designs sequentially maximizes the number of clear main effects and the number of clear two-factor interactions. Zhang et al. (2008) pointed out that $^{\#}_2C^0_2$ is the number of clear main effects and $^{\#}_2C^0_2 - {}^{\#}_1C^1_2$ is the number of clear two-factor interactions. For more details about the relationship between the GMC criterion and MA and clear effects criteria, see Zhang et al. (2008).

3. Relationships Between AENPs

It is well known that when the signs of all the factors of an initial design are reversed, all the words containing odd number of factors disappear in the combined foldover design and all the words that contain even number of factors in the initial design are still in the combined foldover design. Let ${}_i^{\#}C_j^{(k)}(d)$ and ${}_i^{\#}C_j^{(k)}(c)$ denote the number of ith-order effects that is aliased with k jth-order effects in the initial design d and the combind foldover design c, respectively. Note that ${}_l^{\#}C_0^{(0)} = \binom{n}{l} - A_l$ or ${}_l^{\#}C_0^{(1)} = A_l$ by Theorem 2 in Zhang et al. (2008). From the well known result, we obtain some relationships between the AENPs of initial designs and combined foldover designs as shown in Result 1.

Result 1, Assume that a combined foldover design is obtained by reversing the signs of all the factors in the initial design. Then,

(1) if l is odd, then ${}_l^{\#}C_0^{(0)}(c) = \binom{n}{l}$ or ${}_l^{\#}C_0^{(1)}(c) = 0$.

(2) if $i + j$ is odd, then ${}_i^{\#}C_j^{(0)}(c) = r$, where r is the number of i-th order effects of the design d and ${}_i^{\#}C_j^{(k)}(c) = 0$ for $k = 1, 2, ...$

(3) if $i + j$ is even, then ${}_i^{\#}C_j^{(k)}(d) = {}_i^{\#}C_j^{(k)}(c)$ for $k = 0, 1, 2, ...$

Since some effects are de-aliased after folding an initial design, the number of **i**-order effects that are not aliased with any **j**-th order effects in a combined foldover design is always greater than or equal to that of its corresponding initial design. Therefore, we have Result 2.

Result 2. ${}_i^{\#}C_j^{(0)}(c) \geq {}_i^{\#}C_j^{(0)}(d)$ for any $i, j = 1, 2, ...$

The resolution of a design is defined as the length of the shortest word of the design. Note that the results 1 and 2 are true for designs with any resolution.

4. Optimal Foldover Designs

Zhang et al. (2008) presented a catalogue of 16- and 32-run GMC designs. We search optimal foldover designs from the designs in Zhang et al. (2008) using GMC criterion, and compare them with the optimal foldover designs obtained using MA and clear effects criteria. For each initial design, we consider all core foldover plans and calculate the AENP for each combined foldover design. Then the AENPs are compared and the optimal combined foldover designs are obtained. Similarly, the optimal MA foldover designs and the optimal clear effects foldover designs are also obtained. Tables 1 and 2 present the optimal foldover designs obtained from the 16- ($6 \leq n \leq 12$) and 32-run ($7 \leq n \leq 15$) designs, respectively, in Zhang et al. (2008).

In Tables 1 and 2, the first column lists the initial designs in Zhang et al. (2008); the second column lists additional columns, which represent the generators of each design, from the design matrix (Table 1 in Chen et al. Chen *et al.* (1993)); the third column lists AENP of the initial design. To save space, we list only $({}_1^{\#}C_2\,,\, {}_2^{\#}C_2)$. The fourth and fifth columns represent the optimal

foldover plans based on GMC criterion and AENP of the corresponding optimal combined foldover designs, respectively. The sixth column shows the word length pattern (A_4, A_5, A_6) of the optimal foldover designs chosen based on MA criterion. We do not show A_3 since it is zero for any optimal foldover designs in the table. To save space, the corresponding optimal foldover plans are not listed. The last column presents the number of clear main effects c_1 and the number of clear two-factor interactions c_2 of the optimal foldover designs based on clear effects criterion. Again, to save space, the corresponding optimal foldover plans are not listed.

For example, for 16-run design 7.3.1, the AENP of the initial design is $({}^{\#}_{1}C_2; {}^{\#}_{2}C_2) = (7; 0, 0, 21)$. To save space, we write it as $(7; 0^2, 21)$. The optimal foldover plans based on GMC criterion are $5, 6, 7, 56, 57, 67, 567$ and the AENP of the corresponding optimal foldover designs is $(7; 6, 12, 3)$. The word length pattern of the optimal foldover designs based on MA criterion is $(A_4, A_5, A_6) = (3, 0, 0)$. For the optimal foldover designs obtained using clear effects criterion, the number clear main effects is $c_1 = 7$ and the number of clear two-factor interactions is $c_2 = 6$.

For the optimal GMC foldover designs, we find that most of the 16-run designs considered have only one optimal foldover plan except for designs 6.2.1, 7.3.1 and 8.4.1; for 32-run designs, most of them have more than one optimal foldover plans. One can see that ${}^{\#}_{i}C_j^{(0)}$ of all the optimal foldover designs are the same or larger than that of the corresponding initial designs.

Although the optimal foldover plans of MA foldover designs are not listed, MA and GMC criteria choose the same foldover plans as optimal for all the designs considered except for the 16-run design 8.4.1 and 32-run designs 9.4.3, 11.6.1, 12.7.1, 12.7.2, 13.8.1 and 15.10.1, for which, the two criteria choose completely different optimal foldover plans. This shows that the GMC criterion can choose completely different foldover plans as the optimal from MA criterion. For example, for design 8.4.1, eight foldover plans 5, 6, 7, 8, 567, 568, 578, and 678 are chosen as optimal according to GMC criterion while six foldover plans 56, 57, 58, 67, 68, and 78 are selected as optimal according to MA criterion. The $AENP's$ of the optimal foldover designs chosen by GMC and MA criteria are $(8; 7, 0, 21)$ and $(8; 0, 24, 0, 4)$, respectively. Clearly, the foldover designs chosen by GMC criterion has seven clear two-factor interactions and the optimal foldover designs selected by MA criterion has no clear two-factor interactions. Therefore, GMC criterion chooses better designs than MA criterion in terms of estimation of effects. For 32-run designs, we search optimal designs for 13 designs. The two criteria choose complete different optimal foldover plans for six designs 9.4.3, 11.6.1, 12.7.1, 12.7.2, 13.8.1 and 15.10.1. For each of the six designs, there are more than one optimal MA foldover plans. We present only one for each design here, they are 67, 69$\underline{10}$, 67$\underline{10}$ $\underline{12}$, 67$\underline{12}$, 67$\underline{11}$ $\underline{13}$, and 67$\underline{11}$ $\underline{14}$ $\underline{15}$, respectively. The results show that when the number of runs becomes larger, the two criteria tends to choose different optimal foldover plans.

For the optimal foldover designs chosen by the clear effects criterion, their optimal foldover plans always include the ones chosen by the GMC criterion. In fact, the two criteria choose the same optimal foldover plans for all the designs except for the 16-run design 9.5.1 and 32-run designs 9.4.1, 11.6.2, 12.7.2, and 13.8.1. For instance, for design 9.5.1, the GMC criterion chooses 589 as the optimal foldover plan while the clear effect criterion chooses 5 and 589 as the optimal foldover plans. The $AENP's$ of the optimal foldover designs obtained by foldover plans 5 and 589 are $(9; 8, 0, 0, 28)$ and $(9; 8, 24, 0, 4)$, respectively. Even though both foldover designs have the same number of clear main effects and two-factor interactions, the former have 24 two-factor interactions aliased with only 1 two-factor interaction whiles the latter have 28 two-factor

interactions aliased with 3 two-factor interactions. The alias structure in latter is more severe than in the former, thereby making it less preferable. In general, when the run size of a design is large, the GMC criterion tends to choose less optimal foldover plans than the clear effects criterion.

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Table 1: Optimal foldover designs for 16-run initial designs

Initial designs			Optimal foldover designs			
Design	Additional Columns	AENP $(^{\#}_{1}C_2; ^{\#}_{2}C_2)$	OFP	ANEP $(^{\#}_{1}C_2; ^{\#}_{2}C_2)$	WLP (A_4, A_5, A_6)	CE c_1, c_2
6.2.1	7,14	$6; 0, 12, 3$	5,6,56	$6; 9, 6$	$(1, 0, 0)$	6,9
6.2.3	6,12	$1, 4, 1; 9, 6$	56	$6; 9, 6$	$(1, 0, 0)$	6,9
6.2.4	3,6	$6; 15$	56	$6; 15$	$(0, 0, 1)$	6,15
7.3.1	7,11,14	$7; 0^2, 21$	5,...,567[1]	$7; 6, 12, 3$	$(3, 0, 0)$	7,6
7.3.3	6,10,12	$1, 0, 6; 6, 12, 3$	567	$7; 6, 12, 3$	$(3, 0, 0)$	7,6
7.3.5	3,6,12	$0, 5, 2; 9, 12$	567	$7; 9, 12$	$(2, 0, 1)$	7,9
8.4.1	7,11,13,14	$8; 0^3, 28$	5,..., 678[2]	$8; 7, 0, 21$	$(6, 0, 0)$	8,7
8.4.2	3,5,7,14	$2, 0, 6; 0, 24, 0, 4$	568	$8; 13, 12, 3$	$(3, 4, 0)$	8,13
8.4.3	3,7,11,14	$1, 6, 0, 1; 7, 0, 21$	58	$8; 13, 12, 3$	$(3, 4, 0)$	8,13
8.4.4	6,10,12,14	$1, 0^2, 7; 7, 0, 21$	567	$8; 7, 0, 21$	$(7, 0, 0)$	8,7
8.4.5	3,7,12,14	$0, 4, 4; 4, 18, 16$	57	$8; 4, 18, 6$	$(5, 0, 2)$	8,4
9.5.1	3,7,11,13,14	$0, 8, 0^2, 1; 8, 0^2, 28$	589	$9; 8, 24, 0, 4$	$(6, 8, 0)$	9,8
9.5.2	3,6,7,11,14	$0, 2, 5, 2; 2, 12, 18, 4$	56	$9; 2, 12, 18, 4$	$(10, 0, 4)$	9,2
9.5.3	3,6,10,12,14	$0, 2, 0, 6, 1; 2, 12, 18, 4$	5678	$9; 2, 12, 18, 4$	$(10, 0, 4)$	9,2
9.5.4	3,7,9,12,14	$0^2, 9; 0, 18, 18$	578	$9; 0, 18, 18$	$(9, 0, 6)$	9,0
9.5.5	3,6,7,12,14	$0^2, 6, 3; 0, 18, 18$	568	$9; 0, 18, 18$	$(9, 0, 6)$	9,0
10.6.1	3,6,7,11,13,14	$0^2, 8, 0, 2; 0, 16, 0, 24, 5$	56	$10; 0, 16, 0, 24, 5$	$(18, 0, 8)$	10,0
10.6.3	3,5,6,10,12,14	$0^2, 3, 4, 3; 0, 6, 27, 12$	56789	$10; 0, 6, 27, 12$	$(16, 0, 12)$	10,0
10.6.4	3,6,7,12,14,15	$0^3, 10; 0^2, 45$	56810	$10; 0^2, 45$	$(15, 0, 15)$	10,0
11.7.1	3,6,7,11,12,13,14	$0^3, 8, 3; 0^2, 24, 16, 15$	569	$11; 0^2, 24, 16, 15$	$(26, 0, 24)$	11,0
11.7.2	3,5,6,7,11,13,14	$0^3, 8, 0, 3; 0^2, 24, 16, 15$	567	$11; 0^2, 24, 16, 15$	$(26, 0, 24)$	11,0
11.7.3	3,5,6,7,9,12,14	$0^3, 5, 6; 0^2, 15, 40$	567910	$11; 0^2, 15, 40$	$(25, 0, 27)$	11,0
12.8.1	3,6,7,9,11,12,13,14	$0^4, 12; 0^3, 48, 0, 18$	56810	$12; 0^3, 48, 0, 18$	$(39, 0, 48)$	12,0

Note: [1]The complete set is: 5,6,7,56,57,67,567. [2]The complete set is: 5,6,7,8,567,568,578,678.

Table 2: Optimal foldover designs for 32-Run initial designs

Initial designs			Optimal foldover designs			
Design	Additional Columns	AENP $(^{\#}_{1}C_2; ^{\#}_{2}C_2)$	OFP	ANEP $(^{\#}_{1}C_2; ^{\#}_{2}C_2)$	WLP (A_4, A_5, A_6)	CE c_1, c_2
7.2.1	7,30	$7; 15, 6$	6, 67	$7; 21$	(0, 1, 0)	7, 21
8.3.1	7,11,30	$8; 13, 12, 3$	6, 7, 67, 68 78, 678	$8; 22, 6$	(1, 2, 0)	8, 22
9.4.1	7,11,13,30	$9; 15, 0, 21$	67, 68, 69, 78 79, 89, 6789	$9; 21, 12, 3$	(3, 3, 0)	9, 21
9.4.2	7,11,19,30	$9; 8, 24, 0, 4$	67, 68, 78 679, 689, 789	$9; 24, 12$	(2, 4, 0)	9, 24
9.4.3	14,22,26,28	$9; 8, 0^2, 28$	6, 7, 8, 9, 678 679, 689, 789	$9; 15, 0, 21$	(6, 0, 0)	9, 15
10.5.1	7,11,19,29,30	$10; 0, 40, 0^2, 5$	67, 68, ..., 678910^1	$10; 24, 18, 3$	(4, 8, 0)	10, 24
11.6.1	7,11,14,22,26 28	$11; 0^2, 24, 16, 15$	68, 69, ..., $67910\,11^2$	$11; 12, 18, 21, 4$	(10, 0, 16)	11, 12
11.6.2	7,11,14,19,25 28	$11; 0^2, 15, 40$	6810, 6911,..., $678910\,11^3$	$11; 10, 30, 15$	(10, 0, 16)	11, 10
12.7.1	7,11,13,14,22 26, 28	$12; 0^3, 48, 0, 18$	6, 7, 8, ..., $78911\,12^4$	$12; 11, 0, 24, 16, 15$	(15, 0, 32)	12, 11
12.7.2	7,11,13,14,19 25, 28	$12; 0^3, 36, 30$	10, 11, 12, 10 11 12	$12; 11, 0, 24, 16, 15$	(16, 0, 30)	12, 11
13.8.1	7,11,13,14,19 22,26,28	$13; 0^4, 60, 18$	10	$13; 12, 0^2, 48, 0, 18$	(23, 0, 56)	13, 12
14.9.1	7,11,13,14,19 21,22,26,28	$14; 0^5, 84, 7$	6, 7, 8, ..., $68911\,12\,14^5$	$14; 13, 0^3, 60, 18$	(33, 0, 96)	14, 13
15.10.1	7,11,13,14,19 21,22,25,26,28	$15; 0^6, 105$	6, 7, 8, ..., $10\,11\,12\,13\,14\,15^6$	$15; 14, 0^4, 84, 7$	(45, 0, 160)	15, 14

Note: [1] - [6]The complete sets can be obtained upon request.

