CHARACTERIZATION OF BIB DESIGNS FOR CONSTRUCTING MINIMAL FRACTIONAL COMBINATORIAL TREATMENT DESIGNS

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Damaraju Raghavarao
Temple University
New York, NY

and

Walter T. Federer
Dept. of Biometrics
Cornell University
Ithaca, NY 14853

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Abstract

A characterization of balanced incomplete block (BIB) designs of block sizes three and four for obtaining saturated minimal fractions of m items taken n at a time for estimating the contrasts of item means and two-item, BSMA, and three item, TSMA, specific mixing effects. Such fractions are useful for investigations involving mixtures of crops, drugs, marketing practives, and other systems utilizing mixtures of items. This is a continuation of the work of Federer and Raghavarao (1987) and Federer (2000).

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by

DAMARAJU RAGHAVARAO and WALTER T. FEDERER
Temple University and Cornell University

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1. Introduction

In agricultural, medical, and marketing investigations, often m items will be tested in groups or mixtures of size n items, $2 \leq n \leq m$. In the agricultural context of cropping systems, these are known as intercropping experiments (cf. Federer, 1993, 1999). In a marketing context, these are known as availability designs (cf. Wiley, 2000). In medical experiments, mixtures of drugs have been denoted as "drug cocktails" in some instances. This type of mixture is different from the ones discussed by Cornell (1981), e.g. Different types of statistical design, goals, and analyses are involved for the mixture type discussed herein than for those discussed by Cornell (1981).

As a mode for presentation, we use the terminology of agricultural experiments in this paper. In the agricultural context, it is often possible to obtain a response for each item (cultivar) in the mixture (blend) of n cultivars. For this case, we designate a cultivar mixture as $S_\alpha = \{i_1, i_2, ..., i_n\}$. A response for item i_j in the presence of the other n - 1 items in the mixture is available. That response is composed of the effect of the item when grown alone, the general mixing effect, GMA, a bi-specific mixing ability effect, BSMA, a tri-specific mixing ability effect, TSMA, etc. up to a $(n - 1)^{st}$ order or n-cultivar specific mixing effect. A GMA is a general effect of a cultivar when grown in a mixture. A BSMA effect is a two-cultivar or first order interaction effect of one cultivar in the presence of another cultivar where the interaction effect of each member of a pair is obtainable. This is not the case for two-factor interactions from a factorial experiment where the contribution of each member of a pair to the interaction cannot be determined. A TSMA effect is a three-cultivar or second order interaction effect for one cultivar in the presence of two other cultivars or items; the contribution of each member of the triplet to the interaction is obtainable. Higher factor mixing ability effects are defined in a similar manner (cf. Federer and Raghavarao, 1987; Federer, 1999).

The set of m items taken n at a time is denoted as a *combinatorial* (cf. Federer, 2000) and a subset of a combinatorial is denoted as a *fractional combinatorial* following the convention for fractional factorial treatment designs. Since m may be large, the mixture size n variable, and the experimenter may be willing to assume that certian higher order specific mixing ability effects are not important, a fraction of the combinatorial is desired. Since fractional factorial theory is not usable here, the problem is to construct a fractional combinatorial for estimating item or cultivar effects and BSMA effects, item effects, BSMA effects, and TSMA effects, etc. Often n = 3, n = 4, or more cultivars are grown together in a blend or mixture. In this paper, we characterize classes of BIB designs for constructing minimal treament designs, MTDs, for estimating

item effects and BSMA effects for n = 3 and n = 4

and

item effects, BSMA effects, and TSMA effects for n = 4.

This work opens up many avenues for research in combinatorics to extend our results and to construct saturated or nearly saturated fractional combinatorials for specific objectives for all values of m and n. Some of these topics are discussed in the last section of the paper.

