

## Handout #11 – Confounding: Complete factorial experiments in incomplete blocks

Blocking is one of the important principles in experimental design. In this handout we address the issue of designing complete factorial experiments in incomplete blocks. As the number of factors increases, the total number of treatment combinations soon becomes large. Two challenges to the experimenter arise. There may not be enough resources or time to run a complete factorial experiment, or even if a complete factorial experiment is feasible, incomplete blocks may have to be used since a block accommodating all the treatment combinations may be too large to have acceptable within-block variability. We focus on the latter here and address the former in a later handout. If some factorial effects (for example, the higher-order effects) are deemed less important or are negligible, then one can design an experiment so that these effects are estimated by less precise interblock contrasts. They are said to be *confounded* with blocks and are sacrificed to achieve better precision for the more important ones. We start with a simple example to illustrate the ideas.

### 11.1. An example

Suppose a  $2^2$  experiment is to be performed using a randomized block design with six blocks of size two. In this case there exists a balanced incomplete block design in which each treatment appears in three blocks and every pair of treatments appear together in one block:

(1)	a	(1)	b	(1)	a
b	ab	a	ab	ab	b

A balanced incomplete block design is known to be optimal when the treatments are unstructured and the interest is in, e.g., making all pairwise comparisons. Under a balanced incomplete block design, all normalized treatment contrasts are estimated with the same precision in both the inter- and intrablock strata. Let  $\hat{l}^1$  and  $\hat{l}^2$  be the inter- and intrablock estimator of a treatment contrast  $l = \mathbf{c}'\boldsymbol{\alpha}$ . Then with  $r = 3$  and  $\lambda = 1$ , by (6.15) and (6.12),  $\text{var}(\hat{l}^1) = \|\mathbf{c}\|^2 \xi_1$  and  $\text{var}(\hat{l}^2) = \frac{1}{2} \|\mathbf{c}\|^2 \xi_2$ , where  $\xi_1$  and  $\xi_2$  are the inter- and intrablock variances, respectively, and the efficiency factor of this BIBD in the intrablock stratum is  $\frac{2}{3}$ . It follows that all the factorial effects  $A$ ,  $B$  and  $AB$  are estimated with the same precision: the interblock estimators have variance  $\xi_1/4$ , and the intrablock estimators have variance  $\xi_2/8$ . If the interaction  $AB$  is negligible, then this is a waste of resources since it is not necessary to estimate  $AB$  with the same precision as the main effects. The question is, can we construct a design under which the main effects are estimated more efficiently? Ideally we would want them to be estimated with 100% efficiency in the intrablock stratum, instead of an efficiency factor of  $\frac{2}{3}$ .

Now consider the following alternative design:

(1)	a	(1)	a	(1)	a
ab	b	ab	b	ab	b

Note that the interaction  $AB$  is defined as  $\frac{1}{4}((1) - a - b + ab)$ , and the design is constructed in such a way that in each of the three replicates, the two treatment combinations with the same coefficients in the  $AB$  contrast are placed in the same block. A consequence is that  $AB$  must be estimated by a block contrast. Its information is contained entirely in the interblock stratum, and we say that it is *confounded* with blocks. When written in the form  $\mathbf{c}'_{AB}\boldsymbol{\alpha}$ , the inflated version  $\mathbf{c}^*_{AB}$  of  $\mathbf{c}_{AB}$  as defined in the second paragraph of p.2 of Handout #8 is constant over those entries corresponding to the observations in the same block. Therefore  $\mathbf{c}^* \in \mathcal{B} \ominus \mathcal{G}$ , the interblock stratum. It follows from Theorem 2 in Handout #8 that the best linear unbiased estimator of  $AB$  is obtained by substituting the treatment means into the contrast defining  $AB$ . The variance of this estimator is equal to  $\xi_1/12$ . On the other hand, both  $\mathbf{c}^*_A$  and  $\mathbf{c}^*_B$  are in  $\mathcal{B}^\perp$ . We say that they are *orthogonal* to the blocks. Again by Theorem 2 in Handout #8, they are also estimated by substituting the treatment means into the respective contrasts, and both estimators have variances equal to  $\xi_2/12$ .

Under the second design, the estimators of the main effects of both factors are 50% more efficient than their intrablock estimators under a BIBD. This is achieved by sacrificing the interaction  $AB$  which can only be estimated by a between-block contrast, presumably with a larger variance. Under a model with fixed block effects,  $AB$  is not even estimable under the second design, which is not a connected design in either the inter- or intrablock stratum. For this design, the information matrix for treatment effects in the intrablock stratum has rank equal to 2 and that in the interblock stratum has rank 1. For a BIBD, both information matrices have rank 3.

