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SOME OBSERVATIONS ON THE CONSTRUCTIONS OF CHEMICAL BALANCE WEIGHING DESIGNS

Ratnakaram Nava Mohan,

D. A. R. Department of Mathematics, College, Nuzvid-521201, A.P., India
e-mail: rnmohan@hotmail.com

Bronisaw Ceranka

Department of Mathematical and Statistical Methods
Agricultural University of Poznań
Wojska Polskiego 28, 60–637 Poznań, Poland
e-mail: bronicer@au.poznan.pl

and

Sanpei Kageyama

Department of Mathematics, Graduate School of Education
Hiroshima University, Higashi-Hiroshima 739–8524, Japan
e-mail: ksanpei@hiroshima-u.ac.jp

Abstract

The construction of some optimum chemical balance weighing designs from affine μ-resolvable balanced incomplete block (BIB) designs are discussed in the light of a characterization theorem on the parameters of affine μ-resolvable BIB designs as given by Mohan and Kageyama (1982), for the sake of practical use of researchers who need some selective designs for the construction of chemical balance weighing designs.

Keywords: optimum chemical balance weighing design; BIB design; ARBIB design; μ-ARBIB design.

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1. Introduction

A balanced incomplete block (BIB) design with parameters v, b, r, k, λ is a block design with v treatments and b blocks of size k each such that every treatment occurs in exactly r blocks and that any two distinct treatments occur together in exactly λ blocks. In the BIB design, if the b blocks are partitioned into t sets of m blocks each such that in each of the sets every treatment occurs exactly μ times, then the design is said to be μ-resolvable. Moreover, when any two blocks belonging to the same set (different sets) contain q_1 (q_2, respectively) treatments in common, the μ-resolvable BIB design is called affine μ-resolvable (denoted by μ-ARBIB design). When $\mu = 1$, an (affine) 1-resolvable design is simply called an (affine) resolvable design (see Bose, 1942; Raghavarao, 1988; Kageyama and Mohan, 1983).

In a μ-ARBIB design, it is known that $b = mt, r = \mu t, b\mu = mk, b = v + t - 1$, $q_1 = (\mu - 1)k/(m-1) = k + \lambda - r$, $q_2 = k^2/v$.

Some optimum chemical balance weighing designs were constructed by establishing certain relations between BIB designs and these weighing designs by many authors, for example, see Nigam (1974), Dey (1979), Kageyama and Saha (1983), and Ceranka and Katulska (1987). In this context, Saha (1975) has proved the following two theorems.

Theorem 1.1. *The existence of a* BIB *design with parameters* v, b, r, k, λ *satisfying* $b \leq 4(r - \lambda)$ *implies the existence of an optimum chemical balance weighing design for* v *objects and in* $4(r - \lambda)$ *weighings.*

Theorem 1.2. *The existence of an affine resolvable* BIB (ARBIB) *design with parameters* $v = 2k, b = 2r, r = v - 1,\ k, \lambda$ *implies the existence of an optimum chemical balance weighing design for* r *objects and in* v *weighings.*

Furthermore, Kageyama and Saha (1983), while investigating BIB designs that satisfy $b \leq 4(r - \lambda)$, established the following two propositions using Theorems 1.1 and 1.2.

Proposition 1.1. *An* ARBIB *design with parameters* v, b, r, k, λ *satisfying* $b \leq 4(r - \lambda)$ *has one of the following parameters*

(i) $v = 9, b = 12, r = 4, k = 3, \lambda = 1$;

(ii) $v = 4(t+1), b = 2(4t+3), r = 4t+3, k = 2(t+1), \lambda = 2t+1$

for a non-negative integer t.

Then, by Theorems 1.1 and 1.2, the existence of the BIB designs given in Proposition 1.1 shows the existence of optimum chemical balance weighing designs for $9, 4t+3, 4(t+1)$ objects and in $12, 4(t+1), 8(t+1)$ weighings, respectively.