2. **The model and saturated MTD**

Let $S_\alpha = \{i_1, i_2, ..., i_n\}$be a blend of n cultivars $i_1, i_2, ..., i_n$ from m cultivars 0, 1, 2, ..., m - 1. Let $Y_{i_j(S_\alpha)}$ be the response of the i_j cultivar in the blend S_α. We take a BSMA effect model to be:

$$E[Y_{i_j(S_\alpha)}] = \mu + \tau_{i_j} + \sum_{j'=1, j'\neq j}^{n} \gamma_{i_j(i_{j'})},$$

where E[.] is the expected value of the random variable in the brackets, μ is a general mean effect, τ_{i_j} is the item effect which is the sum of the effect in monoculture (grown alone) and the GMA effect, and $\gamma_{i_j(i_{j'})}$ is the BSMA effect of cultivar i_j in the presence of cultivar $i_{j'}$. Without loss of generality for the over-parameterized model on the right, set the restrictions

$$\sum_{i=1}^{m} \tau_{i_j} = 0 \text{ and } \sum_{j'=1, j'\neq j}^{n} \gamma_{i_j(i_{j'})} = 0.$$

The number of parameters to be estimated with the above restrictions is

$$1 + (m - 1) + m(m - 2) = m(m - 1).$$

Thus, a saturated minimal treatment design, MTD, in blends of size n, needs to be m(m - 1)/n blends where m(m - 1)/n is an integer.

If TSMA effects are also present, our model becomes:

$$E[Y_{i_j(S_\alpha)}] = \mu + \tau_{i_j} + \sum_{j'=1, j'\neq j}^{n} \gamma_{i_j(i_{j'})} + \sum_{j'j''=1, j\neq j'\neq j''}^{n} \delta_{i_j(i_{j'}, i_{j''})},$$

where $\delta_{i_j(i_{j'},i_{j''})}$ is the tri-specific mixing ability, TSMA, effect of i_j in the presence of both $i_{j'}$ and $i_{j''}$ items or cultivars and the other parameters are described above. Without loss of generality, set

$$\sum_{j'=1, j' \neq j, i}^{m} \delta_{i(j,j')} = 0 \quad \text{and} \quad \sum_{j=1,\, j \neq j', i}^{m} \delta_{i(j,j')} = 0$$

The number of parameters to be estimated is

$$1 + (m - 1) + m(m - 2) + m(m - 1)(m - 4)/2 = m(m - 1)(m - 2)/2.$$

Thus, a saturated minimal treatment design in blends of size n for estimating item means, BSMA effects, and TSMA effects must have m(m - 1)(m - 2)/2n blends, where this number is an integer.

3. MTDs for item effects and BSMA effects, n = 3

Let $T_1, T_2, ..., T_{m-1}$ be pairs of symbols from a set {0, 1, 2, ..., m-2}, where every symbol occurs exactly two times. A chain, C, constructed from the set is $\theta_0, \theta_1, \theta_2, ..., \theta_l$, θ_0, where consecutive symbols in the chain occur together in one of the pairs T_i, i = 1, 2, ..., m-1. The chain is said to be complete if $\{\theta_0, \theta_1, \theta_2, ..., \theta_l\} = \{0, 1, 2, ..., m-2\}$. We now have:

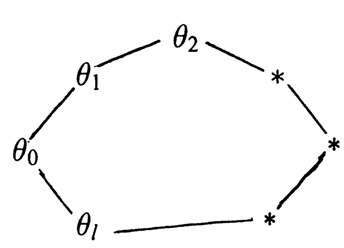
Theorem 1: *If there exists a BIB design with parameters $v = m$, $b = m(m - 1)/3$, $r = m - 1$, $k = 3$, $\lambda = 2$ for m even such that for every symbol θ of the BIB design, the chain is based on the other pair of symbols occurring in the sets of the design is complete; then the sets of the design form a MTD for m items in mixtures of size three that are capable of estimating the contrasts of item effects and BSMA, bi-specific mixing ability, effects.*

Proof: We note that if a BIB design has two sets

$$\{\theta, \phi, \psi_1\} \text{ and } \{\theta, \phi, \psi_2\}$$

where $\psi_1 \neq \psi_2$, the difference of the responses on the item θ estimates the bi-specific mixing ability contrast $\gamma_{\theta(\psi_1)} - \gamma_{\theta(\psi_2)}$.