The sum of squares associated with each factorial effect can be computed easily. Let  $l$  be any of the three effects  $A$ ,  $B$  and  $AB$ . Then  $SS(l) = 12(\widehat{l})^2$ . The two sums of squares  $SS(A)$  and  $SS(B)$  appear in the ANOVA in the intrablock stratum, leaving four degrees of freedom for residual, and  $SS(AB)$  appears in the ANOVA in the interblock stratum, also with four degrees of freedom for residual.

### 11.2. Construction of a $2^n$ design in $2^m$ blocks of size $2^{n-m}$ .

When all the factors have two levels, as shown in Section 9.9 of Handout #9, if each treatment combination is considered as a point in  $EG(n, 2)$ , then each interaction contrast is defined by a nonzero vector  $\mathbf{a} = (a_1, \dots, a_n)^T$  such that all the treatment combinations  $\mathbf{x}$  with  $\mathbf{a}^T \mathbf{x} = 0$  have the same coefficient in the contrast and those with  $\mathbf{a}^T \mathbf{x} = 1$  also have the same coefficient (Throughout this section we have  $1 + 1 = 0$ .) If we put the treatment combinations with  $\mathbf{a}^T \mathbf{x} = 0$  in one block and all the others in another block, then we have constructed a design with two blocks each of size  $2^{n-1}$ . The interaction defined by  $\mathbf{a}$ , which is a  $k$ -factor interaction if  $\mathbf{a}$  contains  $k$  nonzero entries, is confounded with blocks, and all the other factorial effects are orthogonal to the blocks.

To construct a  $2^n$  design in four blocks of size  $2^{n-2}$ , one can choose another nonzero vector  $\mathbf{b}$ . The  $2^n$  treatment combinations are partitioned into four blocks of size  $2^{n-2}$  according to the values of  $\mathbf{a}^T \mathbf{x}$  and  $\mathbf{b}^T \mathbf{x}$ :

$$\begin{aligned} \text{block 1: } & \mathbf{a}^T \mathbf{x} = 0, \mathbf{b}^T \mathbf{x} = 0; \text{ block 2: } \mathbf{a}^T \mathbf{x} = 0, \mathbf{b}^T \mathbf{x} = 1; \\ \text{block 3: } & \mathbf{a}^T \mathbf{x} = 1, \mathbf{b}^T \mathbf{x} = 0; \text{ block 4: } \mathbf{a}^T \mathbf{x} = 1, \mathbf{b}^T \mathbf{x} = 1. \end{aligned}$$

Note that these four blocks are the four  $(n-2)$ -flats in the pencil  $P(\mathbf{a}, \mathbf{b})$  defined by  $\mathbf{a}$  and  $\mathbf{b}$ . Since all the treatment combinations in the same block have the same values of  $\mathbf{a}^T \mathbf{x}$  and  $\mathbf{b}^T \mathbf{x}$ , they have the same coefficients in the two contrasts defined by  $\mathbf{a}$  and  $\mathbf{b}$  respectively. Therefore both of these two contrasts are confounded with blocks. With four blocks, the interblock stratum has three degrees of freedom. It turns out that in addition to the two interaction contrasts defined by  $\mathbf{a}$  and  $\mathbf{b}$ , there is another factorial effect that is also confounded with blocks. Since all the treatment combinations in the same block have the same values of  $\mathbf{a}^T \mathbf{x}$  and  $\mathbf{b}^T \mathbf{x}$ , they also have the same values of  $\mathbf{a}^T \mathbf{x} + \mathbf{b}^T \mathbf{x} = (\mathbf{a} + \mathbf{b})^T \mathbf{x}$ . Therefore the factorial effect defined by  $\mathbf{a} + \mathbf{b}$  is also confounded with blocks. When we choose to confound the interactions defined by  $\mathbf{a}$  and  $\mathbf{b}$  with blocks, we should make sure that the interaction defined by  $\mathbf{a} + \mathbf{b}$  can also be safely confounded.

In general, to construct a  $2^n$  design in  $2^m$  blocks of size  $2^{n-m}$ ,  $m < n$ , we first choose  $m$  linearly independent vectors  $\mathbf{a}_1, \dots, \mathbf{a}_m$  in  $EG(n, 2)$  such that the interaction contrast defined by each of these vectors is to be confounded with blocks. Then the  $2^m$  disjoint  $(n-m)$ -flats in the pencil  $P(\mathbf{a}_1, \dots, \mathbf{a}_m)$  provides a partition of the  $2^n$  treatment combinations into  $2^m$  blocks of size  $2^{n-m}$ . Each block consists of all the treatment combinations  $\mathbf{x}$  satisfying the  $m$  equations