Note that in Proposition 1.1 the series (ii) is self-complementary. It is obvious that any BIB design with parameters v, b, r, k, λ and its complementary BIB design with parameters $v^* = v$, $b^* = b, r^* = b - r$, $k^* = v - k$, $\lambda^* = b - 2r + \lambda$ simultaneously either satisfy or do not satisfy $b \leq 4(r - \lambda)$, because, in case of the complementary design, $b^* = b$ and $r^* - \lambda^* = r - \lambda$. The last observation is helpful for our further characterization in the next section.

Proposition 1.2. *The existence of an affine resolvable s-associate partially balanced incomplete block* (PBIB) *design with parameters v, b, r, k, λ_i, $n_i, p^i_{j\ell}$ $(i, j, \ell = 1, 2, ..., s)$ satisfying $\sum_{\lambda_i>0} n_i \leq 4k(v-k)/v$ implies the existence of an optimum chemical balance weighing design for r objects in $4k(v-k)/v$ weighings, where the summation extends over $i (i = 1, 2, ..., s)$ such that $\lambda_i > 0$.*

Kageyama and Saha (1983, p. 450, lines 34–36) pointed out that the generalization of Propositions 1.1 and 1.2 to the affine μ-resolvability is immediate, for the reason that the complement of an ARBIB design is in general a μ-ARBIB design for some μ. This remark is the starting point for the present discussions.

2. Discussions

Now, regarding the existence of optimum chemical balance weighing designs, we will have a rigorous investigation on all μ-ARBIB designs, in the light of a characterization theorem on the parameters of μ-ARBIB designs as given by Mohan and Kageyama (1982). In fact, there are six series of μ-ARBIB designs, which have to be considered now, for the practical purposes of the researchers to choose the design as per one's need.

In Kageyama and Saha (1983), some of the μ-ARBIB designs are taken as complements of ARBIB designs, as it is a method of construction of those designs. In fact, they have considered these μ-ARBIB designs for some μ, i.e., as in the case (ii) of Theorem 2.1 given by Mohan and Kageyama (1982), $m = \mu + 1$. When an ARBIB design satisfies the condition $b \leq 4(r - \lambda)$, then its complement which is a μ-ARBIB design also satisfies this condition, and hence it needs no further study. For an ARBIB design that is self-complementary, its complement is again an ARBIB design.

But there are some designs which do not satisfy $b = 2r$ and also are μ-ARBIB designs. In the ARBIB designs, i.e., $\mu = 1$, and this is just the first case of the characterization theorem in Mohan and Kageyama (1982). In the other cases depending on the satisfaction of the condition $b \leq 4(r - \lambda)$, we can speak of the existence of the optimum chemical balance weighing designs. But, when we consider μ-ARBIB designs, it is puzzling for the practical researcher for which a μ-ARBIB design is to be selected, for the construction of optimum chemical balance weighing designs. We will aim at bridging this gulf.

The chacterization theorem by Mohan and Kageyama (1982) is stated as follows.

Theorem 2.1. *Let $\mathcal{D}$ be a μ-*ARBIB *design with parameters $v, b = mt, r = \mu t, k, \lambda$, then exactly one of the following is true.*

(1) $\mu = 1$, *i.e., $\mathcal{D}$ is an* ARBIB *design;*

(2) $m = \mu + 1$ *and $\mathcal{D}$ is the complement of an* ARBIB *design;*

(3) $m = 2\mu + 1$ *or* $2\mu - 1$*;*

(4) $m = 2\mu + a_1$ *or* $2\mu - a_1$ *with* $a_1 = m^{1/2}$ *an integer;*

(5) $m = 2\mu + a_2$ *or* $2\mu - a_2$ *with* $a_2 = (2m - 1)^{1/2}$ *an integer;*

(6) $m = 2\mu + a_3$ *or* $2\mu - a_3$ *with* $a_3 = [\ell(m - 1) + m]^{1/2}$ *an integer and* $\ell \geq 2$.