Let the m - 1 sets of the BIB design containing a given symbol θ be $(\theta, \phi_{i1}, \phi_{i2})$ for i = 1, 2, ..., m - 1 and consider the m - 1 pairs $T_i = (\phi_{i1}, \phi_{i2})$ for i = 1, 2, ..., m - 1. Let C be the chain based on T_i and let C be complete. Assume that $C = \theta_0, \theta_1, ..., \theta_l, \theta_0$. If we consider the chain as circular, i.e.,



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and form another chain starting with θ_0 and picking symbols skipping one step, we again get a complete chain if m - 1 is odd. This new chain will have the property that if ϕ_i, ϕ_{i+1} are consecutive pairs of symbols in the chain, then $\gamma_{\theta(\phi_i)} - \gamma_{\theta(\phi_{i+1})}$ is estimable. This in turn implies that BSMA effect contrasts are estimable. Clearly the contrast of item effects is estimable. The theorem is thus proved. It is easy to note that the above theorem does not hold for m odd because the second chain indicated in the proof is not complete for m - 1 even.

Example 1.1: Consider the following BIB design with parameters v = 6, b = 10, k = 3, r = 5 and $\lambda = 2$:

(5, 0, 1)	(5, 1, 2)	(5, 2, 3)	(5, 3, 4)	(5, 4, 0)
(0, 1, 3)	(1, 2, 4)	(2, 3, 0)	(3, 4, 1)	(4, 0, 2)

Consider the pair of symbols occurring with the symbol θ (= 1, say) in the sets of the above BIB design given by

$T_1 = (0, 5)$, $T_2 = (2, 5)$, $T_3 = (0, 3)$, $T_4 = (2, 4)$, and $T_5 = (3, 4)$

The chain based on these five pairs is

$$C = 0, 5, 2, 4, 3, 0$$

and is complete in 0, 2, 3, 4, and 5. We can check that the chain based on pairs for every symbol $\theta = 0, 1, 2, 3, 4, 5$ is complete. Hence the sets form a MTD for m = 6 and n = 3.

The series of BIB designs that are candidates for MTDs with n = 3 are:

$$v = 6t,\ b = 2t(6t - 1),\ r = 6t - 1,\ k = 3,\ \lambda = 2$$

and

$$v = 6t + 4,\ b = (2t + 1)(6t + 4),\ r = 6t + 3,\ k = 3,\ \lambda = 2.$$

4. MTDs for item effects and BSMA effects, n = 4

Consider the BIB design with parameters v = m, b = m(m - 1)/4, r = m - 1, k = 4, and $\lambda = 3$. For every symbol θ, take the m - 1 sets T_1', T_2', T_3', ..., $T_{m-1}'$of three symbols which occur together with θ in the m - 1 sets of the BIB design. In the sets T_i, each of the the m - 1 symbols other than θ occurs in three sets. For every θ_i ($\neq \theta$) form a set $T_i^* = \{\phi_{i1}\psi_{i1}, \phi_{i2}\psi_{i2}, \phi_{i3}\psi_{i3}\}$, where $(\theta_i, \phi_{i1}, \psi_{i1})$, $(\theta_i, \phi_{i2}, \psi_{i3})$, and $(\theta_i, \phi_{i3}, \psi_{i3})$ are three of the $T_{i'}$ sets. If $\phi_{i1}\psi_{i1}, \phi_{i2}\psi_{i2} \in T_i^*$, the BIB design has two sets $(\theta, \theta_i, \phi_1, \psi_1)$ and $(\theta, \theta_i, \phi_2, \psi_2)$ and using the difference of the responses on the symbol θ, we can estimate

$$\gamma_{\theta(\phi_1)} + \gamma_{\theta(\psi_1)} - \gamma_{\theta(\phi_2)} - \gamma_{\theta(\psi_2)}\ .$$