$$\mathbf{a}_i^T \mathbf{x} = b_i, i = 1, \dots, m, \quad (11.2.1)$$

where  $b_1, \dots, b_m = 0$  or  $1$ . The  $2^m$  choices of  $b_1, \dots, b_m$  define the  $2^m$  blocks. Then since all the treatment combinations in the same block have the same value of  $\mathbf{a}_i^T \mathbf{x}$ , they all have the same coefficient in the contrast defined by  $\mathbf{a}_i$ . It follows that the interaction contrast defined by  $\mathbf{a}_i$  is confounded with blocks. Furthermore, for any nonzero vector  $\mathbf{a}$  that is a linear combination of  $\mathbf{a}_1, \dots, \mathbf{a}_m$ , all the treatment combinations in the same block also have the same value of  $\mathbf{a}^T \mathbf{x}$ ; therefore the factorial effect defined by each nonzero vector in the  $m$ -dimensional space generated by  $\mathbf{a}_1, \dots, \mathbf{a}_m$  is also confounded with blocks. This gives a total of  $2^m - 1$  orthogonal contrasts that are confounded with blocks. We call the factorial effect defined by a nonzero linear combination of  $\mathbf{a}_1, \dots, \mathbf{a}_m$  a *generalized interaction* of the  $m$  factorial effects defined by  $\mathbf{a}_1, \dots, \mathbf{a}_m$ . When we choose to confound the interactions defined by  $\mathbf{a}_1, \dots, \mathbf{a}_m$  with blocks, all their generalized interactions are also confounded with blocks.

The block consisting of the solutions of

$$\mathbf{a}_i^T \mathbf{x} = 0, i = 1, \dots, m, \quad (11.2.2)$$

is called the *principal block*. Let this block be denoted by  $B_1$ . Then all the other blocks are of the form  $B_1 + \mathbf{x}$ , where  $\mathbf{x}$  is a nonzero vector in  $\text{EG}(n, 2)$  (see Section 10.4 in Handout #10). Thus one can follow the following procedure to generate the  $2^m$  blocks:

- Step 1: Set  $k = 0$ . Solve the simultaneous equations in (11.2.2) to obtain the initial block  $B_1$ .
- Step 2: Pick a treatment combination  $\mathbf{x}$  that has not appeared in  $\bigcup_{i=1}^{2^k} B_i$  yet. Add  $\mathbf{x}$  to each treatment combination in  $B_1, \dots, B_{2^k}$  to form  $2^k$  additional blocks  $B_{2^k+1}, \dots, B_{2^{k+1}}$ .
- Step 3: Increase  $k$  by 1. Stop if  $k = m$ ; otherwise go to step 2.

If the shorthand notation introduced in the paragraph following (9.6.7) in Handout #9 is used, then the string of capital letters representing the factorial effect defined by  $\mathbf{a} + \mathbf{b}$ , where  $\mathbf{a}, \mathbf{b} \in \text{EG}(n, 2)$ , can be obtained by multiplying those representing the factorial effects defined by  $\mathbf{a}$  and  $\mathbf{b}$ , subject to the rule that the square of any letter is removed; for example,  $(ACD)(CDE) = AE$ . Then the linear independence of  $\mathbf{a}_1, \dots, \mathbf{a}_m$  means that none of the corresponding factorial effects, when written as a string of capital letters, is a product of any number of the other  $m - 1$  effects. In this case, we say that these  $m$  factorial effects are linearly independent. For example,  $AB, BC, ACD$  and  $BCD$  are linearly dependent since  $BCD = (AB)(ACD)$ . For the case of four factors, this corresponds to that  $(0, 1, 1, 1) = (1, 1, 0, 0) + (1, 0, 1, 1)$ . Similarly, the treatment combination  $\mathbf{x} + \mathbf{y}$ , when expressed as a string of lower case letters, is the product of those representing  $\mathbf{x}$  and  $\mathbf{y}$ , again subject to the rule that the square of any letter is removed. If the  $i_1$ th,  $\dots$ , and  $i_k$ th entries of the vector  $\mathbf{a}_i$  in (11.2.2) are nonzero and all the other entries are zero, then the equation  $\mathbf{a}_i^T \mathbf{x} = 0$  means that an even number of  $x_{i_1}, \dots, x_{i_k}$  are equal to 1. This implies that, when the shorthand notation is used, the principal block consists of all treatment combinations that have an even number of letters in common with each of the linearly independent factorial effects defined by  $\mathbf{a}_1, \dots, \mathbf{a}_m$ . One then *multiply* each treatment combination in the blocks that have been generated by a treatment combination that has not appeared yet, until all the blocks have been constructed. We also multiply the strings of capital letters representing the factorial effects defined by  $\mathbf{a}_1, \dots, \mathbf{a}_m$  in all possible ways to obtain their generalized interactions, which are also confounded with blocks.

