CONSTRUCTION OF MINIMAL FRACTIONAL COMBINATORIALS

Walter T. Federer
and
Damaraju Raghavarao

Abstract:
Construction algorithms for minimal fractional combinatorials are described for the following situations:

(i)   General mixing ability (GMA) effects or items means for m items.

(ii)   Item means and bi-specific mixing ability (BSMA) effects.

(iii)   Item means and mixing ability effects up to the kth specific mixing ability (KSMA).

(iv)   Item means, BSMA effects, and tri-specific mixing ability (TSMA) effects.

Numerical examples are given for three situations involving minimal fractional combinatorials for estimating item means, BSMA effects, and TSMA effects.

CONSTRUCTION OF MINIMAL FRACTIONAL COMBINATORIALS

by

Walter T. Federer, Cornell University

and

Damaraju Raghavarao, Temple University

ABSRACT

Construction algorithms for minimal fractional combinatorials are described for the following situations:

(i)   General mixing ability (GMA) effects or items means for m items.
(ii)   Item means and bi-specific mixing ability (BSMA) effects.
(iii)   Item means and mixing ability effects up to the kth specific mixing ability (KSMA).
(iv)   Item means, BSMA effects, and tri-specific mixing ability (TSMA) effects.

Numerical examples are given for three situations involving minimal fractional combinatorials for estimating item means, BSMA effects, and TSMA effects.

INTRODUCTION

The set of all possible combinations of m items taken n at a time, $m!/n!(m-n)!$, is denoted as a *combinatorial*. A subset of a combinatorial is denoted as a *fractional combinatorial*. Mixtures of n of m > n items is a common practice in such areas as intercropping, drugs, diets, education, alloys, marketing, etc. In mixture experiments, various types of effects are involved. A *general mixing ability effect*, GMA, is the effect of an item in a mixture in relation to its effect for the item alone, sole item, i.e., not in a mixture. A *bi-specific mixing ability effect*, BSMA, is an effect peculiar to a specific pair hi of items in a mixture. A *tri-specific mixing ability effect* is an effect pertaining to a triplet hij of items in a mixture. A *KSMA effect* is an effect peculiar to a set of k items in the same mixture. When responses for *each* item in a mixture are obtainable, the KSMA effect for *each* item in the mixture of k items is estimable. It is to be noted that all GMA effects could be positive or negative, i. e., they are not constrained to add to zero. The BSMA, TSMA, etc. effects are constrained to add to zero.

As pointed out in the references cited at the end of this article, the problem of constructing fractional combinatorials for estimating various mixing effects for mixtures of size n is an unresolved problem for general n. We present what has been done on this problem to date as well as three new construction methods for estimating item means, BSMA effects, and TSMA effects for the case when a response is available for each item in a mixture. A characterization of balanced incomplete block designs useful for constructing minimal fractional combinatorials has been presented by Raghavarao and Federer (2000).

ALGORITHMS FOR CONSTRUCTING MIMIMAL FRACTIONAL COMBINATORIALS

Algorithms I, II, and III describe the construction of fractional combinatorials described in the literature to date. Algorithms IV and V are two new procedures for constructing minimal fractional combinatorials for estimating item means, BSMA effects, and TSMA effects. Algorithm VI is used to obtain fractional combinatorials which are not minimal but leave m(m - 1) degrees of freedom for lack of fit or for an error term..

Algorithm I: A minimal fractional combinatorial for estimating item means is one mixture of all m items. If GSMA effects rather than item means are desired, m sole items need to be included (Federer, 1999a, 1999b, 2001).

Algorithm II: A minimal fractional combinatorial for estimating item means and BSMS effects is m mixtures of n = m − 1 items. The treatment design is constructed by taking m − 1 rows of an m × m Latin square. The columns of the Latin square form the m mixtures of size n = m − 1 (Federer 1999a, 1999b, 2001).

Algorithm III: The minimal treatment design for estimating item means and all mixing effects up the $k = n^{th}$ mixing effect is all possible combinations of m items taken n at a time, or $v = m!/n!(m - n)!$ mixtures of size n (Hall, 1975, and Federer and Raghavarao, 1987).

Algorithm IV: A minimal fractional combinatorial treatment design for estimating item means, BSMA, and TSMA effects is obtained by taking $m - 2$ orthogonal $m \times m$ Latin squares (m a prime number), deleting all entries above the main right diagonal from each of the Latin squares, and stacking the Latin squares one upon another. The columns of this array form the $n = m - 2$ items in the $v = m(m - 1)/2$ mixtures. This design is optimal as well as minimal.