Here, Remark 2.2 in Mohan and Kageyama (1982) states that the designs with $m = 2\mu - 1, 2\mu - a_1, 2\mu - a_2$ and $2\mu - a_3$ are the complements of the designs with $m = 2\mu + 1, 2\mu + a_1, 2\mu + a_2$ and $2\mu + a_3$, respectively. Besides $\mu = 1$ and $m = \mu + 1$ are also complements to each other. Thus Proposition 1.1 and the remark of Kageyama and Saha (1983) deal with the cases of (1) and (2) of the above Theorem 2.1, i.e., when $\mu = 1$ the designs are ARBIB designs and when $m = \mu + 1$ these are complements the case (1), i.e., $\mu = 1$. The μ-ARBIB design with parameters $v = 9, b = 12, r = 8, k = 6, \lambda = 5$, where $m = 3$ and $\mu = 2$, are considered there. Now, the remaining cases (3), (4), (5) and (6) are yet to be discussed.

As said earlier, the characterization theorem leads to six series of μ-ARBIB designs for $\mu \geq 1$. We deal with all of them now for the sake of completeness.

Theorem 2.1 Case (1). When $\mu = 1$, the design is an ARBIB design whose parameters are expressed by

$$v = m^2[z(m-1)+1],\ b = m(zm^2+m+1),\ r = zm^2+m+1,$$

$$k = m[z(m-1)+1],\ \lambda = zm+1 \tag{2.1}$$

where z is a non-negative integer (see also Bose, 1942).

Now, it follows that $b \leq 4(r-\lambda)$ iff $z(m-2)^2+m-3 \leq 0$. Hence the solutions are given by (i) $m = 2$ and any z, and (ii) $m = 3$ and $z = 0$. Kageyama and Saha (1983) have already dealt with Case (1), and obtained a subseries out of this series for this purpose in the above two cases.

In the case (i) the ARBIB design we get has the parameters $v = 9, b = 12, r = 4, k = 3, \lambda = 1$, which does not satisfy $b = 2r$, and its complement has $v = 9, b = 12, r = 8, k = 6, \lambda = 5$, which are the parameters of a μ-ARBIB design for $m = 3$ and $\mu = 2$. Again both of these designs satisfy $b \leq 4(r-\lambda)$, and their existence implies the existence of optimum chemical balance weighing designs by Theorem 1.1.

And the case (i), i.e., when $m = 2$, yields the parameters

$$v = 4(z+1),\ b = 2(4z+3),\ r = 4z+3, k = 2(z+1),\ \lambda = 2z+1. \tag{2.2}$$

In fact, the design with parameters (2.2) is of the form $2k, 2r, r, k, \lambda$, and also satisfies the condition $b \leq 4(r-\lambda)$. Hence it follows from Theorems 1.1 and 1.2 that "*the existence of the design with parameters* (2.2) *implies the existence of optimum chemical balance weighing designs for* (a) $4(z+1)$ *objects and in* $8(z+1)$ *weighings, and for* (b) $4z+3$ *objects and in* $4(z+1)$ *weighings.*"

Theorem 2.1 Case (2). When $m = \mu + 1$, the series are expressed by

$$v = m^2(y\mu+1),\ b = m[m^2(y\mu+1)-1]/\mu,\ r = m^2(y\mu+1)-1,$$

$$k = m\mu(y\mu+1),\ \lambda = m\mu(y\mu+1)-1 \tag{2.3}$$

for a non-negative integer y. Then the required condition can be obtained from $b \leq 4(r-\lambda)$ as

$$(\mu-1)^2(y\mu+1) \leq 1 \tag{2.4}$$

which holds only when (i) $y = 0$ and $\mu = 2$, and (ii) $y \geq 1$ and $\mu = 1$.