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Optimality Results of 3^m Fractional Factorial Designs for $N \equiv p$ mod 9 Runs, $p = 1, 2, 3$.

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Abstract

The optimality of fractional factorial designs for $N \equiv p$ mod 9 runs, $p = 1, 2, 3$, is studied, when an experiment involves m factors each at three levels. The optimality criterion used here, is the Φ-optimality employing the notion of majorization. Unlike what happens with orthogonal array plus one run plans, the behavior of plans obtained via augmentation of an orthogonal array by two or three runs depends on the particular runs added.

Key words: Fractional factorial; Orthogonal array; Majorization; Φ-, E-, A-, D-optimality.

1. Introduction

The problem of finding optimal experimental designs for any number N of runs and under different optimality criteria, preoccupies researchers working in this area, almost six decades. Although there are hundreds of papers on 2^m fractional factorial designs (f.f.d. for short), there are few papers on 3^m f.f.d. The extension of theorems concerning 2^m f.f.d. to the 3^m f.f.d. is not evident, since the elements of the design matrix of a 2^m f.f.d. are ± 1, fact which is not valid for the case of 3^m f.f.d. and generally for s^m f.f.d. It is well known that in general s^m setup, when the number of runs is $N \equiv 0$ mod s^2 the corresponding information matrix is diagonal and the optimal designs are constructed via orthogonal arrays (OA for short), Hedayat *et al.* (1999), Raghavarao (1971). For $N \not\equiv 0$ mod s^2, $s > 2$, the problem of finding optimal f.f.d. is partially solved in Chai *et al.* (2002), Chatzopoulos *et al.* (2011), Kolyva-Machera (1989a), Kolyva-Machera (1989b), Mukerjee *et al.* (1999), Pericleous *et al.* (2017) where the authors found the type 1 optimal designs for s^m f.f.d. in the class of O.A. plus p runs. A wide list of optimal f.f.d. can be found in Dey and Mukerjee (1999). In this paper we give Φ-optimal designs for $N \equiv p$ mod 9 runs, $p = 1, 2, 3$ using the notion of majorization.

The paper is organized as follows. The notations and preliminaries are presented in section 2, while section 3 deals with the main results of this paper. Our findings are illustrated with examples in section 4.

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2. Notations and Preliminaries

Consider a factorial experiment involving $m\ (\geq 2)$ factors $F_1, \ldots, F_m$ each at 3 levels, coded $0, 1, 2$. A typical level combination of the factors is denoted as $\ell_1\ell_2\cdots\ell_m$, where $\ell_j = 0, 1, 2$, $j = 1, 2, \ldots, m$. Let $\mathcal{D}_N$ be the class of designs with $N \equiv p \bmod 9$ runs, $p = 1, 2, 3$, consisting of the treatment combinations $\ell_{i1}\ell_{i2}\cdots\ell_{im}$, where $i = 1, 2, \ldots, N$, $j = 1, 2, \ldots, m$, $\ell_{ij} = 0, 1, 2$. For any positive integer t, let $\mathbf{1}_t$ be the $t \times 1$ vector with all elements unity and $\mathbf{I}_t$ (or simply $\mathbf{I}$ if there is no risk for confusion) be the identity matrix of order t and $\mathbf{P} = \begin{pmatrix} \mathbf{p}(0) & \mathbf{p}(1) & \mathbf{p}(2) \end{pmatrix}$ be a 2×3 matrix satisfying

$$\mathbf{P}\mathbf{P}' = 3\mathbf{I}_2, \quad \mathbf{P}\mathbf{1}_3 = \mathbf{0}, \quad \mathbf{p}'(k)\mathbf{p}(l) = 3\delta_{k\ell} - 1, \quad k, \ell = 0, 1, 2, \tag{2.1}$$

where $\mathbf{0}$ is a null vector of an appropriate order, $\mathbf{P}'$ denotes the transpose of matrix $\mathbf{P}$ and $\delta_{k\ell}$ is the Kronecker delta. So, the 2×3 matrix $\mathbf{P}$ satisfying (2.1) is

$$\mathbf{P} = \begin{pmatrix} -\sqrt{\frac{3}{2}} & 0 & \sqrt{\frac{3}{2}} \\ \sqrt{\frac{1}{2}} & -2\sqrt{\frac{1}{2}} & \sqrt{\frac{1}{2}} \end{pmatrix}. \tag{2.2}$$

Let $\mathbf{z}_j$ (or $\mathbf{z}_{jN}$, if needed), $1 \leq j \leq m$ be an $N \times 2$ matrix with rows $\mathbf{p}'(0)$ or $\mathbf{p}'(1)$ or $\mathbf{p}'(2)$ and θ_j be the vector of main effect parameters of factor F_j. Then under the assumption of the absence of interaction effects involving two or more factors, we have the following linear model

$$\left.\begin{array}{lcl} E(\mathbf{Y}) & = & \mathbf{1}_N\mu + \sum_{j=1}^{m} z_j\theta_j, \\ Var(\mathbf{Y}) & = & \sigma^2\mathbf{I}_N, \end{array}\right\} \tag{2.3}$$

where $\mathbf{Y}$ is the $N \times 1$ vector of observations (response).

Define the design matrix $\mathbf{R} = [\mathbf{1}_N, z_1, \cdots, z_m]$. The information matrix of a design $d \in \mathcal{D}_N$ will then be

$$\mathbf{M}_N \quad = \quad \mathbf{R}'\mathbf{R}. \tag{2.4}$$

2.1 Properties of the Information Matrix

Consider two subsets of a design $d \in \mathcal{D}_N$ with $N_1 < N$ and $N_2 = N - N_1$ runs, respectively. For $\ell = 1, 2$ let $\mathbf{z}_{jN_\ell}$ be the $N_\ell \times 2$ matrix with rows $\mathbf{p}(a_{ij})\mathbf{p}'(a_{ij})$, $1 \leq i \leq N_\ell$, $1 \leq j \leq m$ and $N_1 + N_2 = N$. Then:

$$\mathbf{R} = \begin{pmatrix} \mathbf{R}_1 \\ \mathbf{R}_2 \end{pmatrix} = \begin{pmatrix} \mathbf{1}_{N_1} & z_{1N_1} & z_{2N_1} & \cdots & z_{mN_1} \\ \mathbf{1}_{N_2} & z_{1N_2} & z_{2N_2} & \cdots & z_{mN_2} \end{pmatrix} \tag{2.5}$$

and the information matrix of any design $d \in \mathcal{D}_N$ can be written as:

$$\mathbf{M}_N \quad = \quad \mathbf{R}_1'\mathbf{R}_1 + \mathbf{R}_2'\mathbf{R}_2 = \mathbf{M}_1 + \mathbf{M}_2, \tag{2.6}$$

that is $\mathbf{M}_N$ can be decomposed in two (or more) information matrices with N_1 and $N_2 = N - N_1$ runs, respectively.

Remark 2.1. If $\mathbf{M}_1 = N_1\mathbf{I}$, then $N_1 \equiv 0 \bmod 9$ and the off-diagonal elements of the information matrix $\mathbf{M}_2$ are equal to the off-diagonal elements of the information matrix $\mathbf{M}_N$, while the diagonal elements of $\mathbf{M}_2$ are equal to the diagonal elements of $\mathbf{M}_N$ minus N_1.

Definition 2.1. *For $i \neq j = 1, 2, \ldots, m$, $\ell, k = 0, 1, 2$, let $n_i(\ell)$ be the number of runs where the ith factor enters the experiment at level ℓ and $n_{ij}(\ell k)$ be the number of runs where the i-th factor enters the experiment at level ℓ and j-th factor enters the experiment at level k. It holds that*

$$\begin{array}{ll} N = \sum_{\ell=0}^{2} n_i(\ell), & N = \sum_{\ell=0}^{2}\sum_{k=0}^{2} n_{ij}(\ell k), \\ n_i(\ell) = \sum_{k=0}^{2} n_{ij}(\ell k), & n_j(k) = \sum_{\ell=0}^{2} n_{ij}(\ell k). \end{array} \tag{2.7}$$

The information matrix of a design $d \in \mathcal{D}_N$, for the model (2.3), after some simple matrix manipulations, using the parametrization (2.2) can be written as:

$$\mathbf{M}_N = \begin{pmatrix} N & \sqrt{\frac{3}{2}}\mathbf{a}' & \sqrt{\frac{1}{2}}\mathbf{b}' \\ \sqrt{\frac{3}{2}}\mathbf{a} & \frac{3}{2}\mathbf{A} & \frac{\sqrt{3}}{2}\mathbf{C} \\ \sqrt{\frac{1}{2}}\mathbf{b} & \frac{\sqrt{3}}{2}\mathbf{C}' & \frac{1}{2}\mathbf{B} \end{pmatrix}, \tag{2.8}$$

where **a**, **b** are $m \times 1$ vectors , **A** and **B** are $m \times m$ symmetric matrices and **C** is an $m \times m$ matrix. For $i \neq j = 1, 2, \ldots, m$ the elements of the above vectors and matrices are given by the following relations:

$$\begin{array}{ll} a_i = n_i(2) - n_i(0), & b_i = N - 3n_i(1), \\ a_{ii} = N - n_i(1), & a_{ij} = n_{ij}(00) + n_{ij}(22) - n_{ij}(02) - n_{ij}(20), \\ b_{ii} = N + 3n_i(1), & b_{ij} = N - 3n_i(1) - 3n_j(1) + 9n_{ij}(11), \\ c_{ii} = n_i(2) - n_i(0), & c_{ij} = n_i(2) - n_i(0) + 3[n_{ij}(01) - n_{ij}(21)]. \end{array} \tag{2.9}$$

Remark 2.2. From relationships (2.9) it is obvious that trace($\mathbf{M}_N$) $= N + \sum_{i=1}^{m}(\frac{3}{2}a_{ii} + \frac{1}{2}b_{ii}) = (2m+1)N$.

Lemma 2.1. *Let $U_1 = \{a_i, b_i, a_{ii}, b_{ii}, c_{ii}\}$ and $U_2 = \{a_{ij}, b_{ij}, c_{ij}, c_{ji}\}$, $i \neq j = 1, 2, \ldots, m$. The elements of these two sets are all even or all odd.*

Proof. After a simple algebra, using (2.7) and (2.9), for $i \neq j = 1, 2, \ldots, m$, one can easily verify the following relationships:

$$a_i + b_i = 2(n_i(2) - n_i(1)) = 2\widetilde{a}_i. \tag{2.10}$$

$$a_{ii} + b_{ii} + 2c_{ii} = 4(N - n_i(0)) = 4\widetilde{a}_{ii}. \tag{2.11}$$

$$a_{ij} + c_{ij} = 2[n_{ij}(01) + n_{ij}(22) - n_{ij}(02) - n_{ij}(21)]. \tag{2.12}$$

$$a_{ij} + b_{ij} = 2[-n_i(1) - n_j(1) + n_{ij}(00) + n_{ij}(22) + 4n_{ij}(11)]. \tag{2.13}$$

$$c_{ji} + b_{ij} = 2[n_j(2) - n_j(1) + 3n_{ij}(11) - 3n_{ij}(12)] = 2\widetilde{c}_{ji}. \tag{2.14}$$

$$a_{ij} + c_{ij} + c_{ji} + b_{ij} = 4[n_{ij}(11) + n_{ij}(22) - n_{ij}(12) - n_{ij}(21)] = 4\widetilde{a}_{ij}. \tag{2.15}$$

$$c_{ii} + b_{ii} = 2[2n_i(1) + n_i(2)] = 2\widetilde{c}_{ii}. \tag{2.16}$$

From (2.10)-(2.16) the proof of lemma is obvious. □ □

Lemma 2.2. *It holds that det($\boldsymbol{M}_N$) $= 3^{3m}z$, $z \in \mathbb{Z}$.*

Proof. Let us denote:

$$\widetilde{\mathbf{M}}_N = \begin{pmatrix} N & \mathbf{a}' & \mathbf{b}' \\ \mathbf{a} & \mathbf{A} & \mathbf{C} \\ \mathbf{b} & \mathbf{C}' & \mathbf{B} \end{pmatrix}. \tag{2.17}$$

Then, from (2.8) we have:

$$det(\mathbf{M}_N) = \frac{3^m}{2^{2m}} det(\widetilde{\mathbf{M}}_N). \tag{2.18}$$

By adding the $(m+1+j)$-th rows and columns to the $(j+1)$-th rows and columns, $j = 1, 2, \ldots, m$, respectively, from (2.17), we get that:

$$det(\widetilde{\mathbf{M}}_N) = det \begin{pmatrix} N & \mathbf{a}' + \mathbf{b}' & \mathbf{b}' \\ \mathbf{a} + \mathbf{b} & \mathbf{A} + \mathbf{C} + \mathbf{C}' + \mathbf{B} & \mathbf{C} + \mathbf{B} \\ \mathbf{b} & \mathbf{C}' + \mathbf{B} & \mathbf{B} \end{pmatrix},$$

that is from (2.10), (2.11), (2.13)-(2.16), we have:

$$det(\widetilde{\mathbf{M}}_N) = 2^{2m} det \begin{pmatrix} N & \widetilde{\mathbf{a}}' & \mathbf{b}' \\ \widetilde{\mathbf{a}} & \widetilde{\mathbf{A}} & \widetilde{\mathbf{C}} \\ \mathbf{b} & \widetilde{\mathbf{C}}' & \mathbf{B} \end{pmatrix},$$

where for $i \neq j = 1, 2, \ldots, m$ the elements of $m \times m$ matrices $\widetilde{\mathbf{A}} = (\widetilde{a}_{ij})$ and $\widetilde{\mathbf{C}} = (\widetilde{c}_{ij})$ are as defined in (2.11), (2.15) and (2.14), (2.16), respectively, while the elements of the $m \times 1$ vector $\widetilde{\mathbf{a}}$ are given in (2.10). By subtracting the first row and column from the $(m + 1 + j)$-th, $j = 1, 2, \ldots, m$, rows and columns, respectively, we have:

$$det(\widetilde{\mathbf{M}}_N) = 2^{2m} det \begin{pmatrix} N & \widetilde{\mathbf{a}}' & \mathbf{b}' - N\mathbf{1}'_m \\ \widetilde{\mathbf{a}} & \widetilde{\mathbf{A}} & \widetilde{\mathbf{C}} - \widetilde{\mathbf{a}}\mathbf{1}'_m \\ \mathbf{b} - N\mathbf{1}_m & \widetilde{\mathbf{C}}' - \mathbf{1}_m\widetilde{\mathbf{a}}' & \mathbf{B} - \mathbf{b}\mathbf{1}'_m - \mathbf{1}_m\mathbf{b}' + N\mathbf{1}_m\mathbf{1}'_m \end{pmatrix}.$$

It can be easily seen that:

$$b_i - N = -3n_i(1). \tag{2.19}$$

$$\widetilde{c}_{ii} - \widetilde{a}_i = 3n_i(1). \tag{2.20}$$

$$\widetilde{c}_{ji} - \widetilde{a}_j = 3(n_{ij}(11) - n_{ij}(12). \tag{2.21}$$

$$\widetilde{b}_{ii} - 2\widetilde{b}_i + N = 9n_i(1). \tag{2.22}$$

$$\widetilde{b}_{ji} - \widetilde{b}_i - \widetilde{b}_j + N = 9n_{ji}(11). \tag{2.23}$$