Example for m = 7 and n = m – 2 = 5: m – 2 = 5 orthogonal 7 × 7 Latin squares are:

```
1 2 3 4 5 6 7    1 2 3 4 5 6 7    1 2 3 4 5 6 7    1 2 3 4 5 6 7    1 2 3 4 5 6 7
2 3 4 5 6 7 1    3 4 5 6 7 1 2    4 5 6 7 1 2 3    5 6 7 1 2 3 4    6 7 1 2 3 4 5
3 4 5 6 7 1 2    5 6 7 1 2 3 4    7 1 2 3 4 5 6    2 3 4 5 6 7 1    4 5 6 7 1 2 3
4 5 6 7 1 2 3    7 1 2 3 4 5 6    3 4 5 6 7 1 2    6 7 1 2 3 4 5    2 3 4 5 6 7 1
5 6 7 1 2 3 4    2 3 4 5 6 7 1    6 7 1 2 3 4 5    3 4 5 6 7 1 2    7 1 2 3 4 5 6
6 7 1 2 3 4 5    4 5 6 7 1 2 3    2 3 4 5 6 7 1    7 1 2 3 4 5 6    5 6 7 1 2 3 4
7 1 2 3 4 5 6    6 7 1 2 3 4 5    5 6 7 1 2 3 4    4 5 6 7 1 2 3    3 4 5 6 7 1 2
```

Deleting all items above the main right diagonal, stacking the m – 2 = 5 squares upon one another, and taking the n = m – 2 = 5 items in each column as a mixture, we obtain the following m(m – 1)/2 = 7(6)/2 = 21 mixtures of size n = 5:

```
2      3 4    4 5 6    5 6 7 1 6 7 1 2 3      7 1 2 3 4 5
3      5 6    7 1 2    2 3 4 5 4 5 6 7 1      6 7 1 2 3 4
4      7 1    3 4 5    6 7 1 2 2 3 4 5 6      5 6 7 1 2 3
5      2 3    6 7 1    3 4 5 6 7 1 2 3 4      4 5 6 7 1 2
6      4 5    2 3 4    7 1 2 3 5 6 7 1 2      3 4 5 6 7 1
```

For each item, the remaining m – 1 = 6 items form a balanced incomplete block design (BIBD) with b = (m – 1)(m – 2)/2 = 6(5)/2 = 15 incomplete blocks of size m – 3 = 4 with r = (m – 2)(m – 3)/2 = 10 replicates and λ = r(m – 4)/(m – 2) = 10(3)/5 = 6. For each pair of items, the remaining m – 2 = 5 items form a balanced incomplete block design with (m – 2)(m – 3)/2 = 10 incomplete blocks of size m – 4 = 3, r = 6, and λ = 3. Since a BIBD is formed for every pair hi of items, every mean $\mu_{h(ij)}$ for item h in the presence of items i and j is estimable. Since a TSMA effect is equal to $\mu_{h(ij)}$ - $\mu_{h(i.)}$, every TSMA effect is estimable. (The dot notation means summed up over.) Likewise, all BSMA effects are estimable as $\mu_{h(i.)}$ - $\mu_{h(..)}$, and all item means are estimable as $\mu_{h(..)}$. Also, the design for each pair is a BIBD and therefore is optimal.

Algorithm V: A minimal fractional combinatorial for estimating item means, BSMA effects, and TSMA effects is obtained by taking (m - 2)/2 orthogonal Latin squares (m

even), deleting the first row of each of the (m - 2)/2 Latin squares, and stacking the squares one upon another to obtain v = m(m - 1) mixtures of size (m - 2)/2 items.

Example for m = 8 and n = (m - 2)/2 = 3: This design results in all possible combinations of eight choose three at a time. As shown by Hall (1975) and Federer and Raghavarao (1987) this is a minimal design for estimating item means, BSMA effects, and TSMA effects. For any item, the remaining seven items form a balanced incomplete block design with v = 7, k = 2, r = 6, and λ = 1. For any pair of items, each of the remaining six items occurs once.

