

## BALANCE IN DESIGNED EXPERIMENTS WITH ORTHOGONAL BLOCK STRUCTURE

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The notion of general balance due to Nelder is discussed in relation to the eigenvectors of an information matrix, combinatorial balance and the simple combinability of information from uncorrelated sources in an experiment.

**1. Introduction.** This paper is about the notion of general balance (GB) introduced by Nelder (1965) in two papers on designed experiments with orthogonal block structure. Nelder defined (GB) as a relationship between the block structure or dispersion model for the data and the treatment structure or model for the expected value of the data. It embodies and unifies three important and apparently unrelated ideas concerning designed experiments: the usefulness of eigenvectors of the associated information matrices, the combinatorial and statistical notions of balance, and the simple combinability of information from different, uncorrelated, sources in the experiment. These ideas have been discussed independently by a number of authors including Yates (1936, 1939, 1940), Sprott (1956), Morley Jones (1959), Pearce (1963), Martin and Zyskind (1966), Corsten (1976) and many others. We will review the work of these authors in Section 3 and relate it to Nelder's (1965) work.

Nelder (1965, 1968) has shown how a simple and unified approach may be adopted to the analysis of multistratum designed experiments satisfying (GB), including the estimation of stratum variances and the combination of information across strata. We summarise these facts in Section 4 and also prove a useful supplementary result: that (GB) is not only a sufficient but also a necessary condition (assuming known stratum variances) for the simple recovery of all information on every contrast from every stratum in which it is estimable. Our definition of (GB) is slightly different from Nelder's in that we accommodate unequal treatment replications, but it has all the same consequences, and the broad scope of the notion so defined is underlined by the fact that all block designs with equal block size are then generally balanced (assuming the standard dispersion model). It will be seen from our examples and the associated discussion that essentially all designs with orthogonal block structure which have ever been recommended for use satisfy (GB). It also provides a convenient basis for the classification of designs, one which is connected with the simple and directly interpretable analysis.

Section 5 below is devoted to examples, beginning with the balanced incomplete block design (BIBD) which is the prototype of all designs satisfying (GB). Instead of going on to prove directly that partially balanced incomplete block designs (PBIBDs) all satisfy (GB), we obtain the same conclusion for their natural generalisations to more general block structures. Following a brief discussion of some further examples, we close the paper with a row-column design *not* satisfying (GB).

### 2. Basic framework.

2.1. *Treatment structure.* Our data will be viewed as a random array  $y = (y_i)_{i \in \mathbf{I}}$  indexed by a set  $\mathbf{I}$  of  $n = |\mathbf{I}|$  unit labels and taking values in the vector space  $\mathcal{D} = \mathbb{R}^1$

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which has the inner product  $\langle c | d \rangle = \sum_i c_i d_i$  and squared norm  $\|c\|^2 = \langle c | c \rangle$ . The models we consider for  $\tau = \mathbb{E}y$ , termed the *treatment structure*, will all be *linear*, i.e. of the form

$$(2.1) \quad \mathbb{E}y \in \mathcal{T}$$

where  $\mathcal{T} \subseteq \mathcal{D}$  is a linear subspace of  $\mathcal{D}$ . In the theory of designed experiments this usually arises as follows: we have a set  $\mathcal{X}$  of  $v = |\mathcal{X}|$  *treatment labels*, a *design map*  $x: \mathbf{I} \rightarrow \mathcal{X}$  which assigns a treatment to each unit, and a *design matrix*  $X$  satisfying  $X(i, u) = 1$  if  $x(i) = u$ ,  $i \in \mathbf{I}$ ,  $u \in \mathcal{X}$ , and  $= 0$  otherwise. In this case  $\mathcal{T} = \mathcal{R}(X)$ , the range of  $X$ , and  $\tau = X\alpha$  for some  $\alpha \in \mathbb{R}^{\mathcal{X}}$ . However none of the general discussion which follows assumes that  $\mathcal{T}$  arises in this way. The (unweighted) orthogonal projection of  $\mathcal{D}$  onto  $\mathcal{T}$  will be denoted by  $T$ ; if  $\mathcal{T} = \mathcal{R}(X)$  then  $T = X(X'X)^{-1}X'$ .

A vector  $c = (c_i) \in \mathcal{D}$  of constants satisfying  $\sum c_i = 0$  is said to define (or be) a *contrast*; if  $c \in \mathcal{T}$ , then  $c$  defines (or is) a *treatment contrast*. This usage arises because least-squares estimation concentrates on the estimation of linear functions  $\langle t | \tau \rangle$  of  $\tau = \mathbb{E}y$  ( $t \in \mathcal{T}$ ) based upon linear functions  $\langle c | y \rangle$  of the data. Thus the term contrast refers in each case to the coefficients of these linear functions. In many analyses interest focuses on treatment contrasts  $\langle t | \tau \rangle$  defined by elements  $t$  of specific *subspaces* of  $\mathcal{T}$ ; for examples, we refer to Section 5 below. When  $\mathcal{T} = \mathcal{R}(X)$  we say that *simple* treatment contrasts are those elements  $t_{u,v} \in \mathcal{T}$  for which  $\langle t_{u,v} | \tau \rangle$  is proportional to  $\alpha_u - \alpha_v$ ,  $u, v \in \mathcal{X}$ , where  $X\alpha = \tau$ .

2.2. *Block structure.* Following Nelder (1965) we use the term *block structure* to mean the model for the dispersion matrix  $V = \mathbb{D}y$ , and all our models for  $V$  will have the form