Using (2.19)-(2.23), we get

$$det(\widetilde{\mathbf{M}}_N) = 3^{2m}2^{2m} det \begin{pmatrix} N & \widetilde{\mathbf{a}}' & \widetilde{\mathbf{b}}' \\ \widetilde{\mathbf{a}} & \widetilde{\mathbf{A}} & \widetilde{\mathbf{E}} \\ \widetilde{\mathbf{b}} & \widetilde{\mathbf{E}}' & \widetilde{\mathbf{B}} \end{pmatrix}, \tag{2.24}$$

where $\widetilde{\mathbf{b}}$ is a $m \times 1$ vector, $\widetilde{\mathbf{B}}$ is a $m \times m$ symmetric matrix and $\widetilde{\mathbf{E}}$ is a $m \times m$ matrix. For $i \neq j = 1, 2, \ldots, m$ the elements of the above vectors and matrices are given by the following relations:

$$\begin{aligned} &\widetilde{b}_i = -n_i(1), \\ &\widetilde{b}_{ii} = n_i(1), \quad \widetilde{b}_{ij} = n_{ij}(11), \\ &\widetilde{e}_{ii} = n_i(1), \quad \widetilde{e}_{ij} = n_{ij}(11) - n_{ij}(21). \end{aligned}$$

□

From relations (2.18) and (2.24) the result follows. □

2.2 Optimality and Majorization

Definition 2.2. *A design $d^* \in \mathcal{D}_N$, with information matrix M_N^*, is said to be Φ-optimal if it minimizes a functional Φ of the information matrix $\boldsymbol{M}_N$ of any design $d \in \mathcal{D}_N$, that is, $\Phi(\boldsymbol{M}_N) \geq \Phi(\boldsymbol{M}_N^*)$. In other words, d^* minimizes $\phi(\lambda_1)+\phi(\lambda_2)+\ldots+\phi(\lambda_k)$ for all continuous, decreasing and convex functions $\phi(\lambda)$ (Marshall* et al. *(1979), p.11), where λ_i, $i = 1, 2, \ldots, k$ are the latent roots of the information matrix $\boldsymbol{M}_N$. Note that A-, E-, D-optimality are special cases of Φ-optimality. Consideration of the functions $\phi(\boldsymbol{M}) = log\{det(\boldsymbol{M}^{-1})\}$, $\phi(\boldsymbol{M})$ =trace$(\boldsymbol{M}^{-1})$ and $\phi(\boldsymbol{M})$ largest eigenvalue of $\boldsymbol{M}^{-1}$, which are all members of Φ, shows that a Φ-optimal plan is also D-,A-, and E-optimal.*

The following definition 2.3 can be found in Marshall *et al.* (1979), p.7, p.11.

Definition 2.3. *If $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^k$, $\boldsymbol{x} = (x_1, x_2, \ldots, x_k)'$, $\boldsymbol{y} = (y_1, y_2, \ldots, y_k)'$, then $\boldsymbol{x}$ is majorized by $\boldsymbol{y}$ ($\boldsymbol{x} \prec \boldsymbol{y}$) if $x_{(1)} + x_{(2)} + \ldots + x_{(j)} \geq y_{(1)} + y_{(2)} + \ldots + y_{(j)}$, $j = 1, 2, \ldots, k-1$ and $x_{(1)} + x_{(2)} + \ldots + x_{(k)} = y_{(1)} + y_{(2)} + \ldots + y_{(k)}$.*

Lemma 2.3. *The following lemma can be found in (Marshall* et al. *(1979), p.11). For majorization the following conditions are equivalent:*

(a) $\boldsymbol{x} \prec \boldsymbol{y}$.

(b) $\sum_{i=1}^k \phi(x_i) \leq \sum_{i=1}^k \phi(y_i)$ for all continuous convex functions ϕ.

An immediate consequence of lemma 2.3 is the following lemma 2.4.

Lemma 2.4. *A design d^* with $k \times k$ information matrix $\boldsymbol{M}_N^*$ and latent roots $\lambda_1, \lambda_2, \ldots, \lambda_k$, is Φ-optimal in the class $\mathcal{D}_N$ of designs, if the latent roots of $\boldsymbol{M}_N^*$ are majorized by the latent roots of the information matrix $\boldsymbol{M}_N$ of any design $d \in \mathcal{D}_N$.*

Lemma 2.5. *Let $\boldsymbol{Q}$ be a positive definite matrix of order k (pd(k), for short) and $\lambda(\boldsymbol{Q})$ the vector of the latent roots of $\boldsymbol{Q}$. For the completely symmetric matrix $\boldsymbol{Q}^* = (a^* - b^*)I_k + b^* J_k$, where a^* is the mean of the diagonal elements of $\boldsymbol{Q}$ and b^* is the mean of the off diagonal elements of Q, it holds $\lambda(\boldsymbol{Q}^*) \prec \lambda(\boldsymbol{Q})$.*

Proof. See Kiefer (1975). □ □

Lemma 2.6. *If $\boldsymbol{Q} = (q_{ij})$ is a pd(k) matrix with vector of diagonal elements $\delta(\boldsymbol{Q}) = (q_{11}, q_{22}, \ldots, q_{kk})'$ and vector of latent roots $\lambda(\boldsymbol{Q}) = (\lambda_1, \lambda_2, \ldots, \lambda_k)'$, then $\delta(\boldsymbol{Q})$ is majorized by $\lambda(\boldsymbol{Q})$. Equality holds only iff $\boldsymbol{Q}$ is diagonal.*

Proof. See Pukelsheim (1993), p.146. □ □

Lemma 2.7. *If s_1: $x_1 = x_2 = \ldots = x_k = x$, s_2: $y_1, y_2, \ldots, y_k$ not all equal and $y_1+y_2+\ldots+y_k = kx$, then $(x_1, x_2, \ldots, x_k)$ is majorized by $(y_1, y_2, \ldots, y_k)$ or $s_1 \prec s_2$.*

Proof. See Pericleous *et al.* (2017). □ □

Corollary 2.1. *An immediate consequence of lemmas 2.2, 2.4 and 2.7 is that the design d^* with information matrix $\boldsymbol{M}_N^* = N\boldsymbol{I}_k$ is Φ-optimal. However, $\boldsymbol{M}_N^* = \boldsymbol{R}'\boldsymbol{R} = N\boldsymbol{I}_k$, which means that the columns of $\boldsymbol{R}$ are orthogonal.* □

3. Main Results

Let us now consider a $(2m+1)\times(2m+1)$ information matrix $\mathbf{M}_N$ with constant trace($\mathbf{M}_N$) $= (2m+1)N$ and latent roots $\lambda_1, \lambda_2, \ldots, \lambda_{2m+1}$. Without loss of generality we may assume that $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_{2m+1}$. If we denote

$$S_v = (\frac{1}{v}\sum_{i=1}^{v}\lambda_i, \ldots, \frac{1}{v}\sum_{i=1}^{v}\lambda_i, \lambda_{v+1}, \ldots, \lambda_{2m+1}) \tag{3.1}$$

then from definition 2.3 we have $s_1 \succ s_2 \succ \ldots \succ s_{2m+1}$. Moreover, let us denote

$$S_{vu} = (\frac{1}{v}\sum_{i=1}^{v}\lambda_i, \ldots, \frac{1}{v}\sum_{i=1}^{v}\lambda_i, \frac{1}{u}\sum_{i=1}^{u}\lambda_{v+i}, \ldots, \frac{1}{u}\sum_{i=1}^{u}\lambda_{v+i}, \lambda_{v+u+1}, \ldots, \lambda_{2m+1}) \tag{3.2}$$

that is S_{vu} has v components equal to $\frac{1}{v}\sum_{i=1}^{v}\lambda_i$, u components equal to $\frac{1}{u}\sum_{i=1}^{u}\lambda_{v+1}$ and the $(2m+1-v-u)$ components $(\lambda_{v+u+1}, \ldots, \lambda_{2m+1})$. Then, if $S_v = S_{v1}$, from definition 2.3 it holds that $S_v \succ S_{v2} \succ \ldots \succ S_{v(2m+1-u)}$. In what follows $\mathbf{M}_{S_v}$ is the information matrix with latent roots as defined in (3.1) and $\mathbf{M}_{S_{vu}}$ is the information matrix with latent roots as defined in (3.2). Then from lemma 2.3 it holds that:

$$\Phi(\mathbf{M}_N) = \Phi(\mathbf{M}_{S_1}) \geq \Phi(\mathbf{M}_{S_2}) \geq \ldots \geq \Phi(\mathbf{M}_{S_{2m+1}}) \tag{3.3}$$

and for $v = 1, 2, \ldots, 2m$ we have

$$\Phi(\mathbf{M}_{S_v}) \geq \Phi(\mathbf{M}_{S_{v1}}) \geq \ldots \geq \Phi(\mathbf{M}_{S_{v(2m+1-u)}}). \tag{3.4}$$

The information matrix $\mathbf{M}_{S_{2m+1}}$ has $2m+1$ equal latent roots $\lambda_i = N$, $i = 1, 2, \ldots, 2m+1$, minimizes $\Phi(\mathbf{M}_N)$, so the design $d^* \in \mathcal{D}_N$ is Φ-optimal. From relations (2.9), the information matrix M_N, given in (2.8), is diagonal iff $n_i(0) = n_i(1) = n_i(2) = N/3$, $i = 1, 2, \ldots, m$ and $n_{ij}(\ell k) = N/9$, $i \neq j = 1, 2, \ldots, m$, which is true iff $N \equiv 0$ mod 9, and d^* is given by an $OA(N, m, 3, 2)$.

Remark 3.1. For $N \not\equiv 0 \bmod 9$, the information matrix of the Φ-optimal design $d^* \in \mathcal{D}_N$, from (3.3) and (3.4) will be $\mathbf{M}_{S_{v(2m+1-v)}}$, $v < 2m+1$, with v, as close to $2m+1$ as possible. Also, matrix $\mathbf{M}_{S_{v(2m+1-v)}}$ has v latent roots equal to $\lambda < N$, and u latent roots equal to $\lambda_i' = (2m+1)\frac{N-\lambda}{u} + \lambda$, $v + u = 2m + 1$.

Lemma 3.1. *Consider an s^m f.f.d. where $s \geq 3$. Let $1 \leq p \leq s+1$ and $\mathcal{D}_{OA}$ be the class of designs obtained by adding p runs to an OA and $\boldsymbol{M}_{OA}$ be the corresponding information matrix of a design $d \in \mathcal{D}_{OA}$. This design is E-optimal in the class $\mathcal{D}_{OA}$.*

Proof. See [Dey and Mukerjee (1999), p.111]. □

Lemma 3.2. *The information matrix $\boldsymbol{M}_{OA}$ has $2m+1-p$ latent roots equal to $N-p$ and p latent roots $\lambda_i > N-p$, $i = 1, \ldots, p$.*

Proof. See [Chatzopoulos *et al.* (2011), lemma 3]. □

From definition 2.2, design $d \in \mathcal{D}_{OA}$, with information matrix $\mathbf{M}_{OA}$, is E-optimal if d maximizes the smallest eignvalue of $\mathbf{M}_{OA}$. If $\lambda(\mathbf{M}_{OA}) = (\mu_1, \mu_2, \ldots, \mu_{2m+1})$, then from lemmas 3.1 and 3.2, $(\mu_1, \mu_2, \ldots, \mu_{2m+1}) = (N-p, \ldots, N-p, \lambda_1, \lambda_2, \ldots, \lambda_p)$ with $\lambda_i > N-p, i = 1, 2, \ldots, p$. So, it holds that $\text{maxmin}\{\mu_1, \mu_2, \ldots, \mu_{2m+1}\} = N-p$,

Theorem 3.1. *Let $d^* \in \mathcal{D}_N$ be the Φ-optimal design with information matrix M^*. If $N \equiv p$ mod 9, $p \neq 0$, then for the smallest latent root of M^* it holds that $\lambda = N - p$.*

Proof. As E-optimality is a special case of Φ-optimaity and $\mathcal{D}_{OA} \subset \mathcal{D}_N$, for the maximum of the smallest latent root of the Φ-optimal design $d^* \in \mathcal{D}_N$, it holds that $N - p \leq \lambda < N$, where $N \equiv p$ mod 9. On the other hand, from lemma 2.2, for any information matrix $\mathbf{M}_N$ of a 3^m f.f.d, it holds that $\det(\mathbf{M}_N) = 3^{3m}z$, $z \in \mathbb{Z}$, that is, if $\mathbf{M}_N^* = \mathbf{M}_{S_{v(2m+1-v)}}$, then

$$det(\mathbf{M}_N^*) = \lambda^v(\lambda + (2m+1))\frac{N-\lambda}{u}))^u = 3^{3m}z, \tag{3.5}$$

where $z \in \mathbb{Z}$, $v + u = 2m + 1$ and v as close to $2m + 1$ as possible, or u as small as possible. For $N - \lambda \leq p \leq 3$, relation 3.5 holds for $\lambda = N - p$. □

Lemma 3.3. *If a pd(q) matrix $\boldsymbol{M}$ has latent roots: λ with multiplicity $q-k$, $q > k$ and $\lambda_1, \lambda_2, \ldots, \lambda_k$, where $\lambda < \lambda_i$, $1 \leq i \leq k$, then this matrix can be written as $\boldsymbol{M} = \lambda \boldsymbol{I} + \boldsymbol{F}\boldsymbol{F}'$, where $\boldsymbol{F}$ is a $q \times k$ matrix.*

Proof. For any pd(q) matrix $\mathbf{M}$ exists an orthogonal $q \times q$ matrix $\mathbf{W}$, where $\mathbf{W}\mathbf{W}' = \mathbf{I}_q$, such that $\mathbf{W}'\mathbf{M}\mathbf{W} = \mathbf{D}$, where $\mathbf{D}$ is a $q \times q$ diagonal matrix. If $\mathbf{M}$ has latent roots: λ with multiplicity $q-k$, $q > k$ and $\lambda_1, \lambda_2, \ldots, \lambda_k$, where $\lambda < \lambda_i$, $1 \leq i \leq k$, then $\mathbf{D} = \begin{pmatrix} \mathbf{V} & \mathbf{0} \\ \mathbf{0} & \lambda\mathbf{I}_{q-k} \end{pmatrix}$, where $\mathbf{V} = diag(\lambda_1, \lambda_2, \ldots, \lambda_k)$ or $\mathbf{D} = \lambda\mathbf{I}_q + \begin{pmatrix} \mathbf{V} - \lambda\mathbf{I}_k & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}$. Then

$$\mathbf{M} = \mathbf{W}\mathbf{D}\mathbf{W}' = \lambda\mathbf{I}_q + \mathbf{W}\begin{pmatrix} \mathbf{V} - \lambda\mathbf{I}_k & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}\mathbf{W}',$$

that is

$$\mathbf{M} = \lambda \mathbf{I}_q + (\mathbf{W}_1 \quad \mathbf{W}_2) \begin{pmatrix} \mathbf{V} - \lambda \mathbf{I}_k & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{W}_1' \\ \mathbf{W}_2' \end{pmatrix},$$

or

$$\mathbf{M} = \lambda \mathbf{I}_q + \mathbf{W}_1 (\mathbf{V} - \lambda \mathbf{I}_k) \mathbf{W}_1' = \lambda \mathbf{I}_q + \mathbf{F}\mathbf{F}',$$

where $\mathbf{F} = \mathbf{W}_1(\mathbf{V}^{1/2} - \sqrt{\lambda}\mathbf{I}_k)$.□ □

As $\mathcal{D}_{OA} \subset \mathcal{D}_N$, we will try to find a design $d^* \in \mathcal{D}_N$ with information matrix $\mathbf{M}_N^*$, such that $\lambda(\mathbf{M}_N^*) \prec \lambda(\mathbf{M}_{OA}^*)$.

