Statistics and Applications {ISSN 2454-7395 (online)}
Volume 19, No. 1, 2021 (New Series), pp 277–286

An Algorithmic Approach to the Construction of Weighted A-optimal Balanced Treatment Incomplete Block Designs

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Received: 21 November 2020; Revised: 13 January 2021; Accepted: 23 February 2021

Abstract

The purpose of this paper is to present a heuristic algorithm for obtaining weighted A-optimal balanced treatment incomplete block (BTIB) designs for making test versus test and tests versus control comparisons. The proposed algorithm is implemented using R language. The proposed algorithm has been used to obtain weighted A-optimal BTIB designs in a restricted parametric range. A total of 369 weighted A-optimal BTIB designs are obtained in the restricted parametric range.

Key words: Algorithm; BTIB Designs; Linear Integer Programming; Test Treatment; Control; R package.

1. Introduction

There are many experimental situations where the experimenter is interested in comparing a set of new treatments, called tests, with a standard treatment, called control. In the presence of a single nuisance factor, block designs for tests versus control are recommended for conducting such experiments. A number of useful classes of designs such as balanced treatments incomplete block (BTIB) designs, group divisible treatment (GDT) designs, partially balanced treatment incomplete block (PBTIB) designs are available in literature and a lot of research efforts has been made on these designs. One can refer to Hedayat *et al.* (1988), Gupta and Parsad (2001) and Section 5.4 of Dey (2010) for a review on designs for tests versus control comparison.

Consider the experimental setting where v test treatments are to be compared with a control using a block design with b blocks each of size k. Let $D(v, b, k)$ denote the class of connected block designs in $v + 1$ treatments with b blocks with size k each. In the choice of A-optimal designs for tests versus controls comparisons, only comparison between test treatments and the control played the role in the choice of A-optimal designs. No consideration was made for pairwise comparison among test treatments. Since the designs in $D(v, b, k)$ are connected, they permit estimation of test versus test comparisons along with test versus control comparisons. Though, the pairwise comparisons among test versus test treatments would be required with lesser precision. To this end, Gupta *et al.* (1999) introduced weighted A-optimality of the block designs. Gupta *et al.* (1999) derived conditions

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under which a design is weighted A-optimal for estimating these two sets of contrasts with unequal precisions. They provided a method of construction and a catalogue of weighted A-efficient BTIB designs. Parsad *et al.* (2009) proposed an algorithm based on interchange-exchange approach to obtain weighted A-efficient and weighted A-optimal designs for test versus test and tests versus control comparisons. They also obtained 15259 weighted A-efficient designs using the proposed algorithm. However, they reported only 43 weighted A-optimal BTIB designs in Table 3 of their article.

The purpose of this article is to present an algorithm for construction of weighted A-optimal BTIB designs and a list of 369 weighted A-optimal BTIB designs in a restricted parametric range. The article is organized as follows. Section 2 gives the concept of weighted A-optimality. An algorithm is proposed to obtain weighted A-optimal BTIB designs in section 3. The list of weighted A-optimal BTIB designs obtained using the proposed algorithm is presented in section 5. The article is concluded in section 6.

2. Preliminaries

Let the control treatment be indexed as 0 and the test treatments be denoted as $1, 2, ..., v$. Assume the two-way classified fixed effects homoscedastic model

$$y_{ijl} = \mu + \tau_i + \beta_j + \epsilon_{ijl} \tag{1}$$

where y_{ijl} denote the response from the lth experimental units in jth block receiving ith treatment, τ_i is the effect of ith treatment, β_j is the effect of jth block and ϵ_{ijl} are uncorrelated errors with mean zero and constant variance σ^2,$i = 0, 1, 2, ..., v,\ j = 1, 2, ..., b$ and $l = 1, 2, ..., k$. It may be mentioned here that Gupta *et al.* (1999) considered mixed effects model with random block effects. However, we shall restrict ourselves to fixed effects of blocks. A design $d \in D(v, b, k)$ is said to be weighted A-optimal if it minimizes