**Example 11.2.1.** To construct a  $2^5$  design in eight blocks of size four, suppose we pick the three linearly independent interactions  $AC, BD$  and  $ABE$  to be confounded with blocks. Then we will also confound  $(AC)(BD) = ABCD$ ,  $(AC)(ABE) = BCE$ ,  $(BD)(ABE) = ADE$  and  $(AC)(BD)(ABE) = CDE$ . The four treatment combinations that have an even number of letters in common with each of  $AC, BD$  and  $ABE$  are  $(1), ace, bde$  and  $abcd$ . With these four treatment combinations in the principal block, the other seven blocks can easily be constructed:

(1)	$c$	$d$	$cd$	$e$	$ce$	$de$	$cde$
$ace$	$ae$	$acde$	$ade$	$ac$	$a$	$acd$	$ad$
$bde$	$bcde$	$be$	$bce$	$bd$	$bcd$	$b$	$bc$
$abcd$	$abd$	$abc$	$ab$	$abcde$	$abde$	$abce$	$abe$

The second block is obtained by multiplying all the treatment combinations in the first block by the treatment combination  $c$ . The third and fourth blocks are obtained by multiplying all the treatment combinations in the first two blocks by the treatment combination  $d$  and the last four blocks are obtained by multiplying all the treatment combinations in the first four blocks by the treatment combination  $e$ . If we had chosen to confound the highest-order interactions  $ABCD$  and  $ABCDE$  with blocks, then the main effect  $E$  would also be confounded.

### 11.3. Construction of an $s^n$ design in $s^m$ blocks of size $s^{n-m}$ .

The procedure described in the previous section can be extended in a straightforward manner to the case where  $s$ , the number of levels of each factor, is a prime number or power of a prime number. Again, we identify each treatment combination as a point in  $EG(n, s)$ , and start with a set of  $m$  linearly independent vectors  $\mathbf{a}_1, \dots, \mathbf{a}_m$  in  $EG(n, s)$ . The  $m$  vectors define a pencil of  $s^m$  disjoint  $(n - m)$ -flats, each containing  $s^{n-m}$  points (treatment combinations) that are solutions of  $m$  equations  $\mathbf{a}_i^T \mathbf{x} = b_i, i = 1, \dots, m$ , where  $b_i \in GF(s)$ . Each of these  $s^m$   $(n - m)$ -flats is considered as a block. Note that when  $s$  is a prime number, addition and multiplication are carried out as usual except that the results are reduced mod  $s$ . For  $s = p^r$ , where  $p$  is a prime number and  $r > 1$ , more complicated arithmetic operations are required. As in the two-level case, we construct the  $s^m$  blocks as follows:

Step 1: Set  $k = 0$ . Solve the simultaneous equations in (11.2.2) to obtain the initial block  $B_1$ .

Step 2: Pick a treatment combination  $\mathbf{x}$  that has not appeared in  $\bigcup_{i=1}^{s^k} B_i$ . Add each of the  $s - 1$  nonzero multiples of  $\mathbf{x}$  ( $\lambda \mathbf{x}$  with  $\lambda \neq 0$ ) to all the treatment combinations in  $B_1, \dots, B_{s^k}$  to form  $(s - 1)s^k$  additional blocks  $B_{s^k+1}, \dots, B_{s^{k+1}}$ .

Step 3: Increase  $k$  by 1. Stop if  $k = m$ ; otherwise go to step 2.

Under the design so constructed, the interaction contrasts defined by each  $\mathbf{a}_i$  are confounded with blocks. Furthermore, all the interaction contrasts defined by each nonzero linear combination of  $\mathbf{a}_1, \dots, \mathbf{a}_m$  are also confounded with blocks. There are a total of  $s^m - 1$  nonzero linear combinations  $\sum_{i=1}^m \lambda_i \mathbf{a}_i$  of  $\mathbf{a}_1, \dots, \mathbf{a}_m$ , where  $\lambda_i \in GF(s)$ . Each nonzero vector  $\mathbf{a}$  defines  $s - 1$  degrees of freedom; on the other hand, all the  $s - 1$  nonzero multiples of  $\mathbf{a}$  ( $\lambda \mathbf{a}$  with  $\lambda \neq 0$ ) define the same pencil of  $(n - 1)$ -flats, and hence the same treatment contrasts. So the total number of degrees of freedom that are confounded with blocks is equal to  $[(s^m - 1)/(s - 1)](s - 1) = s^m - 1$ .

**Example 11.3.1.** To construct a  $3^3$  design in nine blocks of size three, suppose we choose the two-factor interactions  $AB^2$  and  $AC^2$ , defined by  $\mathbf{a}_1 = (1, 2, 0)$  and  $\mathbf{a}_2 = (1, 0, 2)$ , respectively, to be confounded with blocks. Then the principal block consists of the three solutions of the two equations  $x_1 + 2x_2 = 0$  and  $x_1 + 2x_3 = 0$ :  $\{(0, 0, 0), (1, 1, 1), (2, 2, 2)\}$ . The nine blocks are

000	100	200	021	121	221	012	112	212
111	211	011	102	202	002	120	220	020
222	022	122	210	010	110	201	001	101