Lemma 3.4. *It holds that $\boldsymbol{M}_{S_v} = (N-p)\boldsymbol{I} + \boldsymbol{M}_p$, where $\boldsymbol{M}_p$ is an information matrix such that $\boldsymbol{M}_p = \boldsymbol{R}_1'\boldsymbol{R}_1$ and $\boldsymbol{R}_1'$ is a $(2m+1) \times p$ design matrix.*

Proof. From relation (3.1), theorem 3.1 and lemma 3.3 it holds that $\lambda = N - p$ and $\mathbf{M}_{S_v} = (N-p)\mathbf{I}_q + \mathbf{F}\mathbf{F}'$. Matrix $\mathbf{F}\mathbf{F}'$ has off-diagonal elements the off-diagonal elements of matrix $\mathbf{M}_{S_v}$ and diagonal elements the diagonal elements of matrix $\mathbf{M}_{S_v}$ minus $N-p$. From remark 2.1 matrix $\mathbf{F}\mathbf{F}'$ is an information matrix, say $\mathbf{M}_p$ of a design with p runs and the result follows. □ □

Lemma 3.5. *For $p = 1, 2, 3$ and $w = 1, 2$, let $\boldsymbol{x} = (x_{(1)}, x_{(2)}, \ldots, x_{(p)})$, where $x_{(1)} = g - w(p-1)$, $x_{(i)} = g + w$, $i = 2, 3, \ldots, p$, $\boldsymbol{z} = (z_{(1)}, z_{(2)}, \ldots, z_{(p)})$, where $z_{(p)} = g - (p-1)(w-3)$, $z_{(i)} = g + w - 3$, $i = 1, 2, \ldots, p-1$ and $\sum_{i=1}^p z_{(i)} = \sum_{i=1}^p x_{(i)} = pg$. Then:*

(i) $\boldsymbol{z} \prec \boldsymbol{x}$ for $w = 2$.

(ii) $\boldsymbol{x} \prec \boldsymbol{z}$ for $w = 1$.

Proof. Since $\sum_{i=1}^p z_{(i)} = \sum_{i=1}^p x_{(i)}$, from definition 2.2 we have that:

(i) If $w = 2$ then

$$\begin{aligned} \mathbf{z} \prec \mathbf{x} \Leftrightarrow \sum_{i=1}^{j} z_{(i)} \geq \sum_{i=1}^{j} x_{(i)}, j = 1, 2, \ldots, p-1 \Leftrightarrow \\ \Leftrightarrow j(g-1) \geq j(g+2) - 2p, j = 1, 2, \ldots, p-1 \Leftrightarrow \\ \Leftrightarrow 2p \geq 3j, j = 1, 2, \ldots, p-1, \end{aligned}$$

which is true beacuse $p = 1, 2, 3$, that is $2p \geq 3(p-1) \geq 3j$, $j = 1, \ldots, p-1$.

(ii) If $w = 1$ then

$$\begin{aligned} \mathbf{x} \prec \mathbf{z} \Leftrightarrow \sum_{i=1}^{j} z_{(i)} \leq \sum_{i=1}^{j} x_{(i)}, j = 1, 2, \ldots, p-1 \Leftrightarrow \\ \Leftrightarrow (g-2)j \leq j(g+1) - p, j = 1, 2, \ldots, p-1 \Leftrightarrow \\ \Leftrightarrow p \leq 3j, j = 1, 2, \ldots, p-1. \end{aligned}$$

□ □

Theorem 3.2. *Suppose that the $OA(N-p,m,3,2)$ exists for some p, $p=1,2,3$ and let $\mathcal{D}_{OA}$ be the class of designs obtained by adding p runs to an $OA(N-p,m,3,2)$. Let $d^* \in \mathcal{D}_{OA}$ be the Φ-optimal design in this class and $\boldsymbol{M}^*_{OA} \in \mathcal{M}_{2m+1}$ is the corresponding information matrix. The latent roots of $\boldsymbol{M}^*_{OA}$ are $N-p$ with multiplicity $2m+1-p$, $N-p+2m+1-y$ with multiplicity $p-1$ and $N-p+2m+1+(p-1)y$ with multiplicity 1, where $y=3m_1^*-m+1$ with m_1^* =round$[(m-1)/3]$, and round$[t]$ is the nearest integer to t.*

Proof. From relation (2.5) and (2.6) and remark 2.1 we have $\mathbf{M}_{OA}=(N-p)\mathbf{I}_{2m+1}+\mathbf{R}_1'\mathbf{R}_1$, with $\mathbf{R}_1=(1_p,z_{1p},z_{2p},\ldots,z_{mp})$, where z_{jp}, $1\le j\le m$ are $p\times 2$ matrices as defined in section 2. The latent roots of matrix $\mathbf{M}_{OA}$ are $N-p$ with multiplicity $2m+1-p$ and the latent roots of the $p\times p$ matrix $\mathbf{Q}=(N-p)\mathbf{I}_p+\mathbf{R}_1\mathbf{R}_1'$ (say $\lambda_1,\lambda_2,\ldots,\lambda_p$). From Chai *et al.* (2002) and Chatzopoulos *et al.* (2011), the diagonal elements of $\mathbf{R}_1\mathbf{R}_1'$ are $2m+1$ and the off-diagonal elements are $3m_{ij}-m+1$, $1\le i\ne j\le p$, where m_{ij} is the number of coincidences between level combinations $\ell_{i1}\ell_{i2}\cdots\ell_{im}$ and $\ell_{j1}\ell_{j2}\cdots\ell_{jm}$. Then, $Tr((N-p)\mathbf{I}_p+\mathbf{R}_1\mathbf{R}_1')=p(N-p+2m+1)$, which is independent of the design d.

Let us now consider the matrix $\mathbf{Q}^*$ with diagonal elements the mean of the diagonal elements of $\mathbf{Q}$ and off-diagonal elements the mean of the off-diagonal elements of $\mathbf{Q}$. If we denote $a=N-p+2m+1$ and $b=3m_1-m+1$, where m_1 is the mean number of coincidences between the level combinations $\ell_{i1}\ell_{i2}\cdots\ell_{im}$ and $\ell_{j1}\ell_{j2}\cdots\ell_{jm}$, $1\le i\ne j\le p$, then $\mathbf{Q}^*=(a-b)\mathbf{I}_p+b\mathbf{J}_p$. The latent roots of $\mathbf{Q}^*$ are $a-b$ with multiplicity $p-1$ and $a-b+pb$ with multiplicity one. From lemma 2.5 we have $\lambda(\mathbf{Q}^*)\prec\lambda(\mathbf{Q}))$ and from lemma 2.3 we get $\Phi(\mathbf{Q})\ge\Phi(\mathbf{Q}^*)$.

It holds that:

$$\Phi(\mathbf{M}_{OA})=(2m+1-p)\phi(N-p)+\sum_{i=1}^{p}\phi(\lambda_i)=$$
$$=(2m+1-p)\phi(N-p)+\Phi(\mathbf{Q})\ \ge(2m+1-p)\phi(N-p)+\Phi(\mathbf{Q}^*)=$$

$$=(2m+1-p)\phi(N-p)+(p-1)\phi(N-p+2m+1-(3m_1-m+1))+$$
$$+\phi(N-p+2m+1+(p-1)(3m_1-m+1))\ge$$

$$\ge(2m+1-p)\phi(N-p)+(p-1)\phi(N-p+2m+1-(3m_1^*-m+1))+$$
$$+\phi(N-p+2m+1+(p-1)(3m_1^*-m+1))=\phi(\mathbf{M}^*_{OA}),$$

where m_1^* is the mean value of coincidences minimizing $g(m_1)=(p-1)\phi((N-p+2m+1-(3m_1-m+1))+\phi(N-p+2m+1+(p-1)(3m_1-m+1))$.

Indeed, if $m-1\equiv 0\text{mod}3$, then for $m_1=(m-1)/3$, matrix Q^* is diagonal and $Q^*=(N-p+2m+1)I_p$.

If $(m-1)=3c+w$, $c\in\mathbb{Z}$, $1\le w\le 2$, then $3m_1-(m-1)=3(m_1-c)-w$, that is $c<(m-1)/3<c+1$. Consequently, for $m_1=c$ we have $3m_1-(m_1-1)=-w$, while for $m_1=c+1$ we have $3m_1-(m_1-1)=3-w$ and the corresponding vectors of the latent roots are $\mathbf{x}$ and $\mathbf{z}$, respectively, as defined in lemmma 3.5 for $g=N-p+2m+1$. Moreover,

from lemmma 3.5, if $m \not\equiv 1 \bmod 3$, then m_1 should be the nearest integer to $(m-1)/3$, that is m_1^* =round$[(m-1)/3]$ for $p = 1, 2, 3$. □ □

Theorem 3.3. *Consider an 3^m fractional factorial design and the class of designs $\mathcal{D}_N$ with $N \equiv p$ mod 9 runs, $p = 1, 2, 3$, and that $OA(N-p, m, 3, 2)$ exists. Let also consider the p level combinations $\ell_{j1}\ell_{j2}\cdots\ell_{jm}$, $j = 1, 2, \ldots, p$, such that any two level combinations have an equal number m_1^* =round$[(m-1)/3]$ of coincidences. The design $d^* \in \mathcal{D}_N$ obtained by adding the above p level combinations to an $OA(N-p, m, 3, 2)$ is Φ-optimal*

Proof. From relation (3.1) the Φ-optimal design is the one having information matrix $\mathbf{M}_{s_{2m+1}} = N\mathbf{I}_{2m+1}$ which implies that the design is orthogonal and $N \equiv 0 \bmod 9$. For $N \equiv p \bmod 9$, $p \neq 0$, the optimal design, should have information matrix $\mathbf{M}_{s_v}$, $\mathbf{M}_{s_v} \in \mathcal{M}_{2m+1}$, with $v \leq 2m$ as great as possible. Since M_{s_v} has v equal latent roots λ, from lemma 3.4, we have that matrix $\mathbf{M}_{s_v}$ is decomposed in two information matrices, such that $\mathbf{M}_{s_v} = (N-p)\mathbf{I}_{2m+1} + \mathbf{R}_1'\mathbf{R}_1$. As mentioned in theorem 3.2, the multiplicity of eigenvalue $N-p$ is $v = 2m+1-p$ (the greatest possible). So, from theorem 3.1, we have $\mathbf{M}_{s_v} = \mathbf{M}_{OA}$. Consequently, for any design $d \in \mathcal{D}_N$, with information matrix $\mathbf{M}_N$, $\mathbf{M}_N \in \mathcal{M}_{2m+1}$, from theorems 3.1 and 3.2, it holds:

$$\Phi(\mathbf{M}_N) = \Phi(\mathbf{M}_{s_1}) \geq \Phi(\mathbf{M}_{s_v}) = \Phi(\mathbf{M}_{OA}) \geq$$
$$\geq (2m+1-p)\phi(N-p) + (p-1)\phi(N-p+2m+1-(3m_1^*-m+1)) +$$
$$+\phi(N-p+2m+1+(p-1)(3m_1^*-m+1)) = \Phi(\mathbf{M}_{d^*}),$$

where m_1^* =round$[(m-1)/3]$. Hence, the design $d^* \in \mathcal{D}_N$ obtained as described in the statement of theorem 3.3 is Φ-optimal. □ □

The following examples clarify our main results.

4. Examples

For $N \equiv 1 \bmod s^2$ and $k = (s-1)m + 1$, we have from theorem 3.3 that $\Phi(\mathbf{M}_N) \geq (k-1)\phi(N-1) + \phi(N-p+k)$. The information matrix of a design obtained by adding any run to an $OA(N-1, m, s, 2)$ is $\mathbf{M}_{OA}^* = (N-1)\mathbf{I}_k + \mathbf{f}\mathbf{f}'$, where $\mathbf{f}'$ is any row of matrix $\mathbf{R}$ as defined in (2.4). The latent roots of $\mathbf{M}_{OA}^*$ are, $N-1$ with multiplicity $k-1$ and $1+\mathbf{f}'((N-1)\mathbf{I}_k)^{-1}\mathbf{f} = (N-1+k)$, according to lemma 2.1. So, this design is Φ-optimal. Kolyva-Machera (1989a), Kolyva-Machera (1989b) proved that the design obtained by adding any run to an $OA(N-1, m, 3, 2)$ is D- and G-optimal. Also, Mukerjee *et al.* (1999) proved that the design obtained by adding any run to an $OA(N-1, m, s, 2)$ is type 1 optimal. Note that type 1 optimality includes D-, A- and E-optimality (see Cheng (1978)).

For $N \equiv p \bmod 9$ runs, $p = 2, 3$, a Φ-optimal 3^m f.f.d. can be founded by adding p of the following level combinations: $\ell_{11}\ell_{12}\ldots\ell_{1m}, \ell_{21}\ell_{22}\ldots\ell_{2m}, \ell_{31}$
$\ell_{32}\ldots\ell_{3m}$, where for $h \neq i \neq k \neq h$ $\ell_{hj} \neq \ell_{ij} \neq \ell_{kj} \neq \ell_{hj}$, for $j = 1, 2, \ldots, m - m_1^*$ and $\ell_{ij} = \ell_{kj} = \ell_{hj}$, for $j = m - m_1^* + 1, \ldots, m$ to an $OA(N-p, m, 3, 2)$.

Conclusion. The problem of finding optimal fractional factorial designs for any $N \not\equiv 0 \bmod s^2$, $s > 2$ has stuck for many years. Although this paper solves the problem, the existence

of orthogonal arrays for any $N \equiv 0 \bmod s^2$ and any m, is necessary and the problem of finding optimal designs, remains open for futher research.

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Some Aspects of Optimal Covariate Designs in Factorial Experiments

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Abstract

Following Sinha *et al.* (2014), we initiate a study in the context of 2^n-factorial experiments involving the question of optimal allocation of covariate values. There is one controllable quantitative covariate and it is assumed to 'cover' two experimental units at a time. Earlier we dealt with block design set-up [Sinha *et al.* (2014)]. Here we take up 2^n-factorial set-up and address the question of optimal allocation of the covariate values. Results are illustrated for 2^2- or 2^3-factorial experiments.

Key words: Factorial experiments; Models with covariates; Optimal placement of covariate values.