$$(2.2) \quad \mathbb{D}y \in \mathcal{V}$$

where  $\mathcal{V}$  is a suitably parameterized set of positive semi-definite (p.s.d.) matrices. We will say that we have *orthogonal block structure* (OBS) when  $\mathcal{V}$  consists of all p.s.d. matrices  $V(\xi) = \sum_{\alpha} \xi_{\alpha} S_{\alpha}$ , where  $\xi_{\alpha} \geq 0$  for all  $\alpha$ , and the  $\{S_{\alpha}\}$  are a family of known pairwise orthogonal projectors summing to the identity matrix, i.e.  $S_{\alpha} = S'_{\alpha} = S^2_{\alpha}$ ,  $S_{\alpha} S_{\beta} = S_{\beta} S_{\alpha} = 0$  if  $\alpha \neq \beta$ , and  $\sum_{\alpha} S_{\alpha} = I$ , the identity matrix. We call this representation of  $V(\xi)$  its spectral form. In the theory of designed experiments such models usually arise in the following way: there is a system  $\{A_a\}$  of *association matrices* defined over the set  $\mathbf{I}$  of unit labels, and the dispersion matrix  $V = \mathbb{D}y$  has the form  $V = \sum_a \gamma_a A_a$  where  $\{\gamma_a\}$  is a set of *covariances* varying freely subject only to the constraints ensuring that  $V$  is p.s.d. If the matrices  $\{A_a\}$  satisfy the requirements of an *association scheme* then there always exist matrices  $P = (p_{aa})$  and  $Q = (q_{aa})$  of coefficients such that  $S_{\alpha} = (1/n) \sum_a q_{a\alpha} A_a$  satisfies the properties listed above, and  $\xi_{\alpha} = \sum_a p_{a\alpha} \gamma_a$  constitutes an invertible linear reparametrization; see MacWilliams and Sloane (1978, Chapter 21, especially Section 2) for definitions and the results cited. Once more we remark that the general results which follow do not assume that our orthogonal block structure arose in this way although in practice the vast majority (block, row-column, split-plot designs etc.) do so. For example, any model  $\mathcal{V}$  whose elements have the form  $V = \sum_j \theta_j C_j$ , where the  $\{C_j\}$  are known symmetric idempotent matrices which *commute*, will be a submodel of a model of the form (OBS) above as the  $\{C_j\}$  are simultaneously diagonalizable, but in general there will be more  $\xi$ s than  $\theta$ s.

Summarising, we will be supposing that our data  $y$  is modeled by (2.1) and (2.2) where  $\mathcal{T}$  is a linear subspace of  $\mathcal{D}$  and  $\mathcal{V}$  satisfies (OBS). The subspaces  $\mathcal{L}_{\alpha} = \mathcal{R}(S_{\alpha})$  are termed the *strata* of the dispersion model, the  $\{S_{\alpha}\}$  are *strata projectors* and the  $\{\xi_{\alpha}\}$  the *strata variances* (for it is easy to see that  $\mathbb{D}S_{\alpha}y = \xi_{\alpha} S_{\alpha}$ ). *Multi-strata designs* are those with two or more strata variances in the dispersion model.

2.3. *Examples.*

EXAMPLE 1. The data  $y$  from an experiment consisting of  $v$  treatments applied across  $b$  blocks of  $k$  plots each are usually analysed under the *mixed model*

$$(2.3) \quad y = X\alpha + Z\gamma + \varepsilon,$$

where  $X$  and  $Z$  are the  $n \times v$  and  $n \times b$  treatment and block incidence matrices, respectively,  $\alpha$  is a  $v \times 1$  vector of treatment parameters, and  $\gamma$  is a  $b \times 1$  vector of zero-mean block effects having dispersion matrix  $\sigma_b^2 I_b$ , uncorrelated with the  $n \times 1$  vector  $\varepsilon$  of errors which have dispersion matrix  $\sigma^2 I_n$ .

The dispersion matrix associated with such a model is  $V = \sigma_b^2 Z Z' + \sigma^2 I_n$ , and its spectral form is

$$(2.4) \quad V = \xi_0 G + \xi_1 (B - G) + \xi_2 (I_n - B)$$

where  $G = n^{-1} 11'$  is the grand mean averaging operator (1 is the  $n \times 1$  vector of ones),  $B = k^{-1} Z Z'$  is the block averaging operator,  $\xi_0 = \xi_1 = k\sigma_b^2 + \sigma^2$  and  $\xi_2 = \sigma^2$ . Note that here we have the constraint  $\xi_0 = \xi_1 \geq \xi_2 > 0$ .

A *randomisation model* for  $y$ , see Nelder (1954), would generate a dispersion matrix of the form (2.4).

In order to include both types of model, we will assume when analysing data from block designs with equal block size (which are the only sort we consider) that  $S_0 = G$ ,  $S_1 = B - G$  and  $S_2 = I - B$  defines our block structure satisfying (OBS). It will be simpler, and necessary for most results, to assume  $\xi_0 > 0$ ,  $\xi_1 > 0$  and  $\xi_2 > 0$  as well.  $\square$

**EXAMPLE 2.** The data  $y$  from an experiment in which  $v$  treatments are allocated to the  $n = rc$  plots of a row-column design consisting of  $r$  rows and  $c$  columns are usually analysed under the *mixed model*

$$(2.5) \quad y = X\alpha + Z_1\gamma_1 + Z_2\gamma_2 + \varepsilon$$

where  $X$ ,  $Z_1$  and  $Z_2$  are the treatment, row and column incidence matrices, respectively, and  $\gamma_1$ ,  $\gamma_2$  and  $\varepsilon$  are uncorrelated zero-mean vectors having dispersion matrices  $\sigma_r^2 I_r$ ,  $\sigma_c^2 I_c$  and  $\sigma^2 I_n$ , respectively.

This time the dispersion matrix of  $y$  is  $V = \sigma_r^2 Z_1 Z_1' + \sigma_c^2 Z_2 Z_2' + \sigma^2 I_n$  and its spectral form is

$$(2.6) \quad V = \xi_0 G + \xi_1 (R - G) + \xi_2 (C - G) + \xi_3 (1 - R - C + G)$$

where  $G = (rc)^{-1} 11'$ ,  $R = c^{-1} Z_1 Z_1'$  and  $C = r^{-1} Z_2 Z_2'$ ,  $\xi_0 = c\sigma_r^2 + r\sigma_c^2 + \sigma^2$ ,  $\xi_1 = c\sigma_r^2 + \sigma^2$ ,  $\xi_2 = r\sigma_c^2 + \sigma^2$  and  $\xi_3 = \sigma^2$ . Again we have constraints:  $\xi_1 \geq \xi_3 > 0$ ,  $\xi_2 \geq \xi_3 > 0$  and  $\xi_0 = \xi_1 + \xi_2 - \xi_3$ .