For the case (i), the corresponding design, when $\mu = 1$, i.e., $m = 2$, has $v = 4, b = 6, r = 3, k = 2, \lambda = 1$, which provides an ARBIB design with $b = 2r$. When $\mu = 2$, i.e., $m = 3$, the corresponding design has $v = 9, b = 12, r = 8, k = 6, \lambda = 5$, which is a μ-ARBIB design with $\mu = 2$. Both of these designs satisfy the required condition $b \leq 4(r - \lambda)$, and hence we have that "*the existence of the design with parameters* (2.3) *for* $y = 0$ *and* $\mu = 2$ *implies the existence of three optimum chemical balance weighing designs for* 3 *objects and in* 4 *weighings*, *for* 4 *objects and in* 8 *weighings*, *and for* 9 *objects and in* 12 *weighings*."

In the case (ii), i.e., $\mu = 1$, also the parametric relations are the same as in Case 1. So as $m = 2$, we have

$$v = 4(y + 1),\ b = 2(4y + 3),\ r = 4y + 3, k = 2(y + 1),\ \lambda = 2y + 1. \tag{2.5}$$

As the parametric relations of (2.2) and (2.5) are the same when $m = 2$, no further treatment is required. But when $m \geq 3$, as the condition (2.4), i.e., $(\mu - 1)^2(y\mu + 1) \leq 1$ fails, we can infer that "*the existence of the* μ-ARBIB *design of series* (2.3) (*when* $m \geq 3, y \geq 1$) *does not imply the existence of an optimum chemical balance weighing design*" is dependent on the fulfilment of the codition $b \leq 4(r - \lambda)$. But we consider μ-ARBIB designs in the light of the characterization theorem given by Mohan and Kageyama (1982) for all the cases.

Thus, it is more interesting to investigate further whether there is any design or series which is affine μ-resolvable, and possibly its existence implies the existence of optimum chemical balance weighing designs. So we consider the other cases of Characterization Theorem 2.1.

Theorem 2.1 Case (3). When $m = 2\mu + 1$, the series are expressed by

$$v = m^2(2d\mu + 1),\ b = m[m^2(2d\mu + 1) - 1]/(2\mu),\ r = [m^2(2d\mu + 1) - 1]/2,$$

$$k = m\mu(2d\mu + 1),\ \lambda = [m\mu(2d\mu + 1) - 1]/2 \tag{2.6}$$

for a non-negative integer d. Then the required condition can be obtained from $b \leq 4(r - \lambda)$ as

$$2d\mu + 1 \leq 1.$$

This is valid only when (i) $d = 0$ and any $m \geq 3$. Then the series becomes

$$v = m^2,\ b = m(m+1),\ r = (m^2-1)/2,\ k = m(m-1)/2, \lambda = (m^2-m-2)/4.$$

Since λ is an integer, μ should be an odd integer. When $\mu = 1$ (i.e., $m = 3$) in this series, we get an ARBIB design with parameters

$$\text{(i)} \qquad v = 9,\ b = 12, r = 4,\ k = 3, \lambda = 1$$

which has already been dealt with.

When $\mu = 3$ (i.e., $m = 7$), we get a μ-ARBIB design with parameters

$$\text{(ii)} \qquad v = 49,\ b = 56,\ r = 24,\ k = 21,\ \lambda = 10.$$

For the construction of this design refer to Kageyama and Mohan (1983, p. 119, design no. 184). The existence of this design implies the existence of an optimum chemical balance weighing design for 49 objects and in 56 weighings.

When $\mu = 5$ (i.e., $m = 11$), we get a μ-ARBIB design with parameters

$$\text{(iii)} \qquad v = 121, b = 132, r = 60, k = 55, \lambda = 27.$$

For the construction of this design refer to Kageyama and Mohan (1983, p. 120, design no. 229). The existence of this design implies the existence of an optimum chemical balance weighing design for 121 objects and in 132 weighings.

Thus in this series, "*the existence of the designs with the parameters as mentioned in* (i), (ii), (iii) *above implies the existence of optimum chemical balance weighing designs.*" For odd $\mu \geq 7$, we have big designs and hence they are omitted here. These are not with $b = 2r$ as mentioned earlier in Kageyama and Saha (1983).