The second and third blocks are obtained by adding  $(1, 0, 0)$  and  $2 \cdot (1, 0, 0) = (2, 0, 0)$  to all the treatment combinations in the first block. Blocks 4-6 and 7-9 are obtained by adding  $(0, 2, 1)$  and  $2 \cdot (0, 2, 1) = (0, 1, 2)$ , respectively, to all the treatment combinations in the first three blocks. The two vectors  $\mathbf{a}_1$  and  $\mathbf{a}_2$  have two linear combinations  $\mathbf{a}_1 + \mathbf{a}_2 = (2, 2, 2)$  and  $\mathbf{a}_1 + 2\mathbf{a}_2 = (0, 2, 1)$ . The former defines the same two degrees of freedom of treatment contrasts as  $2 \cdot (2, 2, 2) = (1, 1, 1)$ , which are denoted as  $ABC$ , and the latter defines the same two degrees of freedom of treatment contrasts as  $2 \cdot (0, 2, 1) = (0, 1, 2)$ , which are denoted as  $BC^2$ . Therefore the eight degrees of freedom that are confounded with blocks are  $AB^2, AC^2, ABC$  and  $BC^2$ .

#### 11.4. Analysis

Under an incomplete block design, condition of proportional frequencies cannot be satisfied by the treatment and block factors. It follows that  $\mathcal{T} \ominus \mathcal{G}$  is not entirely in one stratum. Since  $\mathcal{T} \ominus \mathcal{G}$  has nontrivial projections onto both  $\mathcal{B} \ominus \mathcal{G}$  and  $\mathcal{B}^\perp$ , there is treatment information in both the inter- and intrablock strata. When a design is constructed by the method described here, for each contrast  $\mathbf{c}'\boldsymbol{\alpha}$  that is confounded with blocks, the inflated version  $\mathbf{c}^*$  of  $\mathbf{c}$  as defined in Handout #8 belongs to  $\mathcal{B} \ominus \mathcal{G}$ , while those for all the other contrasts fall in  $\mathcal{B}^\perp$ . We say that the latter contrasts are orthogonal to blocks. Theorem 2 in Handout #8 implies that estimates of all the factorial effects and their associated sums of squares can be computed in exactly the same way as when the experiment is not blocked. In particular, the Yates algorithm as described in Handout #9 can be used for two-level designs. In a single-replicate design, each normalized factorial effect that is confounded with blocks is estimated with variance  $\xi_1$ , and those which are orthogonal to blocks are estimated with variance  $\xi_2$ . While  $\mathcal{T} \ominus \mathcal{G}$  is not entirely in one stratum, it can be decomposed as  $\mathcal{T}_1 \oplus \mathcal{T}_2$ , where  $\mathcal{T}_1 \subset \mathcal{B} \ominus \mathcal{G}$  and  $\mathcal{T}_2 \subset \mathcal{B}^\perp$ . Compared with when the experiment is run in complete blocks, the only difference in the ANOVA table is that the sums of squares of the factorial effects that are confounded with blocks now appear in the interblock stratum. For example the following is a skeleton of the ANOVA table for the second design in Section 11.1:

Sources of variation	d.f.
Interblock stratum	
$AB$	1
Residual	4
Intrablock stratum	
$A$	1
$B$	1
Residual	4

The two main effect contrasts  $A$  and  $B$  are tested against the intrablock error, while the interaction contrast  $AB$  should be tested against the interblock error.

### 11.5. Pseudo factors

When the number of levels is of the form  $p^r$ , where  $p$  is a prime and  $r > 1$ , one cannot use the usual arithmetic operations. An alternative approach is to represent each of the  $p^r$  levels as a combination of  $r$   $p$ -level *pseudo factors*. For example, in a  $4^3$  experiment with three four-level factors  $A, B$  and  $C$ , suppose each level of  $A$  ( $B$  and  $C$ , respectively) is represented by a combination of two two-level pseudo factors  $A_1$  and  $A_2$  ( $B_1$  and  $B_2$ ,  $C_1$  and  $C_2$ , respectively). Then  $A_1, A_2$  and  $A_1A_2$  correspond to the three degrees of freedom of the main effect of factor  $A$ , all the nine interactions  $A_1B_1, A_1B_2, A_2B_1, A_2B_2, A_1A_2B_1, A_1A_2B_2, A_1B_1B_2, A_2B_1B_2$  and  $A_1A_2B_1B_2$  correspond to the interaction of factors  $A$  and  $B, \dots$ , etc.

### 11.6. Partial confounding

When the number of replicates  $r > 1$ , one has the option of confounding different factorial effects in different replicates. This is useful when the confounding of some important effects with blocks is inevitable in a single replicate. Both of the two designs in Section 11.1 consist of three replicates of a complete  $2^2$ . If the interaction  $AB$  cannot be ignored, then one may not want to confound it with blocks in all three replicates, as is the case under the second design. The BIBD discussed there, on the other hand, confounds  $A$  with blocks in the first replicate (the first two blocks), confounds  $B$  in the second replicate (the third and fourth blocks) and confounds  $AB$  in the third replicate (the fifth and sixth blocks). This is called *partial confounding*.