A *randomisation model* for  $y$  would also generate a dispersion matrix of the form (2.6). Accordingly we will analyse row-column designs below with  $S_0 = G$ ,  $S_1 = R - G$ ,  $S_2 = C - G$  and  $S_3 = 1 - R - C + G$ , a block structure satisfying (OBS). Again we will usually assume that  $\xi_0 > 0$ ,  $\xi_1 > 0$ ,  $\xi_2 > 0$  and  $\xi_3 > 0$ .  $\square$

**2.4. Designed experiments.** The *design* of an experiment, i.e. the actual allocation of treatments to units, affects the least-squares analysis (under our model) of the data generated through the relationships it determines between the treatment subspace  $\mathcal{T}$  and the strata subspaces  $\{S_\alpha\}$ . For example, it is known that if  $T$  commutes with all the  $\{S_\alpha\}$ , then the analysis is easy; such designs are known as *orthogonal designs*, a class which includes completely randomised, randomised block, latin square and split-plot designs. For other designs, such as the balanced incomplete block designs (BIBDs), this commutativity fails, and a more elaborate analysis is required. Nelder's (1965) notion of general balance (GB) describes a relationship between  $T$  and the  $\{S_\alpha\}$  which generalises, but in a sense is no more difficult than, that which arises with a BIBD, and as a consequence we find that essentially all designed experiments may be analysed in a manner almost identical to that of a BIBD. Note that the  $\{C_i\}$  of Nelder (1965) correspond to our  $\{S_\alpha\}$ . Before giving any further details of these ideas, we devote the next section to reviewing the

antecedents of general balance and clarifying its connections with similar notions which have appeared since 1965. See also Bailey (1981) for a related discussion.

### 3. Eigenvectors, balance and simple combinability.

3.1. *Eigenvectors of information matrices.* It has long been known in linear regression analysis that contrasts which are eigenvectors of the information matrix have special properties which make inference concerning them particularly straightforward; the analogy with principal components analysis explains why this is so. However it appears that Morley Jones (1959) was the first person to examine these ideas in some detail in the context of block experiments, and because of their relevance to general balance we will summarise his results within the framework introduced in Example 1 of the previous section.

Morley Jones analysed the data  $y$  under the "fixed block effects" model:  $\mathbb{E}y \in \mathcal{T} + \mathcal{B}$ ,  $\mathbb{D}y \in \mathcal{V}$  where  $\mathcal{B} = \mathcal{R}(B)$  and  $\mathcal{V} = \{\sigma^2 I : \sigma^2 > 0\}$ , and he concentrated upon the *intra-block analysis*, i.e. that using the reduced data  $\bar{B}y$  ( $\bar{B} = I - B$ ) consisting of the observations adjusted by their block means. Clearly  $\mathbb{E}\bar{B}y \in \bar{B}\mathcal{T}$  and  $\mathbb{D}\bar{B}y \in \bar{B}\mathcal{V}$ , and the task of minimising  $\|\bar{B}y - \bar{B}\tau\|^2$  over  $\tau \in \mathcal{T}$  is equivalent to solving the reduced normal equations ("eliminating blocks"):

$$T\bar{B}T\tau = T\bar{B}y$$

for  $\tau \in \mathcal{T}$ . In this context the eigenvectors and eigenvalues of the information matrix  $T\bar{B}T$  are likely to be of interest. (In fact Morley Jones studied a closely-related matrix with the same eigenvectors but eigenvalues one minus those of  $T\bar{B}T$ .) He made the following observations: (a) an element  $t \in \mathcal{T}$  is an eigenvector of  $T\bar{B}T$  iff there exists a constant  $k$  such that for all  $u \in \mathcal{T}$ ,  $\langle u | (B - G)t \rangle = k\langle u | \bar{B}t \rangle$ ; (b) if one of two orthogonal treatment contrasts  $t$  and  $u$  is an eigenvector of  $T\bar{B}T$ , then their inter-block components  $Bt$ ,  $Bu$  (resp. intra-block components  $\bar{B}t$ ,  $\bar{B}u$ ) are also orthogonal; (c) the best linear unbiased estimators (BLUEs) of contrasts  $\langle t | \tau \rangle$  defined by eigenvectors of  $T\bar{B}T$  are easy to compute, as are their precisions, and these are related to the corresponding eigenvalue; (d) the eigenvalues of  $T\bar{B}T$  are directly related to the Fisher *efficiency factors* describing the relative loss of information occurring by restricting attention only to the intrablock analysis; and (e) normalised contrasts defined by eigenvectors of  $T\bar{B}T$  corresponding to the same eigenvalue are estimated with the same precision; in particular, all contrasts are estimated with the same precision in BIBDs.

Although not explicitly referring to eigenvector contrasts, similar ideas can be found in Kurkjian and Zelen (1963). Their "property A" is equivalent to the spectral decomposition  $T\bar{B}T = \sum_{\beta} \lambda_{\beta} T_{\beta}$  where the  $\{T_{\beta}\}$  are the orthogonal projections decomposing  $\mathcal{T}$  into subspaces  $\{\mathcal{T}_{\beta}\}$  corresponding to main effects and interactions in a factorial experiment laid out in blocks. Their conclusions included (c) above, with the BLUE of  $\langle t_{\beta} | \tau \rangle$  based upon  $\bar{B}y$  being  $\lambda_{\beta}^{-1} \langle t_{\beta} | \bar{B}y \rangle$  for an arbitrary  $t_{\beta} \in \mathcal{T}_{\beta}$ , having variance  $\sigma^2 \lambda_{\beta}^{-1} \|t_{\beta}\|^2$ , and they observed that BLUEs of contrasts defined by elements of the different subspaces  $\{\mathcal{T}_{\beta}\}$  are uncorrelated (cf. (b) above). They also applied their results to other types of incomplete block designs including group divisible and direct product designs. A further paper, Zelen and Federer (1964) extended the same ideas to row-column designs, but still only in the context of the lowest stratum analysis, i.e. that based upon  $(I - R - C + G)y$ ; cf. Example 2 above.

In Pearce, Caliński and Marshall (1974) the eigenvectors of  $T\bar{B}T$  are called "basic contrasts", and these authors note that those with eigenvalue 1 can be estimated with full efficiency in the intra-block analysis, those with eigenvalue 0 are "totally confounded" with blocks, whilst the remainder are "partially confounded". They recommend that the spectral decomposition of  $T\bar{B}T$  be used by experimenters to ensure that the design permits contrasts of particular interest to be estimated with maximum efficiency in the intra-block analysis.

Corsten's (1976) *canonical analysis* is also equivalent to the spectral analysis of  $T\bar{B}T$ . He calls the eigenvectors (with non-zero eigenvalues) "identifiable contrasts" and views the corresponding eigenvalues as the squared cosines of the *canonical angles* between the subspaces  $\mathcal{T}$  and  $\mathcal{B}^\perp$  the orthogonal complement of  $\mathcal{B}$ ; the same geometric approach is used by James and Wilkinson (1971).