$$\beta \sum_{i=1}^{v} \text{var}\left(\hat{\tau}_{d0} - \hat{\tau}_{di}\right) + \alpha \sum_{i=1}^{v-1} \sum_{i'=i+1}^{v} \text{var}\left(\hat{\tau}_{di} - \hat{\tau}_{di'}\right)$$

with $\beta + \alpha = 1$ and $0 \leq \alpha, \beta \leq 1$. The expression above is the weighted sum of the variances of the estimates of test-control contrasts and test-test contrasts, respectively, with weights as β and α, respectively. Clearly, for $\alpha = 0$, the criterion reduces to A-optimality for tests vs controls and for $\alpha = \beta$, the criterion reduces to A-optimality for all pairwise comparisons. Since more precision is required for test-control comparisons than the test-test comparisons, β and α may be so chosen that $\beta > \alpha$.

Let $\mathbf{P}_c = [\mathbf{1}_v : -\mathbf{I}_v]$ and $\mathbf{P}_{T,Z} = [\mathbf{0}_Z : \mathbf{0}_{Z\times(v-Z-1)} : \mathbf{1}_Z : -\mathbf{I}_Z]$, $Z = 1, 2, ..., v-1$. Then

$$\mathbf{P} = \begin{pmatrix} \mathbf{P}_c \\ \mathbf{P}'_{T,1} \\ \mathbf{P}'_{T,2} \\ \vdots \\ \mathbf{P}'_{T,v-1} \end{pmatrix} \tag{2}$$

is the coefficient matrix of the contrasts for test-control and test-test comparisons.

To search for A-optimal block designs in $D(v,b,k)$, Gupta *et al.* (1999) focused their attention in the class of BTIB$(v,b,k;t,s)$ designs which was introduced by Stufken (1987). Gupta *et al.* (1999) presented the following result to characterize weighted A-optimality of BTIB designs.

Theorem 1: A BTIB$(v,b,k;t,s)$ design is A-optimal over $D(v,b,k)$ for fixed value of α if

$$g(t,s)=\min_{(x,z)\in\Delta} g(x,z)$$

where $\Delta=\{(x,z): x=0,1,...,int(k/2)-1; z=0,1,...,b \text{ with } z>0 \text{ when } x=0\}$ and $g(x,z)=\frac{(\beta+\alpha v)(v-1)^2}{A(x,z)}+\frac{\beta b}{B(x,z)}$,
$A(x,z)=k(v-1)[b(k-x)-z]-[v\{b(k-x)-z\}-bk^2-bx^2-2xz-z+2k(bx+z)]$,
$B(x,z)=b[k(bx+z)-(bx^2+2xz+z)]$ and $\alpha/\beta\le\frac{\{(2vk-2v-k+1)^2-(k-1)^2(v-1)^2\}}{v[(k-1)(v-1)]^2}$ when k is odd

and $\alpha/\beta\le\frac{(2vk-2v-k)^2-k^2(v-1)^2}{v[k(v-1)]^2}$ when k is even.

Theorem 1 gives a sufficient condition to check weighted A-optimality of a given BTIB $(v,b,k;t,s)$ design and is useful to see whether a BTIB design is weighted A-optimal or not for given value of α. Gupta *et al.* (1999) used the result to check weighted A-optimality of designs from Parsad *et al.* (1995). The number of weighted A-optimal BTIB designs obtained by them are given below.

α	0	0.1	0.2	0.3	0.4
Number of designs	9	7	8	6	0

It is clear from above that more efforts are required to obtain weighted A-optimal BTIB designs. To this end, we present an algorithm to obtain weighted A-optimal BTIB designs.

3. The Algorithm

In this section, we present the algorithm to obtain weighted A-optimal BTIB designs in $D(v,b,k)$ for test-test and test-control comparisons. Given v,b,k, the algorithm computes the value of t and s which minimize $g(x,z)$ and then obtains other parameters through necessary parametric relations. Then it attempts to obtain the incidence matrix of a weighted A-optimal BTIB design with these parameters through linear integer programming approach.