1. Introduction

The key reference to this article is Sinha *et al.* (2014) dealing with a varietal design set-up. Here we start with a factorial experiment with the level-combinations having standard representations such as $[(0,0),(0,1),(1,0),(1,1)]$ for a 2^2 experiment. There is a controllable covariate x attached to every experimental unit and x assumes values in the closed interval $[-1,1]$. However, every attempt towards choice and application of x necessarily 'covers' a pair of experimental units each time. Thus, for example, we may choose 2 units and apply the level combinations $(0,0)$ and $(0,1)$ and attach a value $x = x_1$ to each of these two units. The mean responses for the two underlying outputs $Y[(0,0);x_1]$ and $Y[(0,1);x_1]$ are assumed to be of the form $\tau(00) + \beta x_1$ and $\tau(01) + \beta x_1$ respectively. Naturally, the contrast $\tau(01) - \tau(00)$ is readily estimated.

Based on the $2^2 = 4$ level combinations, we may form 6 pairs of the above form and make use of $6 \times 2 = 12$ experimental units in pairs and thereby use 6 covariate values. All 'level-combination contrasts' are trivially estimated and hence Main Effects and the 2-factor Interaction are unbiasedly estimated. We wish to provide unbiased estimate of the β-coefficient with utmost precision by suitable choice of the covariate values x's.

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Likewise, we may take up the case of 2^3-factorial experiment and study similar optimality problem involving 28 x-values, all in the closed interval$[-1, 1]$.

While we will develop the theory of optimization for the general case of 2^n-factorial experiment involving $2^{(n-1)}(2^n - 1)$ covariate-values, the cases of $n = 2, 3$ will serve as illustrative examples.

2. Optimal Choice of Covariate Values for 2^n-factorial Design Set-up

For n factors, each at 2-levels, let $N = 2^n$ denote the total number of level combinations. Since the allocation of covariate-values is assumed to 'cover' a pair of experimental units each time, we let $c = \binom{N}{2}$ denote the number of covariates $x_i, i = 1, 2, \cdots, c$ and X denote the $(c \times 1)$ vector $(x_1 x_2 \cdots x_c)'$. Now, it follows that $I(\beta)$ is a quadratic form in X and we denote it by a constant times $Q(X)$.

Construction of the matrix of quadratic form:
$I(\beta) = 2X'IX - [(c_1'X)^2 + \cdots + (c_N'X)^2]/(N-1)$
$= (1/(N-1))X'\{2(N-1)I - [(c_1c_1' + \cdots + c_Nc_N')]\}X = (1/(N-1))Q(X)$,
where c_i is the coefficient vector of order $(c \times 1)$ of i^{th} constraint having $(N-1)$ elements equal to 1 and the rest equal to 0.
Therefore each c_ic_i' is a symmetric matrix of order $(c \times c)$ with only $(N-1)$ nonnull rows (columns) with each nonnull row (column) having $(N-1)$ elements equal to 1 and the rest of $(c - N + 1)$ elements equal to 0.
Thus $Q(X) = X'[2(N-1)I - M]X$ where $M = \Sigma c_ic_i'$.

Notice that M is a symmetric matrix of order $(c \times c)$ wherein each row (column) has diagonal element equal to 2, $2(N-2)$ elements equal to 1 and the rest of $(c - 2N + 3)$ elements equal to 0.

In order to maximize $Q(X)$ for optimal choice of X i.e., of the x_i's, we argue, as in Sinha *et al.* (2014), that $Q(X)$ is maximized only when the x's are each at the extremes i.e., $+/-1$. We skip the proof in general terms. However, we provide all the technical details below for the cases of $n = 2, 3$.

3. Optimal Choice of Covariate Values for 2^2 Factorial Design Set-up

We start with the following Table 1 of x-values :

Standard representation in the form $[Y, A\theta, \sigma^2 I]$ with

$$\theta = (\tau(00), \tau(01), \tau(10), \tau(11), \beta)'$$

suggests a form of the matrix A of order 12×5 and we partition it as usual to derive an expression for Information on β i.e., $I(\beta)$. For simplicity, we drop the multiplier σ^-2. It follows that

$$I(\beta) = 2(\sum x_i^2) - [(x_1 + x_2 + x_3)^2 + (x_1 + x_4 + x_5)^2 + (x_2 + x_4 + x_6)^2 + (x_3 + x_5 + x_6)^2]/3.$$

Table 1

$x-values$	$level-combination(1)$	$level-combination(2)$
x_1	$(0,0)$	$(0,1)$
x_2	$(0,0)$	$(1,0)$
x_3	$(0,0)$	$(1,1)$
x_4	$(0,1)$	$(1,0)$
x_5	$(0,1)$	$(1,1)$
x_6	$(1,0)$	$(1,1)$

Optimality problem centers around optimal choice of the x's so as to maximize $I(\beta)$ when $-1 \leq x_i, i = 1,2,3,4,5,6 \leq 1$.

It follows that $I(\beta)$ can be expressed as a constant times a quadratic form $Q(X)$. $I(\beta) = X'[6I - M]X/3 = Q(X)/3$ where the matrix M with i^{th}column m_i is given in an explicit form as

$$M = \Sigma c_i c_i' = \begin{pmatrix} m_1 & m_2 & m_3 & m_4 & m_5 & m_6 \\ 2 & 1 & 1 & 1 & 1 & 0 \\ 1 & 2 & 1 & 1 & 0 & 1 \\ 1 & 1 & 2 & 0 & 1 & 1 \\ 1 & 1 & 0 & 2 & 1 & 1 \\ 1 & 0 & 1 & 1 & 2 & 1 \\ 0 & 1 & 1 & 1 & 1 & 2 \end{pmatrix}$$

It turns out that a choice of the X's subject to the value of each of the expressions $(x_1 + x_2 + x_3), (x_1 + x_4 + x_5), (x_2 + x_4 + x_6), (x_3 + x_5 + x_6)$ is $+/-1; x_i = +/-1$ serves the purpose and we achieve $I(\beta) = 32/3$. Specifically, one choice is
$x_1 = -1, x_2 = +1, x_3 = -1, x_4 = -1, x_5 = +1, x_6 = +1$ which yields, for the partial sums, $(x_1 + x_2 + x_3) = -1, (x_1 + x_4 + x_5) = -1, (x_2 + x_4 + x_6) = +1, (x_3 + x_5 + x_6) = +1$.

We give a proof of the above claim below.

Lemma 1 : Let $X_0 = (x_1 x_2 \cdots x_c)'$ be the vector with elements in the interval $[-1, +1]$ which maximizes $Q(X) = X'(tI - M)X$, where $t \geq max(m_{ii})$ is a positive constant. Then each component x_i of X_0 is $+/-1$.

Proof: Write $X_0 = U_i + x_i e_i$ where e_i is the i^{th} column of I. Then
$Q(X_0) = (U_i + x_i e_i)'(tI - M)(U_i + x_i e_i) = U_i'(tI - M)U_i + x_i^2(t - m_{ii}) + 2x_i U_i'(tI - M)e_i$
$= U_i'(tI - M)U_i + x_i^2(t - m_{ii}) + 2x_i U_i'(-M)e_i = p_i + (t - m_{ii})x_i^2 + 2x_i q_i$,
where $p_i = U_i'(tI - M)U_i$ and $q_i = -U_i' M e_i = -U_i' m_i$ do not involve x_i.
Now it is clear that for $Q(X_0)$ to be maximum the value of x_i should be $+/-1$ with sign as that of the constant q_i. In case $q_i = 0$, x_i can be given any of $+1$ or -1.

Algorithm: Start with $U_0 = \phi$. For $i = 1, 2, \cdots, c$, in i^{th} step, calculate $q_i = -U_{i-1}' m_i$. Replace ith element of U_{i-1} with $+/-1$, the sign being that of q_i and denote this new vector by U_i. If $q_i = 0$ then any sign can be chosen. Add $|q_i|$ to q. Increase i by 1 and repeat.
After c steps, check the vector $X = U_c$ is a vector which maximizes $Q(X)$ or not.

The following lemma is useful for checking whether the vector computed using above algorithm maximizes $Q(X)$ or not.

Lemma 2 : Starting with $U_0 = \phi$, the final vector U_c obtained after c steps of above algorithm maximizes $Q(X)$ if and only if 2q=$2\Sigma|q_i| = \Sigma m_{ii} - N$.
Proof: Let Q_i denote $Q(U_i)$, for $i = 1, 2, \cdots, c$. Notice that at i^{th} step
$Q_i = Q_{i-1} + (t - m_{ii})x_i^2 + 2x_i q_i$. Hence the increment at i^{th} step is $(t - m_{ii})x_i^2 + 2x_i q_i$. Thus $Q_c = \sum((t - m_{ii})x_i^2 + 2x_i q_i) = t \times c - \Sigma m_{ii} + 2 \times \Sigma|q_i|$. Comparing this with the maximum value $t \times c - N$ of $Q(X)$, we get the required result.

For $n = 2$, $N = 4$, $c = 6$, $t = 6$, each $m_{ii} = 2$ and $\Sigma|q_i| = 4$ (from the table).Therefore, $2\Sigma|q_i| = 8 = \Sigma m_{ii} - N$. Hence $Q(U_c)$ maximizes $Q(X)$.

In order to achieve the solution, it is now a matter of verification of the conditions

$$(u_1 + u_2 + u_3) = (u_1 + u_4 + u_5) = (u_2 + u_4 + u_6) = (u_3 + u_5 + u_6) = +/-1; x_i = +/-1.$$

Example: For the case $n = 2$, the successive U vectors along with k_2 values are as follows:

q_i	0	-1	0	0	-1	2
U_0	U_1	U_2	U_3	U_4	U_5	U_6
0	1	1	1	1	1	1
0	0	-1	-1	-1	-1	-1
0	0	0	1	1	1	1
0	0	0	0	-1	-1	-1
0	0	0	0	0	-1	-1
0	0	0	0	0	0	1

The first row gives the values of $q_i = -U'_{i-1}m_i$, for $i = 1, 2, \cdots, c$, and the last column displays the optimum choice of U since the conditions are readily verified to hold.
For the first step when $q_1 = 0$, we chose the value $+1$ for the first element of U_1. Next step $q_2 = -1$ and we take the second element of $U_2 = -1$. For the third step, $q_3 = 0$ and we choose the third element of $U_3 = 1$ and so on. The solution is not unique though. For example, another choice of the final vector is $(1\ -1\ 1\ 1\ -1\ 1)$ which also maximizes $Q(x)$.

4. Optimal Choice of Covariate Values in A 2^3 Factorial Experiment

We now discuss similar result for the case of 2^3 factorial experiment. A version of Table 1 would be Table 2 as shown below. This time the matrix A is of order 28×9 and $I(\beta)$ is given by the expression [again ignoring σ^-2]

$$I(\beta) = 2\sum x_i^2 - [(x_1 + x_2 + \ldots\ldots + x_7)^2 + \ldots + (x_7 + x_{13} + x_{18} + x_{22} + x_{25} + x_{27} + x_{28})^2]/7$$

It turns out that $I(\beta)$ attains its maximum value of $56 - 8/7 = 384/7$ for a choice of the x's at the extreme values $+/-1$ subject to

$$\begin{aligned}
(000): &\quad x_1 + x_2 + x_3 + x_4 + x_5 + x_6 + x_7 = &+/-1,\\
(001): &\quad x_1 + x_8 + x_9 + x_{10} + x_{11} + x_{12} + x_{13} = &+/-1,\\
(010): &\quad x_2 + x_8 + x_{14} + x_{15} + x_{16} + x_{17} + x_{18} = &+/-1,\\
(011): &\quad x_3 + x_9 + x_{14} + x_{19} + x_{20} + x_{21} + x_{22} = &+/-1,\\
(100): &\quad x_4 + x_{10} + x_{15} + x_{19} + x_{23} + x_{24} + x_{25} = &+/-1,\\
(101): &\quad x_5 + x_{11} + x_{16} + x_{20} + x_{23} + x_{26} + x_{27} = &+/-1,\\
(110): &\quad x_6 + x_{12} + x_{17} + x_{21} + x_{24} + x_{26} + x_{28} = &+/-1,\\
(111): &\quad x_7 + x_{13} + x_{18} + x_{22} + x_{25} + x_{27} + x_{28} = &+/-1.
\end{aligned}$$

One such (optimal) choice is given in the same Table 2.

The realized values of various partial sums of the x's corresponding to the above solution to the x's are given below.

$$\begin{aligned}
(000): &\quad x_1 + x_2 + x_3 + x_4 + x_5 + x_6 + x_7 = &-1,\\
(001): &\quad x_1 + x_8 + x_9 + x_{10} + x_{11} + x_{12} + x_{13} = &-1,\\
(010): &\quad x_2 + x_8 + x_{14} + x_{15} + x_{16} + x_{17} + x_{18} = &-1,\\
(011): &\quad x_3 + x_9 + x_{14} + x_{19} + x_{20} + x_{21} + x_{22} = &-1,\\
(100): &\quad x_4 + x_{10} + x_{15} + x_{19} + x_{23} + x_{24} + x_{25} = &-1,\\
(101): &\quad x_5 + x_{11} + x_{16} + x_{20} + x_{23} + x_{26} + x_{27} = &+1,\\
(110): &\quad x_6 + x_{12} + x_{17} + x_{21} + x_{24} + x_{26} + x_{28} = &-1,\\
(111): &\quad x_7 + x_{13} + x_{18} + x_{22} + x_{25} + x_{27} + x_{28} = &+1.
\end{aligned}$$

5. Proof of Claim for 2^3 Case

The expression for $Q(x)$ given for 2^2 factorial set-up generalizes itself naturally to the case of 2^3 factorial set-up and is given by $I(\beta) = X'[14I - M]X/7 = Q(X)/7$ where all the diagonal elements of the matrix M are each equal to 2 while its off-diagonal elements are a known combination of 0s and 1s. The Lemma 1 and the algorithm stated above both work in this set-up as well. In the above, we have given one solution and there are other solutions too.

Table 3 gives the matrix M along with the final vector U_c (obtained using the above algorithm with initial vector as null vector), the values of q_i and $|q_i|$. $Q(X)$ attains maximum at $X = U$.

For $n = 3$, $N = 8$, $c = 6$, $t = 14$, each $m_{ii} = 2$ and $\Sigma|q_i| = 24$ (from the table).Therefore, $2\Sigma|q_i| = 48 = \Sigma m_{ii} - N$. Hence U_c maximizes $Q(X)$.

For the choice vector displayed above, various partial sums, as realized, are shown below.