Example for m = 12 and n = (m - 2)/2 =5: Using the OLS(12, 5) set given by Johnson *et al.* (1961), and the above algorithm, we obtain the following m(m - 1) = 132 mixtures of size n = (m - 2)/2 = 5:

```
5  0  1  2  3  4 11  6  7  8  9 10        4  5  0  1  2  3 10 11  6  7  8  9
6  7  8  9 10 11  0  1  2  3  4  5       10 11  6  7  8  9  4  5  0  1  2  3
3  4  5  0  1  2  9 10 11  6  7  8        6  7  8  9 10 11  0  1  2  3  4  5
10 11  6  7  8  9  4  5  0  1  2  3        5  0  1  2  3  4 11  6  7  8  9 10
2  3  4  5  0  1  8  9 10 11  6  7        7  8  9 10 11  6  1  2  3  4  5  0

3  4  5  0  1  2  9 10 11  6  7  8        2  3  4  5  0  1  8  9 10 11  6  7
4  5  0  1  2  3 10 11  6  7  8  9       11  6  7  8  9 10  5  0  1  2  3  4
5  0  1  2  3  4 11  6  7  8  9 10        9 10 11  6  7  8  3  4  5  0  1  2
7  8  9 10 11  6  1  2  3  4  5  0        1  2  3  4  5  0  7  8  9 10 11  6
8  9 10 11  6  7  2  3  4  5  0  1        4  5  0  1  2  3 10 11  6  7  8  9

1  2  3  4  5  0  7  8  9 10 11  6        6  7  8  9 10 11  0  1  2  3  4  5
5  0  1  2  3  4 11  6  7  8  9 10        9 10 11  6  7  8  3  4  5  0  1  2
7  8  9 10 11  6  1  2  3  4  5  0        4  5  0  1  2  3 10 11  6  7  8  9
9 10 11  6  7  8  3  4  5  0  1  2        3  4  5  0  1  2  9 10 11  6  7  8
11  6  7  8  9 10  5  0  1  2  3  4       10 11  6  7  8  9  4  5  0  1  2  3

11  6  7  8  9 10  5  0  1  2  3  4       10 11  6  7  8  9  4  5  0  1  2  3
7  8  9 10 11  6  1  2  3  4  5  0        2  3  4  5  0  1  8  9 10 11  6  7
10 11  6  7  8  9  4  5  0  1  2  3        1  2  3  4  5  0  7  8  9 10 11  6
8  9 10 11  6  7  2  3  4  5  0  1        4  5  0  1  2  3 10 11  6  7  8  9
6  7  8  9 10 11  0  1  2  3  4  5        9 10 11  6  7  8  3  4  5  0  1  2

9 10 11  6  7  8  3  4  5  0  1  2        8  9 10 11  6  7  2  3  4  5  0  1
8  9 10 11  6  7  2  3  4  5  0  1        1  2  3  4  5  0  7  8  9 10 11  6
2  3  4  5  0  1  8  9 10 11  6  7       11  6  7  8  9 10  5  0  1  2  3  4
11  6  7  8  9 10  5  0  1  2  3  4        6  7  8  9 10 11  0  1  2  3  4  5
5  0  1  2  3  4 11  6  7  8  9 10        3  4  5  0  1  2  9 10 11  6  7  8

7  8  9 10 11  6  1  2  3  4  5  0
3  4  5  0  1  2  9 10 11  6  7  8
8  9 10 11  6  7  2  3  4  5  0  1
```

2 3 4 5 0 1 8 9 10 11 6 7
1 2 3 4 5 0 7 8 9 10 11 6

The above forms a BIBD with v = 12, k = 5, r = 55, and λ = 20. For any item h, an incomplete block design with v = 11, k = 4, and r = 20. This design is not balanced. For any pair of items hi = 10, an incomplete block design for v = 10, b = 20, and k = 3 of the following nature is formed:

3 8 10	6 8 9	4 10 11	5 9 10	2 10 11
8 9 10	3 8 10	6 7 9	3 6 7	2 4 5
2 3 5	2 3 4	3 4 5	3 8 9	7 10 11
3 6 9	3 8 10	5 6 11	2 6 7	6 7 8

The concurrence matrix NN' is:

$$
\begin{array}{cccccccccc}
5 & 2 & 2 & 2 & 1 & 1 & 0 & 0 & 1 & 1 \\
2 & 9 & 2 & 2 & 2 & 2 & 4 & 2 & 3 & 0 \\
2 & 2 & 4 & 2 & 0 & 0 & 0 & 0 & 1 & 1 \\
2 & 2 & 2 & 5 & 1 & 0 & 0 & 1 & 1 & 1 \\
1 & 2 & 0 & 1 & 7 & 4 & 3 & 2 & 0 & 1 \\
1 & 1 & 0 & 0 & 4 & 5 & 1 & 1 & 1 & 1 \\
0 & 4 & 0 & 0 & 2 & 1 & 7 & 3 & 4 & 0 \\
0 & 2 & 0 & 1 & 3 & 1 & 3 & 6 & 2 & 0 \\
1 & 3 & 1 & 1 & 0 & 1 & 4 & 2 & 8 & 3 \\
1 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 3 & 4 \\
\end{array}
$$