The steps of the algorithm are detailed below.

Step 1: Given v,b,k and α, first check whether α satisfies the condition of Theorem 1. If α satisfies the condition of Theorem 1, obtain t and s which minimize $g(x,z)$.

Step 2: Compute $r_0=s+bt, r=(bk-r_0)/v, \lambda_0=(s(t+1)(k-t-1)+(b-s)t(k-t))/v$ and $\lambda_1=(r(k-1)-\lambda_0)/(v-1)$. If all of r,r_0,λ and λ_0 are integers then proceed, else a weighted A-optimal BTIB does not exist.

Step 3: (i) Create the first row of the incidence matrix **N** by assigning $t+1$ in s randomly chosen columns and by assigning t in the remaining $b-s$ columns of the row. The first row of incidence matrix indicates the allocation of the control to b blocks.

(ii) Obtain the ith $(i = 2, 3, \ldots, v+1)$ row for allocation of $(i-1)$th test treatment to blocks by solving the following linear integer programming formulation with respect to *binary* decision variables $x_1, x_2, \ldots, x_b$:

$$\begin{aligned} &\text{Maximize } \phi = \sum_{j=1}^{b} w_j x_j \\ &\text{subject to constraints} \\ &\sum_{j=1}^{b} x_j = r \\ &x_j \leq k - k_j \forall j = 1, 2, \ldots, b \\ &\sum_{j=1}^{b} n_{1j} x_j = \lambda_0 \\ &\sum_{j=1}^{b} n_{i'j} x_j = \lambda_1, \ \forall i' = 2, 3, \ldots, i-1 \end{aligned} \tag{3}$$

where $w_j = \frac{1}{k_j}$ if $k_j > 0$ and $w_j = 1$ if $k_j = 0$, with k_j being the size of the jth block up to $(i-1)$ row and $n_{i'j}$ is the element at the i'th row and the jth column of **N**.

(iii) If there is no optimal solution of the formulation (3), delete a random row m between 2 to $(i-1)$th row of the incidence matrix, store the deleted row in a matrix **T**, update k_j values and try to obtain a newer solution to mth row by solving the formulation (4):

$$\begin{aligned} &\text{Maximize } \phi = \sum_{j=1}^{b} w_j x_j \\ &\text{subject to constraints} \\ &\sum_{j=1}^{b} x_j = r \\ &x_j \leq k - k_j \ \forall j = 1, 2, \ldots, b \\ &\sum_{j=1}^{b} n_{1j} x_j = \lambda_0 \\ &\sum_{j=1}^{b} n_{i'j} x_j = \lambda_1 \ \forall i' = 2, 3, \ldots, m-1, m+1, \ldots, i-1 \\ &\sum_{j=1}^{b} t_{uj} x_j < r \ \forall u = 1, 2, \ldots, p \end{aligned} \tag{4}$$

where p is the number of rows of the matrix **T** and t_{uj} is the element at the

uth row and the jth column of $\mathbf{T}$ matrix. If there is a solution then update the incidence matrix. If there is no solution, repeat this step by drawing another random number m. Once the mth row is obtained, then go back to step ii) to obtain the ith row.

Step 4: If all the $v+1$ rows of the matrix $\mathbf{N}$ are obtained, then compute the A-efficiency by using the formula $A_e = \text{trace}(\mathbf{PC}_{d*}^{-}\mathbf{P}')/\text{trace}(\mathbf{PC}_{d}^{-}\mathbf{P}')$ to confirm weighted A-optimality of the design. Here d^* is a hypothetical A-optimal design in $D(v,b,k)$ for which $\text{trace}(\mathbf{PC}_{d*}^{-}\mathbf{P}')$ is minimum. If $A_e = 1$, then the design is weighted A-optimal.