Theorem 2.1 Case (4). When $\mu = (m + m^{1/2})/2$, i.e., $2\mu = m + m^{1/2}$, the series are expressed by

$$v = m^2[\alpha(m-1)+1],\ b = m(\alpha m^2 + m + 1),\ r = \mu(\alpha m^2 + m + 1),$$

$$(2.7) \qquad k = m\mu[\alpha(m-1)+1],\ \lambda = \mu\{[\alpha(m-1)+1]m\mu - 1\}/(m-1)$$

for a non-negative integer α. Then the required condition in this case can also be obtained from $b \leq 4(r - \lambda)$ as $m(m-1)(\alpha+1) \leq 0$, which is impossible. Hence we have the following observation that "*the existence of* *the* μ-ARBIB *design of this series* (2.7) *does not imply the existence of an optimum chemical balance weighing design.*"

Theorem 2.1 Case (5). When $\mu = [m + (2m-1)^{1/2}]/2$, the series are expressed by

$$v = m^2[\beta(m-1)+1],\ b = m(\beta m^2 + m + 1),\ r = \mu(\beta m^2 + m + 1),$$

$$k = m\mu[\beta(m-1)+1],\ \lambda = \mu\{[\beta(m-1)+1]m\mu - 1\}/(m-1) \tag{2.8}$$

for a non-negative integer β. Then the required condition can also be obtained from $b \leq 4(r-\lambda)$ as $m(m-1)[\beta(2m-1)+2] \leq 0$, which is impossible. Hence this leads to a statement "*the existence of the* μ-ARBIB *design of this series* (2.8) *does not imply the existence of an optimum chemical balance weighing design.*"

Theorem 2.1 Case (6). When $\mu = \{m + [\ell(m-1)+m]^{1/2}\}/2$, the series are expressed by

$$v = m^2[\varepsilon(m-1)+1],\ b = m(\varepsilon m^2 + m + 1),\ r = \mu(\varepsilon m^2 + m + 1),$$

$$k = m\mu[\varepsilon(m-1)+1],\ \lambda = \mu\{[\varepsilon(m-1)+1]m\mu - 1\}/(m-1) \tag{2.9}$$

for non-negative integers ε and $\ell(\geq 2)$. It follows that $b \leq 4(r-\lambda)$ iff $m\{[\varepsilon(m-1)+1][\ell(m-1)+m]-1\} \leq 0$, which is impossible. This fact leads to the statement that "*the existence of the* μ-ARBIB *design of this series* (2.9) *does not imply the existence of an optimum chemical balance weighing design.*"

Thus, for all μ-ARBIB designs we can speak of the existence or non-existence of optimum chemical balance weighing designs by considering all the cases of Characterization Theorem 2.1 for the sake of practical purposes.

Note 2.1. In the case of PBIB designs, unlike the case of μ-ARBIB designs, it may be difficult to assess the possibilities of existence or non- existence of optimum chemical balance weighing designs in terms of PBIB designs. But, as an example, if we take the series from the following, which was given in Kageyama and Mohan (1980, Theorem 2.2), then the existence of a symmetrical BIB design with parameters $v = b$ (being a prime), $r = k, \lambda$ implies the existence of an affine r-resolvable semi-regular group divisible design with parameters $v' = b' = v^2$, $r' = k' = vk$, $\lambda_1 = v\lambda, \lambda_2 = k^2$,

$q_1 = \lambda v (= \lambda_1)$, $q_2 = k^2 (= \lambda_2)$. This resulting design is a symmetrical PBIB design and its existence implies the existence of an optimum chemical balance weighing design for v^2 objects and in $4k(v-k)$ weighings, as we require only linked block type for our purposes (see Kageyama and Saha, 1983, Proposition 4).

Thus the present discussions revealed the existence or non-existence of optimum chemical balance weighing designs, depending on the existence or non-existence of μ-ARBIB designs.

Also it needs further study regarding whether the existence of those μ-ARBIB designs implies the existence of at least best weighing designs as given in Raghavarao (1959, 1960) also the second best weighing designs as given in Bhaskararao (1966). However, in the case of μ-ARPBIB designs a further investigation is still needed.