Table 2

$generic\, x-values$	$level-combination(1)$	$level-combination(2)$	$optimal\, x-values$
x_1	$(0,0,0)$	$(0,0,1)$	-1
x_2	$(0,0,0)$	$(0,1,0)$	-1
x_3	$(0,0,0)$	$(0,1,1)$	-1
x_4	$(0,0,0)$	$(1,0,0)$	-1
x_5	$(0,0,0)$	$(1,0,1)$	1
x_6	$(0,0,0)$	$(1,1,0)$	1
x_7	$(0,0,0)$	$(1,1,1)$	1
x_8	$(0,0,1)$	$(0,1,0)$	1
x_9	$(0,0,1)$	$(0,1,1)$	1
x_{10}	$(0,0,1)$	$(1,0,0)$	1
x_{11}	$(0,0,1)$	$(1,0,1)$	1
x_{12}	$(0,0,1)$	$(1,1,0)$	-1
x_{13}	$(0,0,1)$	$(1,1,1)$	-1
x_{14}	$(0,1,0)$	$(0,1,1)$	-1
x_{15}	$(0,1,0)$	$(1,0,0)$	-1
x_{16}	$(0,1,0)$	$(1,0,1)$	-1
x_{17}	$(0,1,0)$	$(1,1,0)$	1
x_{18}	$(0,1,0)$	$(1,1,1)$	1
x_{19}	$(0,1,1)$	$(1,0,0)$	1
x_{20}	$(0,1,1)$	$(1,0,1)$	1
x_{21}	$(0,1,1)$	$(1,1,0)$	1
x_{22}	$(0,1,1)$	$(1,1,1)$	-1
x_{23}	$(1,0,0)$	$(1,0,1)$	-1
x_{24}	$(1,0,0)$	$(1,1,0)$	-1
x_{25}	$(1,0,0)$	$(1,1,1)$	1
x_{26}	$(1,0,1)$	$(1,1,0)$	-1
x_{27}	$(1,0,1)$	$(1,1,1)$	1
x_{28}	$(1,1,0)$	$(1,1,1)$	-1

$$
\begin{aligned}
(000): &\quad x_1+x_2+x_3+x_4+x_5+x_6+x_7 = 1,\\
(001): &\quad x_1+x_8+x_9+x_{10}+x_{11}+x_{12}+x_{13} = 1,\\
(010): &\quad x_2+x_8+x_{14}+x_{15}+x_{16}+x_{17}+x_{18} = 1,\\
(011): &\quad x_3+x_9+x_{14}+x_{19}+x_{20}+x_{21}+x_{22} = 1,\\
(100): &\quad x_4+x_{10}+x_{15}+x_{19}+x_{23}+x_{24}+x_{25} = 1,\\
(101): &\quad x_5+x_{11}+x_{16}+x_{20}+x_{23}+x_{26}+x_{27} = 1,\\
(110): &\quad x_6+x_{12}+x_{17}+x_{21}+x_{24}+x_{26}+x_{28} = 1,\\
(111): &\quad x_7+x_{13}+x_{18}+x_{22}+x_{25}+x_{27}+x_{28} = 1.
\end{aligned}
$$

It may be seen that this solution is different from the one shown earlier.

Table 3

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	U_c	q_i	$\lvert q_i \rvert$
1	2	1	1	1	1	1	1	1	1	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0
2	1	2	1	1	1	1	1	1	0	0	0	0	0	1	1	1	1	1	0	0	1	1	0	0	0	0	0	0	−1	−1	1
3	1	1	2	1	1	1	1	0	1	0	0	0	0	1	0	0	0	0	1	1	1	1	0	0	0	0	0	0	1	0	0
4	1	1	1	2	1	1	1	0	0	1	0	0	0	0	1	0	0	0	1	0	0	0	1	1	1	0	0	0	−1	−1	1
5	1	1	1	1	2	1	1	0	0	0	1	0	0	0	0	1	0	0	0	1	0	0	1	0	0	1	1	0	1	0	0
6	1	1	1	1	1	2	1	0	0	0	0	1	0	0	0	0	1	0	0	0	1	0	0	1	0	1	0	1	−1	−1	1
7	1	1	1	1	1	1	2	0	0	0	0	0	1	0	0	0	0	1	0	0	0	0	0	0	1	0	1	1	1	0	0
8	1	1	0	0	0	0	0	2	1	1	1	1	1	1	1	0	1	1	0	0	0	0	0	0	0	0	0	0	1	0	0
9	1	0	1	0	0	0	0	1	2	1	1	2	1	1	0	0	0	0	1	1	0	0	0	0	0	0	0	0	−1	−3	3
10	1	0	0	1	0	0	0	1	1	2	1	1	1	0	1	0	0	0	1	0	0	0	1	1	1	0	0	0	1	0	0
11	1	0	0	0	1	0	0	1	1	1	2	1	1	0	0	0	0	0	0	1	0	0	0	1	1	0	1	0	−1	−3	3
12	1	0	0	0	0	1	0	1	1	1	1	2	1	0	0	0	1	0	0	0	1	0	0	1	0	1	0	0	1	0	0
13	1	0	0	0	0	0	1	1	1	1	1	1	2	0	0	0	0	1	0	0	0	1	0	0	1	0	1	0	−1	−3	3
14	0	1	1	0	0	0	0	1	1	0	0	0	0	2	1	1	1	2	0	0	1	1	0	0	0	0	0	0	1	0	0
15	0	1	0	1	0	0	0	1	0	1	0	0	0	1	2	1	1	1	1	0	0	0	1	1	1	0	0	0	−1	−1	1
16	0	1	0	0	1	0	0	1	0	0	1	0	0	1	1	2	1	1	0	1	0	0	0	1	0	1	0	0	1	0	0
17	0	1	0	0	0	1	0	1	0	0	0	0	1	1	1	1	2	1	0	1	0	0	0	1	0	1	0	1	−1	−1	1
18	0	1	0	0	0	0	1	1	0	0	0	0	1	1	1	1	1	2	0	0	0	1	0	0	1	0	1	1	1	0	0
19	0	0	1	1	0	0	0	0	1	1	0	0	0	1	1	0	0	0	2	1	1	1	1	1	1	0	0	0	1	0	0
20	0	0	1	0	1	0	0	0	1	0	1	0	0	1	1	1	0	0	1	2	1	1	1	0	0	1	1	0	−1	−3	3
21	0	0	1	0	0	1	0	0	1	0	0	0	0	1	0	0	1	1	1	1	2	1	0	1	0	1	0	1	1	0	0
22	0	0	1	0	0	0	1	0	1	0	0	0	1	1	0	0	0	1	1	1	1	2	0	0	1	0	1	1	−1	−3	3
23	0	0	0	1	1	0	0	0	0	1	1	0	0	0	1	1	0	0	1	1	0	0	2	1	1	1	1	0	1	0	0
24	0	0	0	1	0	1	0	0	0	1	0	1	0	0	0	1	1	0	1	1	1	0	1	2	1	1	0	1	−1	−1	1
25	0	0	0	0	1	0	1	0	0	0	0	1	0	1	0	0	1	0	0	0	1	1	1	1	2	0	1	1	1	0	0
26	0	0	0	0	0	1	0	0	0	0	1	1	0	0	0	1	1	1	0	1	1	1	0	1	0	2	1	1	1	0	0
27	0	0	0	0	1	0	1	0	0	0	1	0	1	0	0	1	0	1	0	1	0	1	1	0	1	1	2	1	−1	−3	3
28	0	0	0	0	0	1	1	0	0	0	0	1	1	0	0	0	1	1	0	0	1	1	0	1	1	1	1	2	1	0	0

Table 4

$x-values$	$level-combination(1)$	$level-combination(2)$	$level-combination(3)$
x_1	$(0,0)$	$(0,1)$	$(1,0)$
x_2	$(0,0)$	$(0,1)$	$(1,1)$
x_3	$(0,0)$	$(1,0)$	$(1,1)$
x_4	$(0,1)$	$(1,0)$	$(1,1)$

6. Generalization to 'triplets'

We now contemplate a situation when every single application of the covariate value x encompasses three experimental units i.e., 'covers the eu's in triplets'. What would be the optimal choice of covariate values for most efficient estimation of the β co-efficient ? We study the cases of 2^2 and 2^3 factorials in this section.

(A) The case of 2^2 factorial

It follows that we need 4 covariate-values x_1, x_2, x_3, x_4 as are indicated in the Table 4 below.

It transpires that $I(\beta)$ has the representation

$$I(\beta) = 3\sum x_i^2 - [(T-x_1)^2 + (T-x_2)^2 + (T-x_3)^2 + (T-x_4)^2]/3, T = \sum x_i$$

We readily find that $I(\beta) = [8\sum x_i^2 - 2T^2]/3 \leq 32/3$ with "=" if and only if $T = 0; x_i = +/-1; i = 1,2,3,4$. Any contrast of order 4×1 involving $+/-1$'s such as $(1,1,-1,-1)$ gives a solution.

(B) The case of 2^3 factorial

It follows that we need 56 covariate-values $x_1, x_2, \ldots, x_{56}$ associated with the triplets of the level-combinations as are partially indicated in the Table 5 below.

In the above, we have displayed the first set of 21 x-values corresponding to the triplets starting with $(0,0,0)$. Note that the second set of 15 x-values $[x_{22} - x_{36}]$ correspond to triplets starting with $(0,0,1)$. Likewise, third set of 10 $[X_{37} - x_{46}]$ start with $(0,1,0)$; fourth set of 6 $[x_{47} - x_{52}]$ start with $(0,1,1)$; fifth set of 3 $[x_{53} - x_{55}]$ start with $(1,0,0)$ and the last [sixth] set of a singleton starts with $(1,0,1)$.

Next note that each triplet generates three observations and hence we have a total of $56 \times 3 = 168$ observations in the vector representation Y. Moreover, every x-value will have three replications. It transpires that $I(\beta)$ has the representation

$$I(\beta) = 3\sum x_i^2 - [T_1^2 + T_2^2 + \ldots + T_8^2]/21.$$

Table 5

$x-values$	$level-combination(1)$	$level-combination(2)$	$level-combination(3)$
x_1	$(0,0,0)$	$(0,0,1)$	$(0,1,0)$
x_2	$(0,0,0)$	$(0,0,1)$	$(0,1,1)$
$-$	$-$	$-$	$-$
x_6	$(0,0,0)$	$(0,0,1)$	$(1,1,1)$
x_7	$(0,0,0)$	$(0,1,0)$	$(0,1,1)$
$-$	$-$	$-$	$-$
x_{11}	$(0,0,0)$	$(0,1,0)$	$(1,1,1)$
x_{12}	$(0,0,0)$	$(0,1,1)$	$(1,0,0)$
$-$	$-$	$-$	$-$
x_{15}	$(0,0,0)$	$(0,1,1)$	$(1,1,1)$
x_{16}	$(0,0,0)$	$(1,0,0)$	$(1,0,1)$
x_{17}	$(0,0,0)$	$(1,0,0)$	$(1,1,0)$
x_{18}	$(0,0,0)$	$(1,0,0)$	$(1,1,1)$
x_{19}	$(0,0,0)$	$(1,0,1)$	$(1,1,0)$
x_{20}	$(0,0,0)$	$(1,0,1)$	$(1,1,1)$
x_{21}	$(0,0,0)$	$(1,1,0)$	$(1,1,1)$

There are eight level-combinations and therefore, eight T_i's. Every T_i contains 21 terms and we demand it to assume the value $+/-1$. In the above expression, each T_i is a linear combination of x_is. The Lemma holds true once again. Each x_i has to be necessarily $+/-1$. Now writing $T_i = c_i'x$ for $i = 1, 2, \cdots, 8$, the following table gives the 8 these coefficient vectors c_i, along with a solution vector X.

References

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Table 6

	c_1	c_2	c_3	c_4	c_5	c_6	c_7	c_8	X
1	1	1	1	0	0	0	0	0	1
2	1	1	0	1	0	0	0	0	−1
3	1	1	0	0	1	0	0	0	1
4	1	1	0	0	0	1	0	0	−1
5	1	1	0	0	0	0	1	0	1
6	1	1	0	0	0	0	0	1	−1
7	1	0	1	1	0	0	0	0	1
8	1	0	1	0	1	0	0	0	−1
9	1	0	1	0	0	1	0	0	1
10	1	0	1	0	0	0	1	0	−1
11	1	0	1	0	0	0	0	1	1
12	1	0	0	1	1	0	0	0	−1
13	1	0	0	1	0	1	0	0	1
14	1	0	0	1	0	0	1	0	−1
15	1	0	0	1	0	0	0	1	1
16	1	0	0	0	1	1	0	0	−1
17	1	0	0	0	1	0	1	0	1
18	1	0	0	0	1	0	0	1	−1
19	1	0	0	0	0	1	1	0	1
20	1	0	0	0	0	1	0	1	−1
21	1	0	0	0	0	0	1	1	1
22	0	1	1	1	0	0	0	0	−1
23	0	1	1	0	1	0	0	0	1
24	0	1	1	0	0	1	0	0	−1
25	0	1	1	0	0	0	1	0	1
26	0	1	1	0	0	0	0	1	−1
27	0	1	0	1	1	0	0	0	1
28	0	1	0	1	0	1	0	0	−1
29	0	1	0	1	0	0	1	0	1
30	0	1	0	1	0	0	0	1	−1
31	0	1	0	0	1	1	0	0	1
32	0	1	0	0	1	0	1	0	−1
33	0	1	0	0	1	0	0	1	1
34	0	1	0	0	0	1	1	0	−1
35	0	1	0	0	0	1	0	1	1
36	0	1	0	0	0	0	1	1	−1
37	0	0	1	1	1	0	0	0	1
38	0	0	1	1	0	1	0	0	−1
39	0	0	1	1	0	0	1	0	1
40	0	0	1	1	0	0	0	1	−1
41	0	0	1	0	1	1	0	0	1
42	0	0	1	0	1	0	1	0	−1
43	0	0	1	0	1	0	0	1	1
44	0	0	1	0	0	1	1	0	−1
45	0	0	1	0	0	1	0	1	1
46	0	0	1	0	0	0	1	1	−1
47	0	0	0	1	1	1	0	0	−1
48	0	0	0	1	1	0	1	0	1
49	0	0	0	1	1	0	0	1	−1
50	0	0	0	1	0	1	1	0	1
51	0	0	0	1	0	1	0	1	−1
52	0	0	0	1	0	0	1	1	1
53	0	0	0	0	1	1	1	0	−1
54	0	0	0	0	1	1	0	1	1
55	0	0	0	0	1	0	1	1	−1
56	0	0	0	0	0	1	1	1	1

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Optimality of Binary Periodic Sequences of Odd Length and Its Applications to Finding Near Optimal 2-symbol Factorial Designs

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Abstract

We propose using periodic binary sequences with optimal correlation energy (CE) to generate near $E(s^2)$-optimal supersaturated designs (SSDs) and near D-optimal 2-symbol fractional factorial designs for the all main effects and the intercept model. We derive a lower bound for the CE of odd length periodic sequences and provide previously unknown odd length periodic sequences with optimal CE up to length 43.

Key words: Factorial designs; Supersaturated designs; Binary periodic sequences; Correlation energy.

1. Introduction

In this section, we provide the background material on binary periodic sequences, their periodic autocorrelations and correlation energy (CE). We also introduce the group ring notation for investigating periodic sequences. Such sequences with optimal CE generate near $E(s^2)$-optimal 2-symbol supersaturated designs (SSDs) and near D-optimal 2-symbol fractional factorial designs for the all main effects and the intercept model. In Section 2, we derive a lower bound for the CE of odd length periodic sequences. In Section 3, we provide previously unknown odd length periodic sequences with optimal CE up to length 43.