The formulations (3) and (4) allocate a particular test treatment to r blocks out of the b blocks. While doing so, the objective function gives less weight to those blocks which already contains more number of treatments compared to other blocks. The first constraint ensures that the number of replications of the treatment is r. The second constraint is to ensure that a block does not contain more than k treatments. The third and fourth set of constraints ensure that for a given test treatment, the concurrences with the control and with the other test treatments are λ_0 and λ_1, respectively. The additional fifth constraint in formulation (4) prevents an already deleted solution for the mth row to recur.

Even if a weighted A-optimal BTIB design exists, sometimes the proposed algorithm may not be able to obtain a weighted A-optimal design. For example, the algorithm may get $u < v+1$ rows of incidence matrix $\mathbf{N}$ and it may not be able to proceed after uth row. This indicates that in these u rows, there may be some row(s) which do not allow the desired structure of the required design. Though step (iii) of Step 3 is there to eliminate such rows, however, it is not known which row(s) are actually the culprit and so step (iii) of Step 3 may not be 100% effective and this is the reason that the algorithm may not be able to get a solution even though a weighted optimal exists for the given parameters.

We have seen that the algorithm works best when $v \leq 30$ and $k \leq 10$. The efficiency of the algorithm to obtain weighted A-optimal design goes down with larger values of v. This is due to the fact that the chances of entering improper candidate rows in the incidence matrix increases with larger v. Further research efforts are required to obtain weighted A-optimal BTIB designs for larger values of v and k.

The integer programming formulations (3) and (4) were solved using lpSolve R package of Berkelaar and Others (2011) and the complete algorithm is implemented using R language. Further, an R package Aoptbdtvc (Mandal *et al.*, 2017a) has been built and published on CRAN. The package is available on cran.r-project.org/web/packages/Aoptbdtvc/index.html. A manual showing the usage of functions to implement the proposed algorithm is also available in the same web page.

4. Working of The Algorithm

In this Section, we illustrate the working of the algorithm with the help of an example.

Example 1: Consider construction of weighted A-optimal BTIB design for $v = 4, b = 4, k = 4, \alpha = 0.4$ The algorithm finds that $t = 0, s = 4$ in Step 1. From Step 2, algorithm gives $r_0 = 4, r = 3, \lambda_0 = 3, \lambda = 2$. Now in Step 3, the algorithm attempts to obtain an treatment-block incidence matrix of such a BTIB design with these parameters.

In the first step of Step 3, the algorithm obtains first row of the treatment-block incidence matrix as $\begin{pmatrix}1 & 1 & 1 & 1\end{pmatrix}$. To obtain the second row of the incidence matrix, following linear integer program is solved:

Maximize $\phi = x_1 + x_2 + x_3 + x_4$ subject to constraints

$$\begin{aligned} &x_1 + x_2 + x_3 + x_4 = 3 \\ &x_1 \leq 4 - 1 \\ &x_2 \leq 4 - 1 \\ &x_3 \leq 4 - 1 \\ &x_4 \leq 4 - 1 \\ &x_1 + x_2 + x_3 + x_4 = 3. \end{aligned}$$

An optimal solution to the above linear program is $\begin{pmatrix}0 & 1 & 1 & 1\end{pmatrix}$. So after two steps, the incidence matrix obtained is $\begin{pmatrix}1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1\end{pmatrix}$. To obtain the third row, the linear integer formulation is Maximize $\phi = x_1 + \frac{1}{2}x_2 + \frac{1}{2}x_3 + \frac{1}{2}x_4$ subject to constraints

$$\begin{aligned} &x_1 + x_2 + x_3 + x_4 = 3 \\ &x_1 \leq 4 - 1 \\ &x_2 \leq 4 - 2 \\ &x_3 \leq 4 - 2 \\ &x_4 \leq 4 - 2 \\ &x_1 + x_2 + x_3 + x_4 = 3 \\ &x_2 + x_3 + x_4 = 2. \end{aligned}$$