3.2. *Balance.* BIBDs were introduced by Yates (1935) as incomplete block designs with equal block sizes, equal replications, and having the combinatorial property that every pair of distinct treatments appeared together in a block the same number of times. It followed that simple treatment contrasts were all estimated with the same precision, and as a consequence, that normalised treatment contrasts were also estimated with the same precision. Thus combinatorial balance was related to the property of sets of contrasts being estimated with the same precision.

Generalised forms of these ideas appeared soon afterwards: PBIBDs were introduced by Bose and Nair (1939); designs with unequally replicated treatments having a restricted form of balance were studied by Nair and Rao (1942); designs with supplemented balance by Hoblyn, Pearce and Freeman (1954), and Pearce (1960, 1963). Morley Jones (1959) continued this line of development.

Balance in block designs was first linked to the spectral properties of the intra-block information matrix (or a closely related matrix) by V. R. Rao (1958) and Morley Jones (1959). The latter proved that a block design is balanced with respect to a set of treatment contrasts iff those contrasts span a subspace of an eigenspace of  $T\bar{B}T$ . The combinatorial aspects of balance are reviewed in Raghavarao (1971), although we will see that the approach through general balance is more relevant to the problem of analysing data from an experiment with a design exhibiting the given type of balance.

3.3. *Simple combinability.* The term *recovery of interblock information* has come to mean the double task of estimating the relevant strata variances and the calculation of weighted combinations of the inter- and intra-block estimates (where this is appropriate) of a given treatment contrast. Following earlier work with cubic lattice designs, Yates (1939), Yates (1940) showed that the overall (weighted least squares) BLUE of any treatment contrast in a BIBD was the linear combination of its BLUE calculated using the intra-block data  $(I - B)y$  and that calculated using the inter-block data  $(B - G)y$ , each weighted inversely according to its variance. We shall call this result, which assumes that the strata variances are known, the property of *simple combinability*, which is valid for *all* contrasts in a BIBD. Yates also gave a method of estimating the usually unknown strata variances from the anova table.

Conditions on a design which ensure the simple combinability in PBIBDs of certain sets of treatment contrasts were described by Spratt (1956) in a paper which gave great insight into the relation between combinability and combinatorial balance. In particular Spratt showed that the property of simple combinability holds for all contrasts in a PBIBD only if the design is actually a BIBD. This and other results along the same lines are special cases of a general theorem proved in the next section.

A link between the spectral properties of  $T\bar{B}T$  and simple combinability in an incomplete block design was established by Zyskind and Martin (1966), who showed that a treatment contrast is simply combinable iff it is an eigenvector of  $T\bar{B}T$ . Thus these three topics: the eigenspaces of  $T\bar{B}T$ , balance, in either the combinatorial sense or in the statistical sense of contrasts being estimable with the same precision, and simple combinability are all seen to be intimately related. With this introduction to general balance we now turn to its definition and study.

4. **General balance.** As we have explained in Section 2 above, our model for the data  $y = (y_i)_{i \in I}$  associated with our designed experiment is given by (2.1)  $\mathbb{E}y \in \mathcal{T}$  and (2.2)  $\text{D}y \in \mathcal{V}$ , where  $\mathcal{T} \subseteq \mathcal{D}$  is a linear subspace and  $\mathcal{V} = \{V(\xi): V(\xi) = \sum_{\alpha} \xi_{\alpha} S_{\alpha},$

$\xi_\alpha > 0$  for all  $\alpha$  is a dispersion model satisfying (OBS). General balance is a structural property relating  $\mathcal{T}$  and the strata  $\{S_\alpha\}$ .

4.1. *Definition of (GB).* We say that a design with (OBS) defined by  $\{S_\alpha\}$  and treatment structure  $\mathcal{T}$  is *generally balanced* with respect to the decomposition  $\mathcal{T} = \bigoplus_\beta \mathcal{T}_\beta$  or just generally balanced if there exists a matrix  $(\lambda_{\alpha\beta})$  of numbers such that for all  $\alpha$

$$(GB) \quad TS_\alpha T = \sum_\beta \lambda_{\alpha\beta} T_\beta,$$

where the  $\{T_\beta\}$  are the orthogonal projectors onto the subspaces  $\{\mathcal{T}_\beta\}$ . It is clear that (GB) is equivalent to the requirement that the matrices  $\{TS_\alpha T\}$  are simultaneously diagonalizable, with the  $\{\mathcal{T}_\beta\}$  as their common eigenspaces. Another equivalent form is the following: there exists numbers  $(\lambda_{\alpha\beta})$  such that for all  $\alpha, \beta$  and  $\beta'$

$$T_\beta S_\alpha T_{\beta'} = \begin{cases} \lambda_{\alpha\beta} T_\beta & \text{if } \beta = \beta', \\ 0 & \text{otherwise.} \end{cases}$$

Since the  $\{S_\alpha\}$  and  $\{T_\beta\}$  are all projectors, we must have  $0 \leq \lambda_{\alpha\beta} \leq 1$  for all  $\alpha$  and  $\beta$ , and it follows from  $\sum_\alpha S_\alpha = I$  that for all  $\beta$ ,  $\sum_\alpha \lambda_{\alpha\beta} = 1$ . A statistical interpretation of the  $\lambda_{\alpha\beta}$  as *efficiency factors* will be explained in Section 4.3 below, and we refer to Fisher (1935) for the first use of such a two-way array. *Orthogonal designs* are just those for which each  $\lambda_{\alpha\beta}$  is 0 or 1.

4.2. *Overall analysis assuming (GB): known strata variances.* It is well known that the BLUE of  $\tau = \mathbb{E}y$  based on  $y$  is given by the solution  $\tau \in \mathcal{T}$  of the normal equation

$$(NE) \quad TV^{-1}T\tau = TV^{-1}y;$$

equivalently, that it is given by  $\hat{\tau} = Uy$  where  $U = P_{\mathcal{T}}^V$  is projection of  $\mathcal{D}$  onto  $\mathcal{T}$  orthogonal with respect to the weighted inner product  $\langle c | d \rangle_V := \langle c | V^{-1}d \rangle$ . Yet one further statement of this (Gauss's) result is the following:  $\langle t | \hat{\tau} \rangle$  is the unique BLUE of  $\langle t | \tau \rangle$  for every  $t \in \mathcal{T}$ .