1.1 Sequences and Their Periodic Autocorrelations

A sequence $\mathbf{a} = (a_i)$, where $i = 0, 1, ..., v-1$, is called *periodic* with period (length) v if $a_i = a_{i+v}$ for all i. Such a sequence is also called a $\mathbb{Z}_v$-sequence. In this paper, we consider binary sequences consisting of entries in $\{-1, 1\}$. Let

$$C_{\mathbf{a},\mathbf{b}}(t) = \sum_{i=0}^{v-1} a_{(i+t) \bmod v} \bar{b}_i,$$

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where $\bar{b}_i$ is the complex conjugate of b_i. Then $C_{\mathbf{a},\mathbf{b}}(t)$ is called the *periodic cross-correlation function* of $\mathbf{a}$ and $\mathbf{b}$, where the special case $C_{\mathbf{a},\mathbf{a}}(t)$ is called the *periodic autocorrelation function* (ACF) of $\mathbf{a}$. The sequence $\{C_{\mathbf{a},\mathbf{a}}(t)\}_{t=0}^{\infty}$ is again periodic with period (length) v. It is also easy to verify that $C_{\mathbf{a},\mathbf{a}}(t) = C_{\mathbf{a},\mathbf{a}}(-t)$. Hence, it suffices to find the autocorrelation coefficients $C_{\mathbf{a},\mathbf{a}}(t)$ for $t \in \{0, 1, \ldots, \lfloor v/2 \rfloor\}$. The ACF provides a measure of how much the original sequence differs from its translates. Define $D = \{0 \leq i \leq v-1 : a_i = 1\}$ and $d_D(t) = |(t + D) \cap D|$. Then $d_D(t) = |(t + D) \cap D|$ is called the *difference function* of $D \subseteq \mathbb{Z}_v$. It is easy to show that

$$C_{\mathbf{a},\mathbf{a}}(t) = v - 4(k - d_D(t)), \tag{1}$$

where $k = |D|$. From equation (1) we readily get $C_{\mathbf{a},\mathbf{a}}(t) \equiv v \pmod 4$. We call $C_{\mathbf{a},\mathbf{a}}(v)$, $C_{\mathbf{a},\mathbf{a}}(2v)$, $C_{\mathbf{a},\mathbf{a}}(3v), \ldots$ the *main lobes*, and the remaining $C_{\mathbf{a},\mathbf{a}}(i)$ *side lobes*. The value $\max_{g \in G} |C_{\mathbf{a},\mathbf{a}}(g)|$ is called the *peak side lobe*. A sequence $\mathbf{a}$ is said to have *good matched autocorrelation properties* if the peak side lobes in the autocorrelation are small and the sum of the squares of the side lobes in the autocorrelation is small.

Definition 1. *The periodic merit factor (PMF) of a sequence* $\mathbf{a}$ *is defined to be*

$$PMF = \frac{C_{\mathbf{a},\mathbf{a}}^2(0)}{\sum_{l=1}^{v-1} C_{\mathbf{a},\mathbf{a}}^2(l)}.$$

It is desirable to have a large PMF. Hence, our goal is to find sequences with the maximum PMF. Maximizing the PMF is analogous to maximizing the Golay merit factor, where the only difference is that the Golay merit factor is based on a sequence's aperiodic autocorrelation function Green and Green (2002).

Definition 2. *The correlation energy* (CE) *of a sequence* $\mathbf{a}$ *is defined by*

$$CE(\mathbf{a}) = \sum_{l=1}^{v-1} C_{\mathbf{a},\mathbf{a}}^2(l).$$

Maximizing the PMF of a $\{-1, 1\}$ sequence is equivalent to minimizing its CE. A sequence that minimizes the CE is called CE-optimal. We seek to identify what $\{-1, 1\}$ sequence(s) are CE-optimal. A $\{-1, 1\}$ CE-optimal sequence with $C_{\mathbf{a},\mathbf{a}}(i) = 0$ for $i = 1, 2, \ldots, v-1$ is called a *perfect sequence*. The only perfect sequence known is a row of the circulant Hadamard matrix of order 4. For $v \equiv 2 \pmod 4$ CE optimality is guaranteed to occur when $C_{\mathbf{a},\mathbf{a}}(i) = \pm 2$. For $v \equiv 1 \pmod 4$ and $v \equiv 3 \pmod 4$ CE optimality is likely to occur if each $C_{\mathbf{a},\mathbf{a}}(i)$ for $i = 1, 2, \ldots, v-1$ is in $\{-3, 1\}$ and $\{-1, 3\}$.

Next, we introduce the group ring notation that is needed in deriving our results.

Definition 3. *Let* G *be a finite group and* R *a ring, where* $G = \{g_0, g_1, \ldots, g_{n-1}\}$. *Then the group ring of* G *over* R *is the set denoted by* $R[G]$ *defined as:*

$$R[G] = \left\{ \sum_{g \in G} a_g g \mid a_g \in R \right\}.$$

When working with the group ring notation, multiplication and addition are defined in a way similar to those of polynomials. We further define the power of a group ring element in the following way.

Definition 4. *If* $W = \sum_{g\in G} a_g g$ *is an element of* $R[G]$*, and* t *is some integer, then*

$$\left(\sum_{g\in G} a_g g\right)^{(t)} = \sum_{g\in G} a_g g^t.$$

When we refer to a binary $\mathbb{Z}_v$-sequence, we mean a $\mathbb{Z}_v$-sequence with entries from $\{-1, 1\}$ or $\{0, 1\}$. By abuse of notation, we identify a $\mathbb{Z}_v$-sequence $\mathbf{a}$ with the group ring element $S = \sum_{g\in\mathbb{Z}_v} a_g g$. Also, for a $\{0, 1\}$ $\mathbb{Z}_v$-sequence, we identify the group ring element $\sum_{g\in A} g$ with the set A. In particular, $\mathbb{Z}_v$ identifies $\sum_{g\in\mathbb{Z}_v} g$. For a multiplicatively (additively) written cyclic group we use 1 (0) as the identity element. The group ring elements that correspond to $\mathbb{Z}_v$-sequences are used to calculate the autocorrelation of a $\mathbb{Z}_v$-sequence $\mathbf{a}$, where

$$C_{\mathbf{a},\mathbf{a}}(g) = \text{coefficient of } g \text{ in } SS^{(-1)}.$$

Let $A = \{d_0, d_1, \ldots, d_{k-1}\} \subseteq \mathbb{Z}_v$. For each $g \in \mathbb{Z}_v$ let a_g be the number of times g appears in A and $S = \sum_{g\in\mathbb{Z}_v} a_g g$. Then A is a (v, k, λ) *difference set* $\mathrm{DS}(v, k, \lambda)$ if

$$SS^{(-1)} = (k - \lambda)0 + \lambda\mathbb{Z}_v \ \in\ \mathbb{Z}[\mathbb{Z}_v],$$

and A is a $(v, k, \lambda, \lambda + 1)$ *almost difference set* $\mathrm{ADS}(v, k, \lambda, \lambda + 1)$ if

$$SS^{(-1)} = k0 + \lambda B + (\lambda + 1)(\mathbb{Z}_v - B - 0) \ \in\ \mathbb{Z}[\mathbb{Z}_v],$$

for some $B \subset \mathbb{Z}_v \setminus \{0\}$.

Remark 1. *Difference sets and almost difference sets are studied in the more general group theoretic context. The term "array" is used instead of the term "sequence" when the group in question is non-cyclic.*

For more on sequences, arrays, and their interplay with group developed combinatorial designs see Arasu (2011) and Arasu *et al.* (2019).

1.2 Using CE-optimal $\mathbb{Z}_v$-sequences to Construct Near D-optimal Designs and Near $E(s^2)$-optimal SSDs

The Hadamard maximum determinant problem seeks an $N \times N$ matrix of ± 1s with the largest possible determinant. Such matrices are called D-optimal matrices. An online source for this problem can be found at Orrick and Solomon (2018). Multiplying a row or a column of a matrix by -1 does not change its determinant. Hence, an $N \times N$ D-optimal design whose first column is the all 1s column always exists. The last $N - 1$ columns of an $N \times N$ D-optimal matrix whose first column is the all 1s column can be used as an N row, $N - 1$ column

2-symbol factorial design for estimating the all main effects and the intercept model. In fact, such a design minimizes the determinant of the variance-covariance matrix among all possible N row, $N-1$ column, 2-symbol factorial designs for the all main effects and the intercept model.

An N row, k factor, 2-symbol factorial design is called a *supersaturated design* (SSD) if $N < k+1$, i.e., if it does not have enough rows to estimate the all main effects and the intercept model. Most of the literature on SSDs assumes that each column in a 2-symbol SSD is *balanced*, i.e. has an equal number for 1s and -1s. However, recently Bulutoglu *et al.*Bulutoglu *et al.* (2019) considered $\{-1,1\}$ SSDs with a prespecified distribution of column sums. Let $\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_m]$ be an N row, m column, 2-symbol SSD with symbols from $\{-1,1\}$. Then the $E(s^2)$ value of $\mathbf{X}$ is defined as

$$E(s^2) = \frac{\sum_{i\neq j} s_{ij}^2}{m(m-1)},$$

where $s_{ij} = \mathbf{x}_i^T \mathbf{x}_j$ for $1 \leq i < j \leq m$. The $E(s^2)$ value criterion is used to compare two 2-symbol SSDs with the same number of rows and columns, where the SSD with the smaller $E(s^2)$ is more desirable Georgiou (2014). An SSD with the smallest possible $E(s^2)$ is called $E(s^2)$-optimal. For the best known $E(s^2)$-lower bounds of balanced SSDs, see Georgiou (2014) and Bulutoglu *et al.*Bulutoglu *et al.* (2019) for unbalanced SSDs.

A $\{-1,1\}$ $\mathbb{Z}_v$-sequence $\mathbf{a}$ of length v can be used to generate a $v \times v$ matrix of ± 1s by taking the sequence as the first column and obtaining the other columns as cyclic shifts. The resulting $v \times v$ matrix $\mathbf{A}$ is called the *corresponding design* to $\mathbf{a}$. Then $\mathbf{a}$ can either be used to generate a fractional factorial design or as an SSD. In the first case, a subset of A's rows are multiplied by -1 so that its first column is the all 1s column. The remaining $v-1$ columns of $\mathbf{A}$ constitute a v row, $v-1$ column factorial design that can be used for estimating the all main effects and the intercept model. When $\mathbf{A}$ is used as an SSD, the matrix $\mathbf{A}$ is taken as the v row, v column SSD, and the relation

$$\frac{CE(\mathbf{a})}{v-1} = E(s^2)$$

connects the $E(s^2)$ of $\mathbf{A}$ to $CE(\mathbf{a})$. Hence, a CE-optimal sequence $\mathbf{a}$ can be used to generate an SSD that is near $E(s^2)$-optimal.

It is well known that a $v \times v$ matrix $\mathbf{A}$ that has small $E(s^2)$ tends to have large determinant Bulutoglu *et al.* (2019). Hence, we expect that if $\mathbf{A}$ is used to generate a fractional factorial design, then the resulting factorial design will be near D-optimal for estimating the all main effects and the intercept model.

2. CE Lower Bounds

It is easy to see that $\mathbf{x}$ is a CE-optimal $\{0,1\}$ sequence if and only if $2\mathbf{x} - \mathbf{1}$ is a CE-optimal $\{-1,1\}$ sequence, where $\mathbf{1}$ is the all 1s sequence. We say that a $\{0,1\}$ sequence $\mathbf{x}$ *corresponds* to a $\{-1,1\}$ sequence $\mathbf{y}$ if $\mathbf{y} = 2\mathbf{x} - \mathbf{1}$. It is easy to see that the autocorrelation function of a $\{0,1\}$ sequence is $d_D(t)$. We will use the notation $C_{\mathbf{a},\mathbf{a}}(t)$ for $\{-1,1\}$ sequences.

If we refer to $C_{\mathbf{a},\mathbf{a}}(t)$ of a $\{0,1\}$ sequence, we mean the autocorrelation function of its corresponding $\{-1,1\}$ sequence. To find CE-optimal $\{0,1\}$ sequences, we first investigate $\{0,1\}$ sequences of odd length having at most three-valued $d_D(t)$s (at most two distinct non-trivial λs that differ by 1). For such a $\{0,1\}$ sequence $\mathbf{a}$ indexed by $\mathbb{Z}_v$ we have

$$SS^{(-1)} = k0 + \lambda B + (\lambda+1)(\mathbb{Z}_v - B - 0) \tag{2}$$

for some $B \subset \mathbb{Z}_v \setminus \{0\}$ with $|B| = t$. Then, by applying the principal character to both sides of equation (2), we get

$$\begin{aligned} \chi_0\left(SS^{(-1)}\right) =& \chi_0\left(k0 + \lambda B + (\lambda+1)(\mathbb{Z}_v - B - 0)\right) \\ |A|^2 =& k + \lambda|B| + (\lambda+1)(|\mathbb{Z}_v| - |B| - 1) \\ k^2 =& k + \lambda t + (\lambda+1)(v - t - 1). \end{aligned} \tag{3}$$

We refer to equation (3) as the group ring equation. By equation (1)

$$\lambda_1 = \lambda = \frac{4k - v + \gamma_1}{4} \quad \text{and} \quad \lambda_2 = \lambda + 1 = \frac{4k - v + \gamma_2}{4}, \tag{4}$$

where $\gamma_j = C_{\mathbf{a},\mathbf{a}}(i_j)$ for some i_j such that $i_j \neq v$ for $j \in \{1,2\}$. Observe that $\gamma_2 = \gamma_1 + 4$. Upon substituting the right hand side of (4) to the group ring equation we get

$$k^2 = k + \left(\frac{4k - v + \gamma_1}{4}\right) t + \left(\frac{4k - v + \gamma_1}{4} + 1\right)(v - t - 1).$$

We solve for $t(v,k,\gamma)$:

$$\begin{aligned} k^2 =& k + \left(\frac{4k - v + \gamma}{4}\right) t(v,k,\gamma) + \left(\frac{4k - v + \gamma}{4} + 1\right)(v - t(v,k,\gamma) - 1) \\ t(v,k,\gamma) =& k - k^2 + \left(\frac{4k - v + \gamma}{4} + 1\right)(v - 1) \\ t(v,k,\gamma) =& k - k^2 + \left(\frac{4k - v + \gamma + 4}{4}\right)(v - 1). \end{aligned} \tag{5}$$

Now, $\max(|\gamma_1|, |\gamma_2|)$ depends on $v \pmod 4$.