3. A construction of certain chemical balance weighing designs

We can first make use of the method of constructions as given in Kageyama and Mohan (1983) for μ-ARBIB designs and the corresponding optimum chemical balance weighing designs. Secondly, consider either the complete or a part of the array as in Kageyama and Mohan (1983, p. 114) . When the full array is considered, the optimum chemical balance weighing designs that can be obtained have already been discussed here.

When a part of that array has been considered, the designs that can be obtained may not be affine μ-resolvable BIB designs but may be PBIB designs. If such a partial array has been considered, by deleting the first column or by deleting the first row and the first two columns, we can construct certain chemical balance weighing designs. For example, we consider the second row of the array and by deleting the first element alone, we will get an optimum chemical balance weighing design.

Let $\boldsymbol{N}$ be the $v \times b$ incidence matrix of a BIB design with parameters v, b, r, k, λ satisfying $b \leq 4(r-\lambda)$. Further let π be the permutation of the rows $R_1, R_2, ..., R_v$ of $\boldsymbol{N}$ defined by $\pi R_i \equiv R_{i+1} \pmod{v}$. Also let $\boldsymbol{N}_i = \pi^{i-1}\boldsymbol{N}$ for $i = 1, 2, ..., v$, and in each of these matrices $\boldsymbol{N}_i$ replace 0 by -1 and from the following juxtaposition matrix $\boldsymbol{X} = [\boldsymbol{N}_1 : \boldsymbol{N}_2 : \cdots : \boldsymbol{N}_v]$, we can have $\boldsymbol{X}\boldsymbol{X}' = (b-c)\boldsymbol{I}_v + c\boldsymbol{J}_v$, where $c = b - 4(r-\lambda)$, $\boldsymbol{I}_v$ denotes the identity matrix of order v and $\boldsymbol{J}_v$ denotes the $v \times v$ matrix all of whose elements are unity. This gives an optimum chemical balance weighing design by considering the condition $b \leq 4(r-\lambda)$. When $c = 0$, it is trivial. The other cases can be evaluated if the design is known.

The scientists in the field of Nuclear Chemistry require such designs where minute quantities of a very few number of objects are given. Then to avoid hazardous situations and high risk factors in the cases of perilous explosives and super radioactive elements and to achieve accuracy near to perfection and to reduce standard error of estimate they go for more and more weighings.

Example 3.1. Take a BIB design with parameters $v' = b' = 7, r' = k' = 3$, $\lambda' = 1$ with its incidence matrix $\boldsymbol{N}$. Then we can obtain by Theorem 1.1 an optimum chemical balance weighing design for 7 objects and in 8 weighings. If we use the above method, we have $\boldsymbol{X} = [\boldsymbol{N}_1 : \boldsymbol{N}_2 : \cdots : \boldsymbol{N}_7]$ which gives a BIB design with parameters $v = 7, b = 49, r = 21, k = 3$, $\lambda = 7$. This produces an optimum chemical balance weighing design for 7 objects and in 56 weighings, which may be of our need and choice with the help of Characterization Theorem 2.1 and from the methods of construction of Kageyama and Mohan (1983).

We attain greater efficiency in estimating the weights by weighing the objects in sets rather than by weighing them just separately. Hence there will be more weighings. Even though the number of weighings is greater we can build up the plan of weighings. Consequently we can obtain bounds for the variance of thus estimated weights.

Note 3.1. In the Remark of Dey (1970), it was stated that as repeated designs take one or more repetitions it will overcome the drawback for the estimation of error variance. And then these designs are of much use in the direction of the optimum chemical balance weighing designs. Furthermore, in Ceranka and Katulska (1987), they have given a construction of optimum chemical balance weighing designs, taking various BIB designs with the same number of treatments. In this the number of copies is fixed as v only.

The discussions regarding the existence or non-existence of optimum chemical balance weighing designs for other combinatorial configuration are still open.

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