Now  $TV^{-1}T = \sum_\beta \nu_\beta T_\beta$  under (GB), where we write  $\nu_\beta = \sum_\alpha \lambda_{\alpha\beta} \xi_\alpha^{-1}$ , and so the unique matrix inverse of  $TV^{-1}T$  on the subspace  $\mathcal{T}$  is  $\sum_\beta \nu_\beta^{-1} T_\beta$ . Consequently the solution  $\hat{\tau} = Uy$  of (NE) is given by

$$(4.1) \quad U = \sum_{\alpha,\beta} w_{\alpha\beta} \lambda_{\alpha\beta}^{-1} T_\beta S_\alpha$$

where we have written  $w_{\alpha\beta} = \nu_\beta^{-1} \xi_\alpha^{-1} \lambda_{\alpha\beta}$ . This expression is called the *weight* for the treatment term  $\beta$  within stratum  $\alpha$ , a name which we will shortly justify. Here and later all summations involving  $\lambda_{\alpha\beta}^{-1}$  will be restricted only to those  $\alpha$  or  $\beta$  for which  $\lambda_{\alpha\beta} > 0$ .

As we have already observed, the unique BLUE of  $\langle t | \tau \rangle$  for  $t \in \mathcal{T}$  is  $\langle t | \hat{\tau} \rangle$  and by (4.1) this is just

$$(4.2) \quad \langle t | \hat{\tau} \rangle = \sum_{\alpha,\beta} w_{\alpha\beta} \lambda_{\alpha\beta}^{-1} \langle t | T_\beta S_\alpha y \rangle$$

with variance  $\sum_\beta \nu_\beta^{-1} \| T_\beta t \|^2$ . If  $t = t_\beta \in \mathcal{T}_\beta$ , the BLUE simplifies to

$$(4.3) \quad \langle t_\beta | \hat{\tau} \rangle = \sum_\alpha w_{\alpha\beta} \lambda_{\alpha\beta}^{-1} \langle t_\beta | S_\alpha y \rangle$$

with variance  $\nu_\beta^{-1} \| t_\beta \|^2$ .

Finally, the *covariance* between two BLUEs  $\langle t_1 | \hat{\tau} \rangle$  and  $\langle t_2 | \hat{\tau} \rangle$  is just

$$\sum_\beta \nu_\beta^{-1} \langle T_\beta t_1 | T_\beta t_2 \rangle,$$

and if  $t_1 \in \mathcal{T}_\beta, t_2 \in \mathcal{T}_{\beta'}, \beta \neq \beta'$ , this reduces to zero.

It is clear from the above that as long as the strata variances are known (up to a common scalar multiplier) and we can readily effect the projections  $\{S_\alpha\}$  and  $\{T_\beta\}$ , the

weighted least squares analysis of data from a designed experiment with generally balanced block structure is particularly simple. We will deal with the problem of unknown strata variances in the next subsection and in Section 4.5 below. On the issue of the ease of calculation and computation of the projections we can say this: the  $\{S_\alpha\}$  are commonly built up from simple averaging operators such as  $G$  and  $B$  in Example 1 or  $R$ ,  $C$  and  $G$  in Example 2 above, and rarely give any difficulties. The common decompositions  $\{T_\beta\}$  relative to which designed experiments satisfy (GB) are also of this form, although there are some that are quite different, and in general the problem is not: "how do we compute the projections  $\{T_\beta\}$ ?" but: "how do we discover them?" This is essentially a combinatorial problem, which needs to be done for each new design or class of designs. The usual mathematical skills (trial and error, ingenuity, etc.) help, as does the occasional computer-aided spectral analysis, and it is only the broader classes of block designs for which general solutions are unavailable; see Section 5.4.

4.3. *Within strata analysis assuming (GB).* A reduction of the full data  $y$  to its strata projections  $S_\alpha y$  permits analyses *within strata* without knowledge of the strata variances, for  $\mathbb{E}S_\alpha y \in S_\alpha \mathcal{T}$  and  $\mathbb{D}S_\alpha y = \xi_\alpha S_\alpha$ ; in particular, the dispersion matrix of  $S_\alpha y$  is known up to a scalar, and this is adequate for the usual least-squares analyses.

The least-squares *fitted value*  $\hat{y}_\alpha$  of  $y$  in stratum  $\alpha$  is  $\hat{y}_\alpha = P_{S_\alpha \mathcal{T}} y$ , the unweighted projection of  $y$  onto  $S_\alpha \mathcal{T}$ , unweighted because the subspace  $S_\alpha \mathcal{T}$  is invariant under  $\mathbb{D}S_\alpha y$  whence unweighted and weighted projectors coincide. The normal equation within  $\mathcal{S}_\alpha$  is

$$(NE_\alpha) \quad TS_\alpha T\tau = TS_\alpha y$$

and its solution  $\hat{\tau}_\alpha = U_\alpha y$  is given by (cf. Nelder (1965) equation 3.3)

$$(4.4) \quad U_\alpha y = \sum_\beta \lambda_{\alpha\beta}^{-1} T_\beta S_\alpha y$$

where the sum is only over those  $\beta$  for which  $\lambda_{\alpha\beta} > 0$ . We can readily prove that  $P_{S_\alpha \mathcal{T}} = S_\alpha U_\alpha$ . It follows from (4.4) that the unique BLUE of a contrast  $\langle t | \tau \rangle$  which is estimable in  $\mathcal{S}_\alpha$  (i.e. for which there exists a BLUE based on  $S_\alpha y$ ) is

$$(4.5) \quad \langle t | \hat{\tau}_\alpha \rangle = \sum_\beta \lambda_{\alpha\beta}^{-1} \langle T_\beta t | S_\alpha y \rangle$$

with variance  $\xi_\alpha \sum_\beta \lambda_{\alpha\beta}^{-1} \|T_\beta t\|^2$ . If  $t = t_\beta \in \mathcal{T}_\beta$  the BLUE simplifies to

$$(4.6) \quad \langle t_\beta | \hat{\tau}_\alpha \rangle = \lambda_{\alpha\beta}^{-1} \langle t_\beta | S_\alpha y \rangle \quad (\text{provided } \lambda_{\alpha\beta} > 0)$$

with variance  $\lambda_{\alpha\beta}^{-1} \xi_\alpha \|t_\beta\|^2$ , and if  $\lambda_{\alpha\beta} = 0$  then *no* contrast  $\langle t_\beta | \tau \rangle$  is estimable in  $\mathcal{S}_\alpha$ . Finally, we remark that the covariance between two BLUEs  $\langle t_1 | \hat{\tau}_\alpha \rangle$  and  $\langle t_2 | \hat{\tau}_\alpha \rangle$  is  $\xi_\alpha \sum_\beta \lambda_{\alpha\beta}^{-1} \langle T_\beta t_1 | T_\beta t_2 \rangle$  and if  $t_1 \in \mathcal{T}_\beta$ ,  $t_2 \in \mathcal{T}_{\beta'}$ ,  $\beta \neq \beta'$ , this again reduces to zero.