The BIB design is said to have RF property if for every $\theta, \theta_1, \theta_2$ ($\theta \neq \theta_1 \neq \theta_2 \neq \theta$), we can form a chain of pairs of symbols and T* sets in any of the following ways:

$$\theta_1\phi_1 T^*_{i_1}\theta_2\phi_2,\ \theta_1\phi_2 T^*_{i_2}\theta_2\phi_1,$$

or

$$\theta_1\phi T^*_{i_1}\phi_1\phi_2 T^*_{i_2}\phi\theta_2\ ,$$

or

$$\theta_1\phi_0 T^*_{i_1}\phi_0\phi_1,\ \phi_1\phi_2 T^*_{i_2}\phi_2\phi_3, \dots, \phi_{l-1}\phi_l T^*_{i_l}\phi_l\theta_2$$

Any one of the above chains provide an estimate of $\gamma_{\theta(\theta_1)} - \gamma_{\theta(\theta_2)}$. Thus we have

Theorem 2: *A BIB design with parameters $v = m$, $b = m(m - 1)/4$, $r = m = 1$, $k = 4$, $\lambda = 3$, and with the RF property is a MTD in m items with mixtures of size four that is capable of estimating the contrasts of item effects and BSMA effects.*

<u>Example 2.1</u>: Consider the following BIB design

(0, 1, 4, 8)	(0, 1, 3, 7)
(1, 2, 5, 0)	(1, 2, 4, 8)
(2, 3, 6, 1)	(2, 3, 5, 0)
(3, 4, 7, 2)	(3, 4, 6, 1)
(4, 5, 8, 3)	(4, 5, 7, 2)
(5, 6, 0, 4)	(5, 6, 8, 3)
(6, 7, 1, 5)	(6, 7, 0, 4)
(7, 8, 2, 6)	(7, 8, 1, 5)
(8, 0, 3, 7)	(8, 0, 2, 6)

with parameters $v = 9$, $b = 18$, $r = 8$, $k = 4$, and $\lambda = 3$. The eight sets where the symbol 0 occurs in the BIB design and excluding 0 are:

$T_1' = (1, 4, 8)$, $T_2' = (1, 2, 5)$, $T_3' = (4, 5, 6)$, $T_4' = (3, 7, 8)$, $T_5' = (1, 3, 7)$,
$T_6' = (2, 3, 5)$, $T_7' = (4, 6, 7)$, and $T_8' = (2, 6, 8)$.

In the T_i' sets 1 occurs with the pair of symbols 48, 25, and 37, and we form $T_1^* = \{48, 25, 37\}$of pairs of symbols. Similarly, we form

$T_2^* = \{15, 35, 68\}$, $T_3^* = \{78, 17, 25\}$, $T_4^* = \{18, 56, 67\}$, $T_5^* = \{12, 46, 23\}$,
$T_6^* = \{45, 47, 28\}$, $T_7^* = \{38, 13, 46\}$, and $T^*_8 = \{14, 37, 26\}$.

$\gamma_{0(6)} - \gamma_{0(1)}$ is estimable as $26T_8{*}14$, $46T_5{*}12$,
$\gamma_{0(1)} - \gamma_{0(3)}$ is estimable as $17T_3{*}25T_1{*}37$,
$\gamma_{0(3)} - \gamma_{0(8)}$ is estimable as $37T_1{*}25T_3{*}78$,
$\gamma_{0(8)} - \gamma_{0(2)}$ is estimable as $38T_7{*}$ $46T_5{*}23$,
$\gamma_{0(2)} - \gamma_{0(4)}$ is estimable as $28T_6{*}45$, $25T_1{*}48$,
$\gamma_{0(4)} - \gamma_{0(7)}$ is estimable as $48T_1{*}25T_3{*}78$,
$\gamma_{0(7)} - \gamma_{0(5)}$ is estimable as $47T_6{*}45$, and
$\gamma_{0(5)} - \gamma_{0(6)}$ is estimable as $25T_1{*}37T_8{*}26$.