The inverse of the above matrix is

$$
\begin{array}{cccccccccc}
0.30 & -0.04 & -0.09 & -0.06 & -0.02 & -0.04 & 0.03 & 0.03 & -0.02 & -0.00 \\
-0.04 & 0.20 & -0.07 & -0.04 & -0.06 & 0.02 & -0.07 & 0.03 & -0.07 & 0.10 \\
-0.09 & -0.07 & 0.40 & -0.09 & 0.07 & -0.01 & 0.01 & -0.01 & 0.04 & -0.09 \\
-0.06 & -0.04 & -0.09 & 0.30 & -0.07 & 0.08 & 0.06 & -0.04 & -0.03 & -0.02 \\
-0.02 & -0.06 & 0.07 & -0.07 & 0.50 & -0.40 & -0.10 & -0.20 & 0.30 & -0.30 \\
-0.04 & 0.02 & -0.01 & 0.08 & -0.40 & 0.50 & 0.07 & 0.10 & -0.20 & 0.09 \\
0.03 & -0.07 & 0.01 & 0.06 & -0.10 & 0.07 & 0.40 & -0.03 & -0.20 & 0.20 \\
0.03 & 0.03 & -0.01 & -0.04 & -0.20 & 0.10 & -0.03 & 0.30 & -0.10 & 0.10 \\
-0.02 & -0.07 & 0.04 & -0.03 & 0.30 & -0.20 & -0.20 & -0.10 & 0.50 & -0.40 \\
-0.00 & 0.10 & -0.09 & -0.02 & -0.30 & 0.09 & 0.20 & 0.10 & -0.40 & 0.60 \\
\end{array}
$$

This incomplete block design has the RF property described by Raghavarao and Federer (2000). This property is shared by every one of the 132 pairs hi incomplete block designs. As can be seen this design is not optimal but every $\mu_{h(ij)}$ is estimable, and hence all TSMA effects, all BSMA effects, and all item means are estimable.

Algorithm VI: A fractional combinatorial for estimating items means, BSMA, and TSMA effects is obtained by taking m/2 orthogonal m × m Latin squares (m even), deleting the first row of each of the m/2 Latin squares, and stacking the squares one upon another to obtain v = m(m – 1) mixtures of size n = m/2 items. This design is not minimal but will leave m(m - 1) degrees of freedom for lack of fit or for an error variance.

Example for m = 8 and n = 4: Consider the following four orthogonal 8 × 8 Latin squares:

```
1 2 3 4 5 6 7 8     1 2 3 4 5 6 7 8     1 2 3 4 5 6 7 8     1 2 3 4 5 6 7 8
2 1 7 5 4 8 3 6     8 6 4 3 7 2 5 1     7 3 2 6 8 4 1 5     6 8 5 7 3 1 4 2
3 7 1 8 6 5 2 4     2 1 7 5 4 8 3 6     8 6 4 3 7 2 5 1     7 3 2 6 8 4 1 5
4 5 8 1 2 7 6 3     3 7 1 8 6 5 2 4     2 1 7 5 4 8 3 6     8 6 4 3 7 2 5 1
5 4 6 2 1 3 8 7     4 5 8 1 2 7 6 3     3 7 1 8 6 5 2 4     2 1 7 5 4 8 3 6
6 8 5 7 3 1 4 2     5 4 6 2 1 3 8 7     4 5 8 1 2 7 6 3     3 7 1 8 6 5 2 4
7 3 2 6 8 4 1 5     6 8 5 7 3 1 4 2     5 4 6 2 1 3 8 7     4 5 8 1 2 7 6 3
8 6 4 3 7 2 5 1     7 3 2 6 8 4 1 5     6 8 5 7 3 1 4 2     5 4 6 2 1 3 8 7
```