There are a number of points in the formulae above and in the corresponding ones in the previous sub-section which are worth noting. First, it is clear from both (4.6) and (4.3) that estimation *is* especially simple for contrasts which are eigenvectors of *all* the information matrices  $TS_\alpha T$ , cf. Section 3.1 point (c). Secondly, BLUEs of contrasts from distinct (common) eigenspaces of the  $TS_\alpha T$  are orthogonal, cf. Section 3.1 point (b), and so the BLUEs of contrasts  $\langle t | \tau \rangle$  for arbitrary  $t \in \mathcal{T}$  are sums of the uncorrelated BLUEs of  $\langle T_\beta t | \tau \rangle$  which have the simple form. And finally, the overall BLUE (4.3) of  $\langle t_\beta | \tau \rangle$  for  $t_\beta \in \mathcal{T}_\beta$  is quite clearly the simple combination of its BLUEs (4.6) in each stratum in which it is estimable, each weighted inversely according to its variance:  $\langle t_\beta | \hat{\tau} \rangle = \sum_\alpha w_{\alpha\beta} \langle t_\beta | \hat{\tau}_\alpha \rangle$ . This justifies our use of the term *weight* for  $w_{\alpha\beta}$  introduced following equation (4.1). Similarly we can compare the variance of  $\langle t_\beta | \hat{\tau}_\alpha \rangle$  to that of  $\langle t_\beta | \hat{\tau} \rangle$  when the  $\xi_\alpha$  are assumed equal, and see why  $\lambda_{\alpha\beta}$  is termed the *efficiency factor* for treatment term  $\beta$  in stratum  $\alpha$ , cf. point (d) in Section 3.1.

In a sense there is no single analysis of variance table which summarises all aspects of the least-squares analysis of a designed experiment satisfying (GB), but rather one for each stratum and one overall. See Table 1, the anova table within stratum  $\alpha$ . Examples of

TABLE 1  
Anova table within stratum  $\alpha$

Source	d.f.	Sum of squares	$\mathbb{E}\{\text{Mean square}\}$
$\vdots$	$\vdots$	$\vdots$	$\vdots$
Treatment term $\mathcal{T}_\beta$ (assuming $\lambda_{\alpha\beta} > 0$ )	$\dim \mathcal{T}_\beta$	$\lambda_{\alpha\beta}^{-1} \ T_\beta S_\alpha y\ ^2$	$\xi_\alpha + \frac{\lambda_{\alpha\beta}}{\dim \mathcal{T}_\beta} \ T_\beta \tau\ ^2$
$\vdots$	$\vdots$	$\vdots$	$\vdots$
Residual	$d_\alpha$ : By difference $\uparrow$ may be zero	By difference $\uparrow$	$\xi_\alpha$ (if $d_\alpha > 0$ )
Total	$\dim \mathcal{S}_\alpha$	$\ S_\alpha y\ ^2$	

designs with residual degrees of freedom  $d_\alpha = 0$  in some strata are quite common, e.g. symmetric BIBDs, double, triple, ... lattice designs, rectangular lattice designs all have zero residual d.f. in the inter-block stratum, and the best general way to estimate  $\xi_\alpha$  is certainly not via the anova table for stratum  $\alpha$ . For further comments on the estimation of  $\xi_\alpha$ , see Section 4.5 below.

4.4. *Simple combinability: a converse to (GB).* We now prove a result asserting that under certain general circumstances, if a set of contrasts spanning  $\mathcal{T}$  is simply combinable, then the design satisfies (GB). The following lemma has its straightforward proof omitted. Our framework is that of Section 2.4 without assuming (GB).

LEMMA. *If the treatment contrast  $\langle t | \tau \rangle$  is estimable in stratum  $\alpha$ , then there exists a unique  $c_\alpha = c_\alpha(t) \in \mathcal{R}(S_\alpha T)$  such that  $Tc_\alpha = t$ . Furthermore, the unique BLUE of  $\langle t | \tau \rangle$  based on  $S_\alpha y$  is then  $\langle c_\alpha | y \rangle$ .  $\square$*

PROPOSITION 4.1. *Let  $\langle t | \tau \rangle$  be a treatment contrast such that for each stratum  $\mathcal{S}_\alpha$  it is either estimable in or orthogonal to  $\mathcal{S}_\alpha$ , and suppose that there is a set  $\{w_\alpha\}$  of non-negative weights summing to unity such that*

$$(4.7) \quad \langle t | \hat{\tau} \rangle = \sum_\alpha w_\alpha \langle c_\alpha | y \rangle, \quad (y \in \mathcal{D})$$

where  $\langle c_\alpha | y \rangle$  is the BLUE of  $\langle t | \tau \rangle$  based on  $S_\alpha y$ , if  $\langle t | \tau \rangle$  is estimable in  $\mathcal{S}_\alpha$ , and  $w_\alpha = 0$  if  $t$  is orthogonal to  $\mathcal{S}_\alpha$ . Then for all  $\alpha$ ,  $t$  is an eigenvector of  $TS_\alpha T$  with eigenvalue  $\lambda_\alpha = \xi_\alpha w_\alpha (\sum_\alpha \xi_\alpha w_\alpha)^{-1}$ .