An optimal solution to this formulation is $\begin{pmatrix}1 & 0 & 1 & 1\end{pmatrix}$ which gives incidence matrix up to third row as $\begin{pmatrix}1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1\end{pmatrix}$. For obtaining the fourth row, the formulation is Maximize $\phi = \frac{1}{2}x_1 + \frac{1}{2}x_2 + \frac{1}{3}x_3 + \frac{1}{3}x_4$ subject to constraints

$$\begin{aligned} &x_1 + x_2 + x_3 + x_4 = 3 \\ &x_1 \leq 4 - 2 \\ &x_2 \leq 4 - 2 \\ &x_3 \leq 4 - 3 \\ &x_4 \leq 4 - 3 \\ &x_1 + x_2 + x_3 + x_4 = 3 \\ &x_2 + x_3 + x_4 = 2 \\ &x_1 + x_3 + x_4 = 2. \end{aligned}$$

The algorithm gives an optimal solution to this formulation as $\begin{pmatrix}1 & 1 & 0 & 1\end{pmatrix}$ and hence, the incidence matrix obtained till fourth row is $\begin{pmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \end{pmatrix}$. For getting the last row of the incidence matrix, the formulation is as follows: Maximize $\phi = \frac{1}{3}x_1 + \frac{1}{3}x_2 + \frac{1}{4}x_3 + \frac{1}{4}x_4$ subject to constraints

$$
\begin{aligned}
&x_1 + x_2 + x_3 + x_4 = 3 \\
&x_1 \leq 4 - 3 \\
&x_2 \leq 4 - 3 \\
&x_3 \leq 4 - 3 \\
&x_4 \leq 4 - 4 \\
&x_1 + x_2 + x_3 + x_4 = 3 \\
&x_2 + x_3 + x_4 = 2 \\
&x_1 + x_3 + x_4 = 2 \\
&x_1 + x_2 + x_4 = 2.
\end{aligned}
$$

An optimal solution to this formulation is $\begin{pmatrix} 1 & 1 & 1 & 0 \end{pmatrix}$. As a result, the algorithm gives treatment-block incidence matrix as $\begin{pmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix}$ and the corresponding design is

Block-1	(0	2	3	4)
Block-2	(0	1	3	4)
Block-3	(0	1	2	4)
Block-4	(0	1	2	3)

For confirmation of A-optimality, A_e is computed which is $A_e = \text{trace}(\mathbf{PC}_{d*}^{-}\mathbf{P}')/\text{trace}(\mathbf{PC}_d^{-}\mathbf{P}')$ $= g(t,s)/\text{trace}(\mathbf{PC}_d^{-}\mathbf{P}') = 3.2/3.2 = 1$. Thus, the design so obtained is weighted A-optimal BTIB design for $v = b = k = 4, \alpha = 0.4$.

Let us consider another example with $\alpha = 0.5$.

Example 2: Consider $v = 6, b = 7, k = 4, \alpha = 0.5$. In Step 1, it can be found that $t = 0, s = 4$ which gives $r = r_0 = 4, \lambda_0 = \lambda_1 = 2$. Step 3 gives us the following design.

Block-1	(2	3	4	6)
Block-2	(0	2	3	4)
Block-3	(0	2	5	6)
Block-4	(1	2	4	5)
Block-5	(0	1	4	6)
Block-6	(1	2	3	6)
Block-7	(0	1	3	5)

Clearly, the design is a balanced incomplete block design and is A-optimal for all possible pair wise comparisons.

5. List of Weighted A-optimal BTIB Designs

The proposed algorithm in Section 3 can be used to construct weighted A-optimal BTIB designs for given parameters v, b, k, and α. We utilized the algorithm to obtain weighted A-optimal BTIB designs in a limited parametric range $2 \leq v \leq 30, v+1 \leq b \leq 50, 2 \leq k \leq min(10, v), \alpha = 0.2, 0.4, 0.6, 0.8$. We denote this parametric range as $\mathfrak{P}$ for further reference.

Within $\mathfrak{P}$, we obtained 369 A-optimal designs out of which 70 are R-type and 299 are S-type. The list of designs along with the layouts is available at `https://drs.icar.gov.in/WAoptBTIB/WAoptBTIB.htm`, (Mandal *et al.*, 2017b). The distribution of the designs according to various values of block size k and α is given in Table 1.