Although estimates of the factorial effects under this BIBD can be computed as in Handout #6, one can take advantage of the factorial structure to compute the interblock estimate of a factorial effect and the associated sum of squares (as if there were no blocking) from the replicate in which it is confounded with blocks, and compute the intrablock estimate and the associated sum of squares (as if there were no blocking) from the two replicates in which it is orthogonal to blocks. This results in a variance of  $\xi_1/4$  for the interblock estimate and  $\xi_2/8$  for the intrablock estimate. The following gives a skeleton of the ANOVA which is different from the one shown in Section 11.4 for the design which confounds  $AB$  in all three replicates:

Sources of variation	d.f.
Interblock stratum	
$A$	1
$B$	1
$AB$	1
Residual	2

Intrablock stratum	
<i>A</i>	1
<i>B</i>	1
<i>AB</i>	1
Residual	3
Total	11

If the randomization is carried out in each replicate separately, i.e., the block structure is 3 replicates/2 blocks/2 units. Then there is an additional inter-replicate stratum with two degrees of freedom. The ANOVA in the intrablock stratum remains the same, but two degrees of freedom for residual in the interblock stratum move up to the inter-replicate stratum, leaving no residual degree of freedom in the interblock stratum for the BIBD and two degrees of freedom for the other design.

### 11.7. Design keys

We present an alternative but equivalent construction of complete factorial designs in incomplete blocks based on the method of *design key* due to H. D. Patterson. We have seen that in order to partition the  $2^n$  treatment combinations into  $2^m$  blocks of equal size, we first pick  $m$  linearly independent interactions to be confounded with blocks, and use them to construct the blocking scheme. In the meantime, an additional set of  $2^m - 1 - m$  factorial effects will also be confounded with blocks. Let the factorial effects which can be safely confounded with blocks be called *eligible* effects. We need to check that all the  $2^m - 1$  effects confounded with blocks are eligible. In the current context, typically we avoid confounding the main effects with blocks, and so the main effects are ineligible.

The method of design key, however, first designates the strata where the main effects will be estimated. If we want to estimate the main effects in the intrablock stratum, we can designate a set of  $n$  linearly independent contrasts in the intrablock stratum to be *aliases* of the main effects, to be described more precisely later. This guarantees that the main effects will be estimated in the intrablock stratum, and the specified aliasing of main-effect contrasts with intrablock contrasts can be used to construct the blocking scheme in a straightforward manner, and can also be used to obtain *aliases* of all the other factorial effects to determine in which stratum each of them will be estimated.

The method of design key can be applied more generally to designs with simple block structures. In this section we only discuss the application to the construction of single-replicate complete factorial designs in incomplete blocks. A more general treatment of the method will be presented in a later handout.



Suppose the  $s^n$  treatment combinations are to be partitioned into  $s^m$  blocks of size  $s^{n-m}$ . The  $s^n$  experimental units can be thought of as all the combinations of an  $s^m$ -level factor  $B$  and an  $s^{n-m}$ -level factor  $U$ , with the levels of  $U$  nested within each level of  $B$ . The combination where  $B$  is at level  $i$  and  $U$  is at level  $j$  corresponds to the  $j$ th unit in the  $i$ th block. Ignore the nesting structure and define the "main-effect" and "interaction" contrasts of  $B$  and  $U$  as if they were crossed. Then the "main-effect" contrasts of  $B$ , which have  $s^m - 1$  degrees of freedom, are the inter-block contrasts, and the main-effect contrasts of  $U$  and the interaction contrasts of  $B$  and  $U$  are intrablock contrasts. If a design is constructed so that each main-effect treatment contrast coincides with a contrast representing either the main effect of  $U$  or interaction of  $B$  and  $U$ , then all the treatment main effects are estimated in the intrablock stratum. For ease of construction, we further consider each block as a combination of  $m$   $s$ -level pseudo factors  $B_1, \dots, B_m$  and each level of  $U$  as a combination of  $n - m$   $s$ -level pseudo factors  $U_1, \dots, U_{n-m}$ . Then a main-effect or interaction contrast of the  $n$  factors  $B_1, \dots, B_m, U_1, \dots, U_{n-m}$  represents an interblock (respectively, intrablock) contrast if and only if it involves none (respectively, at least one) of the  $U_j$ 's. We call  $B_1, \dots, B_m, U_1, \dots, U_{n-m}$  the *unit factors*. For a reason to be explained later, we place  $U_1, \dots, U_{n-m}$  before  $B_1, \dots, B_m$  and label each experimental unit by  $(u_1, \dots, u_{n-m}, b_1, \dots, b_m)$ , where  $0 \leq u_i, b_j \leq s - 1$ .