PROOF. It is not hard to prove that the transpose  $U'$  of  $U = P_{\mathcal{V}_\tau}^V$  coincides with  $V^{-1}UV$ . It follows from equation (4.7) that  $V^{-1}UVt = \sum_\alpha w_\alpha c_\alpha$  and so

$$(4.8) \quad UVt = (\sum_\alpha \xi_\alpha S_\alpha)(\sum_\alpha w_\alpha c_\alpha) = \sum_\alpha \xi_\alpha w_\alpha c_\alpha.$$

Now  $TU = U$  and since  $Tc_\alpha = t$  for all  $\alpha$ , (4.8) implies

$$(4.9) \quad UVt = (\sum_\alpha \xi_\alpha w_\alpha)t.$$

On the other hand, (4.8) also implies that  $S_\alpha UVt = \xi_\alpha w_\alpha c_\alpha$ , and so

$$(4.10) \quad TS_\alpha UVt = \xi_\alpha w_\alpha t.$$

The conclusion now follows from (4.9) and (4.10).  $\square$

Now let us suppose that the subspace  $\mathcal{T}$  has a basis consisting of vectors  $t$  satisfying



the hypotheses of Proposition 4.1. Then for each such  $t$  there is a set  $\{\lambda_{\alpha t}\}$  eigenvalues, and we can obtain a pairwise orthogonal system  $\{\mathcal{T}_\beta\}$  of subspaces of  $\mathcal{T}$  by grouping together all  $t$ s with a common set of eigenvalues, say  $\{\lambda_{\alpha\beta}\}$  for each  $t \in \mathcal{T}_\beta$ . It is clear that the system  $\{\mathcal{T}_\beta\}$  forms a complete set of eigenspaces common to all the matrices  $\{TS_\alpha T\}$  and also that  $\mathcal{T} = \bigoplus_\beta \mathcal{T}_\beta$ . Thus we can obtain the following converse to (GB) implying equation (4.1).

**PROPOSITION 4.2.** *If there exists an orthogonal decomposition  $\mathcal{T} = \bigoplus_\beta \mathcal{T}_\beta$  of  $\mathcal{T}$  and a set  $\{w_{\alpha\beta}^*\}$  of weights such that for all  $V \in \mathcal{V}$  the projection  $U$  onto  $\mathcal{T}$  orthogonal with respect to  $\langle \cdot | \cdot \rangle_V$  is  $U = \sum_{\alpha,\beta} w_{\alpha\beta}^* T_\beta S_\alpha$ , where  $w_{\alpha\beta}^* \xi_\alpha$  is independent of  $\alpha$ , then the design satisfies (GB) with respect to  $\{\mathcal{T}_\beta\}$ .  $\square$*

The proof will be omitted; it can be found in Houtman (1980). A stronger result can be obtained when there are only two effective strata, i.e.  $\mathcal{V}$  is spanned by  $S_0 = G, S_1, S_2$ ; for this case the hypothesis “for all  $V \in \mathcal{V}$ ” in Proposition 4.2 is not required, as one suitable  $V$  leads to the same conclusion.

4.5. *The estimation of strata variances under (GB).* We remarked in Section 4.3 above that the residual operator  $R_\alpha = S_\alpha - P_{S_\alpha \mathcal{T}}$  in stratum  $\alpha$  may be zero, equivalently, that  $d_\alpha = \text{tr } R_\alpha = \dim \mathcal{L}_\alpha - \sum \{\dim \mathcal{T}_\beta : \lambda_{\alpha\beta} > 0\}$  may be zero. The reason for this is not hard to see: if  $0 < \lambda_{\alpha\beta} < 1$ , then treatment term  $T_\beta \tau$  is being fitted and its full d.f.  $\dim \mathcal{T}_\beta$  removed not only in stratum  $\alpha$ , but also in one or more other strata in which it is estimable. In a sense we should only remove that fraction  $w_{\alpha\beta}(\dim \mathcal{T}_\beta)$  of the d.f. corresponding to the amount of information on  $\mathcal{T}_\beta$  in  $\mathcal{L}_\alpha$  and the approach of Nelder (1968) amounts to just this.

More precisely, Nelder’s approach is based upon equating the observed with expected mean square of the *actual* residual  $S_\alpha(I - U)y = S_\alpha \bar{U}y$  in stratum  $\alpha$  rather than doing so with the *apparent* residual  $R_\alpha y$  as is done if only the anova table is consulted. To illustrate the difference between the two we cite the following without proof:

- LEMMA** (i)  $\|S_\alpha \bar{U}y\|^2 = \|R_\alpha y\|^2 + \|(P_{S_\alpha \mathcal{T}} - S_\alpha U)y\|^2$ .  
 (ii)  $d'_\alpha = \text{tr}(S_\alpha \bar{U}) = d_\alpha + \sum_\beta (1 - w_{\alpha\beta}) \dim \mathcal{T}_\beta$ .  
 (iii) *When every treatment term is estimated in one of two strata,  $\alpha$  and  $\alpha'$  say, then*

$$\|(P_{S_{\alpha'} \mathcal{T}} - S_\alpha U)y\|^2 = \sum_\beta w_{\alpha'\beta} \lambda_{\alpha\beta} \|\Delta_\beta y\|^2$$

where  $\Delta_\beta y = \lambda_{\alpha\beta}^{-1} T_\beta S_\alpha y - \lambda_{\alpha'\beta}^{-1} T_\beta S_{\alpha'} y$  is the difference between the estimates of treatment term  $\beta$  in the two strata, and a similar equation holds with the roles of  $\alpha$  and  $\alpha'$  reversed.  $\square$

Now both  $U$  and  $d'_\alpha$  involve the weights  $\{w_{\alpha\beta}\}$  so if we are to make use of the identity  $\mathbb{E} \|S_\alpha \bar{U}y\|^2 = d'_\alpha \xi_\alpha$  in estimating  $\xi_\alpha$ , an *iterative* approach must be used. We proceed as follows:

(0) Begin with initial estimates  $\{\xi_\alpha^{(0)}\}$  or  $\{w_{\alpha\beta}^{(0)}\}$  of the strata variances or weights, possibly making use of the strata anova tables;

(1) Given a set  $\{\xi_\alpha\}$  and  $\{w_{\alpha\beta}\}$  of *working* estimates of the strata variances and weights, calculate  $U$  and  $d'_\alpha$  and obtain *revised* estimates  $\{\xi_\alpha^*\}$  by solving for  $\{\xi_\alpha\}$  in

$$(4.11) \quad \|S_\alpha \bar{U}y\|^2 = \xi_\alpha d'_\alpha, \quad \alpha = 0, 1, \dots$$

It is interesting to note that equation (4.11) is in fact the likelihood equation for  $\{\xi_\alpha\}$  based upon  $\|(I - T)y\|^2$  under the assumption that  $y$  has a multivariate normal distribution, see Patterson and Thompson (1971) for details. The information matrix corre-

sponding to these *restricted ML estimates*  $\{\hat{\xi}_\alpha\}$  under normality has elements

$$-2\mathbb{E}\left\{\frac{\partial^2 \log l}{\partial \xi_\alpha \partial \xi_{\alpha'}}\right\} = \frac{1}{\xi_\alpha \xi_{\alpha'}} \times \begin{cases} [d_\alpha + \sum_\beta (1 - w_{\alpha\beta})^2 (\dim \mathcal{T}_\beta)] & \text{if } \alpha = \alpha' \\ [\sum_\beta w_{\alpha\beta} w_{\alpha'\beta} (\dim \mathcal{T}_\beta)] & \text{if } \alpha \neq \alpha' \end{cases}$$

where the sums are over all  $\beta$  for which  $\lambda_{\alpha\beta}$  (or  $\lambda_{\alpha'\beta}$ )  $> 0$ .