Case 1: $v \equiv 1 \pmod 4$, $\max(|\gamma_1|, |\gamma_2|) = \max(|\gamma_1|, |\gamma_1 + 4|) = |\gamma_1|$, where $\gamma_1 = -3$. Then

$$t(v,k,-3) = k - k^2 + \left(\frac{4k - v + 1}{4}\right)(v - 1).$$

In this case, minimizing the CE is equivalent to minimizing $t(v,k,-3)$. Solving for k when

$t(v,k,-3)=0$, we get

$$\begin{aligned} 0 &= k-k^2+\left(\frac{4k-v+1}{4}\right)(v-1) \\ k^2-k &= \left(\frac{4k-v+1}{4}\right)(v-1) \\ 4k^2-4k &= (4k-v+1)(v-1) \\ 4k^2-4vk+(v-1)^2 &= 0 \\ k &= \frac{4v\pm\sqrt{16v^2-16(v-1)^2}}{8} \\ k &= \frac{v\pm\sqrt{2v-1}}{2}. \end{aligned} \tag{6}$$

Hence, k should be rounded to the closest integer k^* to

$$\frac{v\pm\sqrt{2v-1}}{2}$$

so that $t(v,k^*,-3)$ is a nonnegative integer less than v.

Case 2: $v\equiv 3 \pmod 4$, $\max(|\gamma_1|,|\gamma_2|)=\max(|\gamma_2-4|,|\gamma_2|)=|\gamma_2|$, where $\gamma_2=3$. Thus, we have to minimize

$$\begin{aligned} t^*(v,k,3)=v-t(v,k,3)-1 &= v-\left(k-k^2+\left(\frac{4k-v+3+4}{4}\right)(v-1)\right)-1 \\ &= v-k+k^2-\left(\frac{4k-v+7}{4}\right)(v-1)-1 \\ &= k^2-k-\left(\frac{4k-v+7}{4}\right)(v-1)-1. \end{aligned}$$

Now $t^*(v,k,3)$ has a minimum at

$$k=-\frac{-1-(v-1)}{2}=\frac{v}{2}. \tag{7}$$

In light of equations (6) and (7), we determine what number of elements are required to minimize the CE for a given length. So, k should be rounded to the closest integer k^* to $v/2$ such that $t(k^*)$ is a nonnegative integer less than v. Based on the knowledge gained thus far, we provide the following table for the parameters of the odd length sequences up to length 49 that are CE-optimal when they exist.

Theorem 1. *When a sequence with the parameters in a row of Table 1 exists, then it is CE-optimal.*

Proof. The result is obvious for cases in which the correlation $|\gamma_j|=3$ count is 0 or 2. For all the remaining cases, $v\equiv 1 \pmod 4$. So, for each of these cases the next best possibility with $C_{\mathbf{a},\mathbf{a}}(t')\notin\{-3,1\}$ for some t' is when the frequency of $C_{\mathbf{a},\mathbf{a}}(t)=\gamma_2=5$ is 2 and the frequency of $C_{\mathbf{a},\mathbf{a}}(t)=\gamma_1=1$ is $v-3$. For each v such that the correlation $|\gamma_j|=3$ count is 4 or larger, the CE of a sequence with the frequency of $\gamma_2=5$ equal to 2 is larger or equal to the corresponding CE in Table 1. □

Table 1: The optimal parameters for odd length sequences up to length 49

v	k^*	Correlation $\lvert\gamma_j\rvert = 3$ count	CE
5	1	0	4
7	4	0	6
9	3	2	24
11	6	0	10
13	4	0	12
15	8	0	14
17	6	2	32
19	10	0	18
21	8	4	52
23	12	0	22
25	9	0	24
27	14	0	26
29	11	2	44
31	16	0	30
33	13	4	64
35	18	0	34
37	15	6	84
39	20	0	38
41	16	0	40
43	22	0	42
45	18	2	60
47	24	0	46
49	20	4	80

3. CE-optimal Sequences

We present Table 2 containing sequences with minimum CE (maximum periodic merit factor) by length, v. The remaining columns show the elements of the sequence that are 1, CE, number of 1s k in the sequence, and a column indicating if the sequence is optimal and has the parameters in Table 1. All lengths for which the column labeled "Conform?" is answered with "Y" are optimal as each has a set of parameters that appears in Table 1. If the column contains an "N", then the sequence listed is still optimal, it just does not have the parameters in Table 1. In other words, just because the equations indicate a particular parameter set as being optimal does not mean that such a sequence exists.

The length $v = 17$ is the shortest length for in which the Table 1 hypothetical optimal sequence fails to exist. The Table 1 hypothetical optimal sequence for this length should have $k = 6$ and a CE of 32. The indices of the 1 entries of such a sequence constitutes an ADS$(17, 6, 1, 2)$. However, a computer search revealed that this sequence does not exist. To search for a sequence with the next best possible CE, we must add an element to a hypothetical

ADS$(17, 6, 1, 2)$. For $k = 7$ the group ring equation

$$49 = 7 + 2t + 3(17 - t - 1)$$

gives $t = 6$, and a sequence with the next best possible CE is an ADS$(17, 7, 2, 3)$ with $CE = 64$. We found such a sequence by using a computer search.

For $v = 39$ and $v = 41$, the group ring equations and arguments for the CE-optimal sequences indicate that each of DS$(39, 20, 10)$ and DS$(41, 16, 6)$ is CE-optimal if it exists. Both of these are known not to exist by the Mann test Baumert and Gordon (2004). The nonexistence of DS$(39, 20, 10)$ requires that we look for a sequence with two different non-trivial autocorrelation values. The group ring equations give that the next best possible case is when $k = 18$, and from

$$18^2 = 18 + 8t + 9(39 - t - 1)$$

we get that $t = 36$. This particular sequence was not found by an exhaustive computer search. The next best case can be found by removing another element from the set making $k = 17$. Using the group ring equation,

$$17^2 = 17 + 7t + 8(39 - t - 1)$$

gives that $t = 32$. This sequence was found and is listed in Table 2.

A CE-optimal solution to the length $v = 41$ case has been open Luke and Schotten (2003). An optimal solution based on a DS$(41, 16, 6)$ is known not to exist Lander (1983). If we decrease k by 1 to $k = 15$, then the group ring equation

$$15^2 = 15 + 4t + 5(41 - t - 1)$$

implies $t = -10$. This is not possible. Thus, we must increase k by 1 to $k = 17$. When $k = 17$,

$$17^2 = 17 + 6t + 7(41 - t - 1)$$

giving $t = 8$. Such a sequence was found and is listed in Table 2. The autocorrelation of our length 41 $\{-1, 1\}$ sequence contains 8 $-$3s and 32 $+$1s. There is another distribution of autocorrelation values with 2 $-$3s, 2 $+$5s, 36 $+$1s, and $CE = 104$. A computer search proved that such a sequence does not exist.

A DS$(25, 9, 3)$ does not exist by the Mann test Baumert and Gordon (2004). A DS$(27, 14, 7)$ does not exist Lander (1983). We proved that an ADS$(29, 11, 3, 4)$ does not exist by an exhaustive computer search. In fact, to check the correctness of our exhaustive search implementation, we proved the existence/non-existence of each of the corresponding hypothetical difference set or almost difference set in each row of Table 1 by using our computer program. Hence, none of the hypothetical CE-optimal sequences in Table 1 for $v = 25, 27, 29$ exists. The solutions in Table 2 for the $v = 25, 27, 29$ cases are constructed similar to the $v = 17, 39, 41$ cases.

Theorem 2. *Each sequence in Table 2 is CE-optimal.*

Table 2: Optimal sequences of odd length up to length 43

v	Sequence elements	CE	k	Conform?
5	{0}	4	1	Y
7	{1,2,4}	6	3	Y
9	{0,1,3}	24	3	Y
11	{1,3,4,5,9}	10	5	Y
13	{0,1,5,11}	12	4	Y
15	{0,1,2,7,9,12,13}	14	7	Y
17	{0,1,2,3,5,8,12}	64	7	N
19	{1,4,5,6,7,9,11,16,17}	18	9	Y
21	{7,9,12,13,16,18,19,20}	52	8	Y
23	{1,2,3,4,6,8,9,12,13,16,18}	22	11	Y
25	{0,9,10,12,15,16,18,20,23,24}	72	10	N
27	{0,9,11,12,13,16,18,19,22,24,26}	74	11	N
29	{0,9,10,13,15,18,21,22,23,25,27,28}	92	12	N
31	{1,2,4,7,8,14,15,16,19,23,25,27,28,29,30}	30	15	Y
33	{0,9,13,14,15,19,21,22,24,26,29,30,32}	64	13	Y
35	{0,1,3,4,7,9,11,12,13,14,16,17,21,27,28,29,33}	34	17	Y
37	{0,6,12,14,17,19,23,24,27,28,31,33,34,35,36}	84	15	Y
39	{2,4,5,7,9,10,11,14,15,16,23,24,25,27,31,35,38}	86	17	N
41	{0,9,11,14,15,21,22,24,27,29,31,32,33,35,36,39,40}	104	17	N
43	{1,4,6,9,10,11,13,14,15,16,17,21,23,24,25,31,35,36,38,40,41}	42	21	Y

The CE-optimal sequences constructed in this paper can be used to construct ± 1 matrices with large determinants. These matrices can be used to construct fractional factorial designs that are near D-optimal for estimating the all main effects and the intercept model. In particular, the largest known determinant for ± 1 matrices of order 39 is given by Tamura in Tamura (2006) using group divisible designs. Tamura's record holding matrix has a determinant of $2^{43} \times 3^{36} \times 5$. While we can not beat this record, we come surprisingly close by using our optimal sequence of length 39. By creating a matrix whose first row is the sequence itself followed by each of the next 38 rows being a right-circulant shift of the previous, we generate a circulant matrix of order 39. This matrix has a determinant of $2^{36} \times 3^6 \times 5 \times 7 \times 29^3 \times 3331^3$. This is 95.7% of Tamura's determinant.

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Appendix

Proof of Theorem 2

The only cases that are not covered by Theorem 1 are when $v = 17, 25, 27, 29, 39, 41$. For each of these cases no solution with parameters in Theorem 1 exists. For a $\{-1, 1\}$ sequence $\mathbf{a}$ it is easy to show that

$$\sum_{t=0}^{v-1} C_{\mathbf{a},\mathbf{a}}(t) = (2k - v)^2.$$

Let $\mathbf{a}$ be a CE-optimal sequence. We first consider the cases when $C_{\mathbf{a},\mathbf{a}}(t) \in \{-3,-1,1,3\}$ for each nonnegative $t(v,k,\gamma^*)$, where

$$\gamma^* = \begin{cases} -3 \text{ if } v \equiv 1 \pmod 4, \\ \ \ 3 \text{ if } v \equiv 3 \pmod 4. \end{cases}$$

Let

$$\alpha(v,k,\gamma^*) = \text{number of } -3\text{s in } \{C_{\mathbf{a},\mathbf{a}}(t)\}_{t=0}^{v-1}.$$

Observe that $\alpha(v,k,\gamma^*)$ completely determines $\{C_{\mathbf{a},\mathbf{a}}(t)\}_{t=0}^{v-1}$. Then, for $v \equiv 1 \pmod 4$

$$\begin{aligned} \alpha + \beta &= v-1 \\ -3\alpha + \beta &= (2k-v)^2 - v \end{aligned}$$

and

$$\alpha(v,k,-3) = \frac{(2v-1)-(2k-v)^2}{4}.$$

For fixed $v > 0$, $\alpha(v,k,-3)$ is a quadratic function of k with a maximum at $k = v/2$. Similarly, for $v \equiv 3 \pmod 4$

$$\begin{aligned} \alpha + \beta &= v-1 \\ 3\alpha - \beta &= (2k-v)^2 - v \end{aligned}$$

and

$$\alpha(v,k,3) = \frac{(2k-v)^2-1}{4}.$$

For fixed $v > 0$, $\alpha(v,k,-3)$ is a quadratic function of k with a minimum at $k = v/2$.

In both $v \equiv 1 \pmod 4$ and $v \equiv 3 \pmod 4$ cases $\alpha(v,k,\gamma^*)$ must be a nonnegative integer as small as possible. Moreover, $t(v,k,\gamma^*)$ as in equation (5) must be a nonnegative integer. Also, since $C_{\mathbf{a},\mathbf{a}}(t) = C_{\mathbf{a},\mathbf{a}}(-t)$, $\alpha(v,k,\gamma^*)$ must be even. Then for each fixed $v \in \mathbb{Z}^{\geq 0}$, a solution to the integer nonlinear program (INLP)

$$\begin{aligned} \min_{k} \quad & \alpha(v,k,\gamma^*) \\ \text{subject to:} \quad & t(v,k,\gamma^*) = y, \\ & v-1 \geq \alpha(v,k,\gamma^*) = 2x \geq 0, \ \ v-1 \geq k \geq 2, \\ & v-1 \geq y \geq 0 \quad x,y,k \in \mathbb{Z}, \\ & \text{a sequence } \mathbf{a} \text{ with } \{C_{\mathbf{a},\mathbf{a}}(t)\}_{t=0}^{v-1} \text{ determined by } \alpha(v,k,\gamma^*) \text{ exists} \end{aligned} \tag{8}$$

describes a CE-optimal sequence among all sequences with $\{C_{\mathbf{a},\mathbf{a}}(t)\}_{t=0}^{v-1} \in \{-3,3,1,-1\}$ for each t. Let k^* be a solution of the INLP (8). Then,

$$k^* = \begin{cases} \text{an integer farthest to } v/2 \text{ satisfying constraints of INLP (8) if } v \equiv 1 \pmod 4, \\ \text{an integer closest to } v/2 \text{ satisfying constraints of INLP (8) if } v \equiv 3 \pmod 4. \end{cases} \tag{9}$$

For $v \in \{17,25,27,29,39,41\}$, each value of k in Table 2 satisfies condition (9), and the corresponding sequence is CE-optimal among all sequences $\mathbf{a}$ of the same length such that

$C_{\mathbf{a},\mathbf{a}}(t) \in \{-3,-1,1,3\}$ for $t = 1,2,\ldots,v-1$. For cases $v = 17,25,29,41$, the next best possibility with $C_{\mathbf{a},\mathbf{a}}(t') \notin \{-3,1\}$ for some t' is when the frequency of $C_{\mathbf{a},\mathbf{a}}(t) = \gamma_2 = 5$ is 2 and the frequency of $C_{\mathbf{a},\mathbf{a}}(t) = \gamma_1 = 1$ is $v-3$. The CE resulting from this distribution of autocorrelations is smaller than the CE of the corresponding sequence in Table 2 only when $v = 41$. Hence, the length $17,25,29$ sequences listed in Table 2 are all CE-optimal. Then, for $v = 41$ the distribution of autocorrelations of a sequence with a smaller CE is given by 38 $+1$s and 2 $+5$s. However, by examining the group ring equation and using equations (4) we find that

$$k^2 = k + 38\left(\frac{4k-41+1}{4}\right) + 2\left(\frac{4k-41+5}{4}\right). \tag{10}$$

Equation (10) has no integer solutions. Thus, the length 41 sequence listed in Table 2 is CE-optimal with $CE = 104$.

For cases $v = 27,39$, the next best possibility with $C_{\mathbf{a},\mathbf{a}}(t') \notin \{-1,3\}$ for some t' is when the frequency of $C_{\mathbf{a},\mathbf{a}}(t) = \gamma_2 = -1$ is $v-3$ and the frequency of $C_{\mathbf{a},\mathbf{a}}(t) = \gamma_1 = -5$ is 2. The CE resulting from this distribution of autocorrelations is equal to the CE of the corresponding sequence listed in Table 2 for both $v = 27$ and $v = 39$ cases.

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