Since each experimental unit is a combination of the levels of  $U_1, \dots, U_{n-m}, B_1, \dots, B_m$ , we can describe the relation between the experimental units and the  $n$  unit factors by an  $n \times s^n$  matrix  $\mathbf{Y}$  such that for each  $j$ ,  $1 \leq j \leq s^n$ , the  $j$ th column of  $\mathbf{Y}$  is the corresponding factor-level combination of the unit factors. What we need is an  $n \times s^n$  matrix  $\mathbf{X}$  whose  $j$ th column gives the treatment combination assigned to the  $j$ th unit. The matrix  $\mathbf{X}$  then produces the design. We obtain  $\mathbf{X}$  from  $\mathbf{Y}$  via a matrix multiplication

$$\mathbf{X} = \mathbf{K}\mathbf{Y}, \quad (11.7.1)$$

where  $\mathbf{K}$  is an  $n \times n$  matrix with entries from  $\text{GF}(s)$ . The matrix  $\mathbf{K}$  connects the  $n$  treatment factors to the  $n$  unit factors, and is called a *design key matrix*. By (11.7.1), the design key requires that the treatment combination  $(x_1, \dots, x_n)$  assigned to the experimental unit  $(u_1, \dots, u_{n-m}, b_1, \dots, b_m)$  satisfy

$$x_i = \sum_{j=1}^{n-m} k_{ij} u_j + \sum_{l=1}^m k_{i, n-m+l} b_l. \quad (11.7.2)$$

Equation (11.7.2) shows that under the constructed design, the main effect of the  $i$ th treatment factor coincides with the factorial effect of the unit factors defined by  $(k_{i1}, \dots, k_{i, n-m}, k_{i, n-m+1}, \dots, k_{in})^T$ . We say that the latter is the *unit alias* of the former. The main effect of the  $i$ th treatment factor is estimated in the intrablock stratum if its unit alias involves at least one of the  $U_j$ 's, i.e., at least one of  $k_{i1}, \dots, k_{i, n-m}$  is nonzero. In order to generate all the  $s^n$  treatment combinations, the  $n$  rows of  $\mathbf{K}$  must be linearly independent, i.e.,  $\mathbf{K}$  must be invertible,

**Example 11.7.1.** We revisit Example 11.2.1 and consider the construction of a  $2^5$  design in eight blocks of size four. Let the five treatment factors be  $A, B, C, D, E$ , and the unit factors be  $U_1, U_2$  and  $B_1, B_2, B_3$ . To avoid confounding the treatment main effects with blocks, we need to choose five linearly independent factorial effects of  $U_1, U_2$  and  $B_1, B_2, B_3$ , each involving at least one of  $U_1$  and  $U_2$ , to be the unit aliases of the five treatment main effects. Suppose we choose the unit aliases of  $A, B, C, D, E$  to be  $U_1, U_2, U_1B_1, U_2B_2$ , and  $U_1U_2B_3$ , respectively. Then the design key matrix is

$$\mathbf{K} = \begin{array}{ccccc} & U_1 & U_2 & B_1 & B_2 & B_3 \\ \left[ \begin{array}{ccccc} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 & 1 \end{array} \right] & A & B & C & D & E \end{array} \quad (11.7.3)$$

For example, since the unit alias of  $C$  is  $U_1B_1$ , on the third row, we have 1's at the two entries corresponding to  $U_1$  and  $B_1$ . We use the definition of unit alias for the main effect of each treatment factor to write down the corresponding *row* of  $\mathbf{K}$ , and hence determine the matrix.

The resulting design can be obtained by carrying out the multiplication in (11.7.1) mod 2 which, however, is not necessary. In general, suppose  $s$  is a prime number, then given  $n$  linearly independent vectors  $\mathbf{x}_1, \dots, \mathbf{x}_n$  in  $\text{EG}(n, s)$ , called a set of *independent generators* hereafter, we can generate all the  $s^n$  points in  $\text{EG}(n, s)$  in the following order:

1. Start with  $\mathbf{0}$  which has all the components equal to zero.
2. Set  $k = 1$ . Follow  $\mathbf{0}$  by  $\mathbf{x}_1, \dots, (s - 1)\mathbf{x}_1$ .
3. For each  $1 \leq k \leq n - 1$ , follow the  $s^k$  points that have been generated by their sums with  $\mathbf{x}_k$  in the same order, then the sums with  $2\mathbf{x}_k$  in the same order,  $\dots$ , up to the sums with  $(s - 1)\mathbf{x}_k$  in the same order. This generates a total of  $s^{k+1}$  points.
4. Increase  $k$  by 1. Stop if  $k = n$ ; otherwise go to step 3.

We call the order determined by this procedure the *Yates order* w.r.t. the independent generators  $\mathbf{x}_1, \dots, \mathbf{x}_n$ .

If  $s$  is a prime power but is not a prime number, then one can use pseudo factors as discussed before.