After deleting row one from each of the squares, stack the squares one upon another. There will be n = 4 items in each column. For example, the first mixture of four is obtained as 2 8 7 6. The m(m – 1) = 56 mixtures (in columns) of size n = m/2 = 4 are:

```
2 1 7 5 4 8 3 6     3 7 1 8 6 5 2 4     4 5 8 1 2 7 6 3     5 4 6 2 1 3 8 7
8 6 4 3 7 2 1 5     2 1 7 5 4 8 3 6     3 7 1 8 6 5 2 4     4 5 8 1 2 7 6 3
7 3 2 6 8 4 1 5     8 6 4 3 7 2 5 1     2 1 7 5 4 8 3 6     3 7 1 8 6 5 2 4
6 8 5 7 3 1 4 2     7 3 2 6 8 4 1 5     8 6 4 3 7 2 5 1     2 1 7 5 4 8 3 6

6 8 5 7 3 1 4 2     7 3 2 6 8 4 1 5     8 6 4 3 7 2 5 1
5 4 6 2 1 3 8 7     6 8 5 7 3 1 4 2     7 3 2 6 8 4 1 5
4 5 8 1 2 7 6 3     5 4 6 2 1 3 8 7     6 8 5 7 3 1 4 2
3 7 1 8 6 5 2 4     4 5 8 1 2 7 6 3     5 4 6 2 1 3 8 7
```

For any item, the remaining seven items form a balanced incomplete block design with parameters v = 7 treatments in incomplete blocks of size k = 3 and with r = 12 replicates of each item to form the b = 28 incomplete blocks. Every pair of items occurs together in λ = 4 times in the b = 28 blocks. For any pair of items hi, the remaining m – 2 = 6 items form an incomplete block design with parameters v = 6, k = 2, and r = 4. Each of the six items occurs with four of the items in the blocks and does not occur with one of the items in any block. For example for the pair hi = 12, the b = 12 incomplete blocks of size k = 2 are:

(4, 8) (5, 6) (4, 7) (3, 5) (5, 8) (4, 6) (7, 8) (3, 6) (6, 7) ((3, 8) (3, 4) (5, 7)

This form of a two associate class design occurs for every one of the 56 pairs. For N equal to the 6 × 12 incidence matrix of items and blocks, the inverse of the NN' matrix is

0.3125	0.0625	0.0625	0.0625	0.0625	0.0625
0.0625	0.3125	0.0625	0.0625	0.0625	0.0625
0.0625	0.0625	0.3125	0.0625	0.0625	0.0625
0.0625	0.0625	0.0625	0.3125	0.0625	0.0625
0.0625	0.0625	0.0625	0.0625	0.3125	0.0625
0.0625	0.0625	0.0625	0.0625	0.0625	0.3125

For $\mu_{h(ij)}$ equal to the mean for item h in the presence of items i and j, every $\mu_{h(ij)}$ is estimable. Therefore every TSMA effect is estimable. This also means that every BSMA effect, $\mu_{h(i.)} - \mu_{h(..)}$, and every item mean, $\mu_{h(..)}$, are estimable. The treatment design has $m(m-1)(m-2)/2$ responses and $v = m(m-1)$ mixtures to make this a minimal design capable of estimating item means, BSMA effects, and TSMA effects.

LITERATURE CITED

Federer, W. T. (1999a). *Statistical Design and Analysis for Intercropping Experiments: Volume II. Three or More Crops.* Springer-Verlag, New York, Berlin, and Heidelberg, xxiv + 262 pp.

Federer, W. T. (1999b). Fractional combinatorial treatment design. BU-1467-M in the Technical Report Series of the Department of Biometrics, Cornell University, Ithaca, New York.

Federer, W. T. (2001). Minimal treatment designs for estimating various mixing effects. In *Proceedings of a Conference in Honor of Damaraju Raghavarao's 60ᵗʰ Birthday, 10/3-4/99* (Editors: S. Altan and J. Singh), Nova Science Publishers, pp.

Federer, W. T. and D. Ragahavarao (1987). Response models and minimal designs for mixtures of n of m items useful for intercropping and other investigations. Biometrika **74**, 571-77.

Hall D. G. (1975). Mixing designs: A general model, simplifications, and some minimal designs. M. S. Thesis, Cornell University, Ithaca, New York.

Johnson D. M., A. L. Dulmage, and N. S. Mendelsohn (1961). Orthomorphisms of groups and orthogonal latin squares I. Canadian Journal of Mathematics 13:356-372.

Raghavarao, D. and W. T. Federer (2000). Characterization of BIB designs for constructing minimal fractional combinatorial treatment designs. BU-1492-M in the Technical Report Series of the Department of Biometrics, Cornell University, Ithaca, New York.