Table 1: Distribution of weighted A-optimal designs according to block size and α

	α				
Block size	0.2	0.4	0.6	0.8	Total Number of Designs
3	19	18	17	19	73
4	28	16	14	20	78
5	31	12	11	10	64
6	5	13	8	11	37
7	16	14	7	6	43
8	0	12	6	10	28
9	3	10	6	6	25
10	3	10	3	5	21
Total Number of Designs	105	105	72	87	369

We made a comparison of the weighted A-optimal designs obtained above with those of Gupta *et al.* (1999) and Parsad *et al.* (2009). Out of 15 distinct weighted A-optimal BTIB design given by Gupta *et al.* (1999), 7 fall in the parametric range $\mathfrak{P}$. Out of these 7 designs, we obtained six of them and are shown in Table 2. Out of the 43 designs reported by Parsad *et al.* (2009), only 14 designs fall in the parametric range $\mathfrak{P}$. We have obtained all these 14 designs and are given in Table 3.

Table 2: Weighted A-optimal BTIB designs in $\mathfrak{P}$ from Gupta *et al.* (1999)

v	b	k	t	s	α	Type
6	15	5	0	15	0.2	S
6	18	3	0	12	0.2	S
4	12	4	0	8	0.6	S
4	18	4	0	16	0.4	S
7	7	7	0	7	0.4	S
4	24	4	0	12	0.8	S
4	36	4	0	32	0.4	S

Table 3: Weighted A-optimal BTIB designs in $\mathfrak{P}$ from Parsad *et al.* (2009)

v	b	k	t	s	α	Type
3	3	3	0	3	0.2	S
3	4	3	0	3	0.4	S
6	7	3	0	3	0.4	S
9	18	3	0	9	0.2	S
4	4	4	0	4	0.2	S
4	5	4	0	4	0.4	S
5	5	5	0	5	0.2	S
5	5	5	0	5	0.4	S
7	7	5	0	7	0.2	S
7	7	5	0	7	0.2	S
9	12	7	0	12	0.2	S
8	8	8	0	8	0.4	S
9	9	9	0	9	0.4	S
10	10	10	0	10	0.4	S

An interesting observation is that among the 369 designs in the parametric range $\mathfrak{P}$, we found certain designs with same parametric combinations which are weighted A-optimal for more than one value of α. The list of those designs are depicted in Table 4.

Table 4: Weighted A-optimal designs for multiple values of α

Sr No.	v	b	k	t	s	α	Type
1	3	4	3	0	3	0.4, 0.6	S
2	4	4	4	0	4	0.2, 0.4	S
3	4	4	4	1	0	0.2, 0.4	R
4	4	5	4	0	4	0.4, 0.6	S
5	5	5	5	0	5	0.2, 0.4	S
6	5	5	5	1	0	0.2, 0.4	R
7	6	7	3	0	3	0.4, 0.6	S

6. Concluding Remarks

We have presented an algorithm to construct weighted A-optimal BTIB designs and also listed 369 weighted A-optimal designs. We believe most of the designs, particularly those with $\alpha > 0$ are new and has not been reported elsewhere. The proposed algorithm will be useful for experimenters and statisticians to obtain weighted A-optimal BTIB designs for various values of parameters including other values of weights given to the contrasts. Further efforts are required to devise algorithms which are able to construct weighted A-optimal BTIB designs for larger number of treatments. The proposed algorithm in this article has been restricted to construct weighted A-optimal BTIB designs where only one control is considered. The algorithm may be extended for weighted A-optimal block designs for more than one control treatment. Effort may also be made to obtain weighted A-optimal block designs beyond the class of BTIB designs.

Acknowledgements

Authors are thankful to the reviewer for careful pointing out of a mistake in an important expression in an earlier version of the manuscript. Authors duly acknowledge the support and guidance by the Chair Editor.

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