We have the chain 6 - 1 - 3 - 8 - 2 - 4 - 7 - 5 - 6 such that the contrast of bi-specific mixing ability effects of 0 in the presence of any two consecutive items in the above chain is estimable. Thus all contrasts of $\gamma_{0(\theta_1)} - \gamma_{0(\theta_2)}$, for $\theta_1 \neq \theta_2$ and θ_1 and $\theta_2 \neq 0$, are estimable. Since the design is constructed by the method of differences, all contrasts $\gamma_{\theta(\theta_1)} - \gamma_{\theta(\theta_2)}$ for $\theta \neq \theta_1 \neq \theta_2 \neq \theta$ are estimable and the design has the RF property. The sets of the BIB design form a MTD with $n = 4$ that is capable of estimating contrasts of both item effects (means) and bi-specific mixing ability effects.

The series of BIB designs with $k = 4$ that are candidates for the RF property are

$$v = 4t,\ b = t(4t - 1),\ r = 4t - 1,\ k = 4,\ \lambda = 3$$

and

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

5. MTDs for item means, BSMA effects, and TSMA effects, $n = 4$

Select a BIB design which is a 3-design and has parameters $v = m$, $b = m(m - 1)(m - 2)/8$, $r = (m - 1)(m - 2)/2$, $k = 4$, $\lambda_2 = 3(m - 2)/2$, and $\lambda_3 = 3$. For every pair of symbols i,j ($i \neq j$) form the set T_{ij} of pairs of symbols that go with i and j symbols in the sets of the BIB design. In this set, every symbol other than i and j occurs three times. The BIB design is said to have the RF - 1 property if for every i, j, θ_1, θ_2 ($i \neq j \neq \theta_1 \neq \theta_2 \neq i$)), there exist symbols, ϕ, with the following property

$$\{\theta_1\, \phi_1, \theta_2\, \phi\} \subset T_{ij} \text{ or } \{\theta_1\, \phi, \phi\, \phi_1\}, \{\phi_1\, \phi_2, \phi_2\, \theta_2\} \subset T_{ij}.$$

Similar to the theorems of Sections 3 and 4, we have

Theorem 3: *A BIB design which is a 3-design with parameters $v = m$, $b = m(m - 1)(m - 2)/8$, $r = (m - 1)(m - 2)/2$, $k = 4$, $\lambda_2 = 3(m - 2)/2$ and $\lambda_3 = 3$ with the RF - 1 property, is a MTD for estimating contrasts of item effects, BSMA effects, and TSMA effects.*

It is easy to verify that the irreducible BIB design with parameters $v = 6$, $b = 15$, $r = 10$, $k = 4$, $\lambda_2 = 6$, and $\lambda_3 = 3$ has the RF - 1 property and is a MTD for estimating contrasts of item effects, BSMA effects, and TSMA effects.

Candidate BIB designs for constructing these MTDs are:

$$v = 4t,\ b = t(2t - 1)(4t - 1),\ r = (4t - 1)(2t - 1),\ k = 4,\ \lambda_2 = 3(2t - 1),\ \lambda_3 = 3$$

and

$$v = 4t + 2,\ b = t(2t + 1)(4t + 1),\ r = 2t(4t + 1),\ k = 4,\ \lambda_2 = 6t,\ \lambda_3 = 3.$$

6. CONCLUSION AND SOME UNSOLVED PROBLEMS

BIB designs with block sizes three and four that are MTDs for estimating item, BSMA, and TSMA effects are characterized in this paper. Given a BIB design with block size three or four, methods are given for verifying whether or not it is a MTD for estimating the desired effects. Many unsolved problems remain. For example, it would be useful to give a method for constructing the series of BIB designs indicated in Sections 3, 4, and 5 that are MTDs. What characterizations of designs can be made for values of m not considered above? Is it possible to always obtain saturated or nearly saturated MTDs? How are these to be constructed? Since there is a similarity between fractional replicates of a combinatorial (fractional combinatorials) and fractional replication of a factorial, it would appear that this is a rich area for research in the same manner that fractional replication of factorials has been.

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