Let  $\mathbf{e}_i$  be the vector with the  $i$ th component equal to 1 and all the other components equal to zero. Suppose we place the experimental units in the Yates order w.r.t.  $\mathbf{e}_1, \dots, \mathbf{e}_n$ . Then the first  $s^{n-m}$  units form one block, and each of the succeeding set of  $s^{n-m}$  units is also a block. This is why we place  $U_1, \dots, U_{n-m}$  before  $B_1, \dots, B_m$ . Since  $\mathbf{K}$  is nonsingular,  $\mathbf{K}\mathbf{e}_1, \dots, \mathbf{K}\mathbf{e}_n$  form a set of independent generators for the treatment combinations. Then the treatment combinations assigned to the experimental units arranged in the Yates order w.r.t.  $\mathbf{e}_1, \dots, \mathbf{e}_n$  are themselves in the Yates order w.r.t.

the independent generators  $\mathbf{K}e_1, \dots, \mathbf{K}e_n$ . Now it is easy to see that  $\mathbf{K}e_j$  is exactly the  $j$ th column of the design key matrix. Thus the treatment combinations assigned to the  $s^n$  experimental units can be obtained by writing down all the treatment combinations in the Yates order w.r.t. to the  $n$  columns of  $\mathbf{K}$ . The first  $s^{n-m}$  treatment combinations are those in the first block, and each subsequent set of  $s^{n-m}$  treatment combinations forms a block.

**Example 11.7.1 revisited.** The five columns of the design key matrix  $\mathbf{K}$  in (11.7.3) gives five independent generators  $ace, bde, c, d$  and  $e$ . The first four treatment combinations in the Yates order of the 32 treatment combinations w.r.t.  $ace, bde, c, d$  and  $e$  are  $(1), ace, bde, abcd$ . These form the principal block. The second block can be obtained by multiplying all the treatment combinations in the principal block by the third generator  $c$ . The fourth generator  $d$  generates two more blocks. Finally four additional blocks are constructed by using the last generator  $e$ . This results in the following design:

(1)	$c$	$d$	$cd$	$e$	$ce$	$de$	$cde$
$ace$	$ae$	$acde$	$ade$	$ac$	$a$	$acd$	$ad$
$bde$	$bcde$	$be$	$bce$	$bd$	$bcd$	$b$	$bc$
$abcd$	$abd$	$abc$	$ab$	$abcde$	$abde$	$abce$	$abe$

This is the same design as we have constructed in Example 11.2.1. Note that the unit aliases of all the treatment interactions can be obtained from those of the treatment main effects. For example, the unit aliases of the three interactions  $AC, BD$  and  $ABE$  chosen to be confounded with blocks in Example 11.2.1 are respectively,  $U_1(U_1B_1) = B_1, U_2(U_2B_2) = B_2$  and  $U_1U_2(U_1U_2B_3) = B_3$ , which indeed represent interblock contrasts. The unit aliases of the other four interactions  $ABCD, BCE, ADE$  and  $CDE$  confounded with blocks are respectively,  $B_1B_2, B_1B_3, B_2B_3$  and  $B_1B_2B_3$ .

Thus once the unit aliases of the treatment main effects have been chosen, they can be used to write down the rows of the design key matrix. Then the columns of the matrix can be used to generate the design. One can also determine the treatment interactions that are confounded with blocks by identifying those whose unit aliases only involve  $B_1, \dots, B_m$ .

**Example 11.7.2.** We revisit Example 11.3.1 and consider the construction of a  $3^3$  design in none blocks of size three. Let the treatment factors be  $A, B, C$  and the unit factors be  $U, B_1$  and  $B_2$ . Suppose we choose the unit aliases of  $A, B, C$  to be  $UB_1, UB_2^2$  and  $UB_2$ , respectively. Then the design key matrix is

$$\begin{array}{c}
 U \quad B_1 \quad B_2 \\
 \left[ \begin{array}{ccc|c}
 1 & 1 & 0 & A \\
 1 & 0 & 2 & B \\
 1 & 0 & 1 & C
 \end{array} \right]
 \end{array}$$

Again we use the specified unit aliases of the three treatment main effects to write down three rows and hence determine the design key matrix. The three columns then give the independent generators  $(1, 1, 1)$ ,  $(1, 0, 0)$  and  $(0, 2, 1)$ . The first generator determines the first block  $\{(0, 0, 0), (1, 1, 1), (2, 2, 2)\}$ . The second generator determines two additional blocks and the last generator produces six more:

000	100	200	021	121	221	012	112	212
111	211	011	102	202	002	120	220	020
222	022	122	210	010	110	201	001	101

This is the same design as constructed in Example 11.3.1. Note that the unit aliases of  $AB^2$  and  $AC^2$ , the interactions chosen to be confounded with blocks in Example 11.3.1, are respectively,  $(UB_1)(UB_2)^2 = B_1B_2$  and  $(UB_1)(UB_2)^2 = B_1B_2^2$ , both of which define interblock contrasts.