**4.6. Inferential difficulties under (GB).** Even when a designed experiment with orthogonal block structure defined by the strata  $\{\mathcal{S}_\alpha\}$  and treatment structure  $\{\mathcal{T}_\beta\}$  satisfies (GB), there remain difficulties with estimation and testing the model.

Although the formula (4.1) gives a precise expression for  $\hat{\tau}$  when the strata variances  $\{\xi_\alpha\}$  are *known*, these considerations no longer apply when we use the estimates  $\{\hat{\xi}_\alpha\}$  obtained as in Section 4.5. The general problem of combining information on a common mean when the weights require estimation has a large literature; see Brown and Cohen (1974) for a general discussion and further references. In some of these papers the problem of combining information on treatment contrasts in BIBDs is considered and it would be of interest to extend these conclusions to multi-strata designs with a number of treatment terms.

A second difficulty arises when the analyst wishes to test the hypothesis  $T_\beta \tau = 0$  for some  $\beta$ , say under a normality assumption. This can be done by an  $F$ -test in every stratum  $\alpha$  for which  $\lambda_{\alpha\beta} > 0$  and the stratum residual d.f.  $d_\alpha > 0$ , and although such tests would be *independent*, there appears to be no accepted procedure for combining the tests into a single one. On the other hand, an overall test might be sought, fitting to  $\mathcal{T}$  first and then to the orthogonal complement  $\mathcal{T} \ominus \mathcal{T}_\beta$ , of  $\mathcal{T}_\beta$  in  $\mathcal{T}$  which still satisfies (GB). The problem here is the fact that the likelihood ratio test for such hypotheses does not appear to have been studied when information concerning  $\mathcal{T}_\beta$  resides in more than one stratum.

Both of these problems would seem to warrant further research. Until straightforward exact or approximate solutions are found, most analysts will follow Yates (1940) and others in substituting the estimated weights into (4.1), and testing hypotheses  $T_\beta \tau = 0$  in the stratum  $\alpha$  for which  $\lambda_{\alpha\beta}$  is largest.

## 5. Examples.

**5.1. BIBDs.** The basic notation for block designs was introduced in Section 2.3:  $b$  blocks of  $k$  plots each, and the term *balanced* means that the  $v \geq k$  different treatments are applied to the plots in such a way that each pair of distinct treatments appears together in a block the same number of times,  $\lambda$  say. The strata projections are  $G$ ,  $B - G$  and  $I - B$ , all derived from simple averaging operators, whilst the treatment decomposition  $T = G + (T - G)$  is similarly straightforward. We readily find that

$$(5.1) \quad TGT = G, \quad T(B - G)T = \bar{e}(T - G), \quad T(I - B)T = e(T - G)$$

where  $e = (1 - k^{-1})/(1 - v^{-1}) = 1 - \bar{e}$  is the *efficiency factor* of the design; Yates (1936). The computation which establishes the (GB) conditions most easily is the checking that  $(T - G)B(T - G) = \bar{e}(T - G)$  by applying  $(T - G)B$  to a simple contrast  $t_{u,v}$ ; in this form it is nothing more than checking the balance condition.

The overall BLUE of a treatment contrast  $\langle t | \tau \rangle$  is given by  $\langle t | \hat{\tau} \rangle = \xi_1^{-1}(\bar{e}\xi_1^{-1} + e\xi_2^{-1})^{-1} \langle t | (B - G)y \rangle + \xi_2^{-1}(\bar{e}\xi_1^{-1} + e\xi_2^{-1})^{-1} \langle t | (I - B)y \rangle$ , the correctly weighted linear combination of the inter- and intra-block BLUEs  $\bar{e}^{-1} \langle t | (B - G)y \rangle$ , and  $e^{-1} \langle t | (I - B)y \rangle$ , respectively.

When we turn to the estimation of  $\xi_1$  and  $\xi_2$ , we note that the residual d.f.  $d_1 = (b - 1) - (v - 1)$  in the inter-block stratum is usually small and is zero if  $v = b$ . Nelder's iterative method or its Fisher scoring variant can be used with initial values  $\xi_1^{(0)} = \xi_2^{(0)} = d_2^{-1} \|R_2 y\|^2$  on  $d_2 = b(k - 1) - (v - 1)$  d.f. from the intra-block stratum. The only quantities needed

for this calculation are the residual arrays

$$R_1y = (B - G)y - \bar{e}^{-1}(B - G)T(B - G)y$$

$$R_2y = \bar{B}y - e^{-1}\bar{B}T\bar{E}y$$

and the array of differences of effects estimated in the two strata:

$$\Delta_1y = \bar{e}^{-1}T(B - G)y - e^{-1}T\bar{E}y.$$

The procedure generally converges quickly, and gives estimates which are close, although not identical, to those given by Yates' (1940) method based on anova tables, and the statistical properties of these estimates appear (by simulations) to be very similar to those of Yates' estimates.

5.2. *A natural generalisation of PBIBDs.* PBIBDs were introduced by Bose and Nair (1939) as generalisations of BIBDs and have been the subject of much study since then, mostly devoted to combinatorial aspects of the designs because the combinatorial objects now known as *association schemes* were first defined in this context, see MacWilliams and Sloane (1978) and Raghavarao (1971). The standard reference on the *analysis* of PBIBDs seems to be Clatworthy (1973). The idea behind PBIBDs is quite simple: where it is not possible for every pair of distinct treatment to be together in a block the same number  $\lambda$  of times, the pairs are partitioned into *association classes* forming an association scheme so that this can hold within classes, and the single number  $\lambda$  is replaced by a family  $\lambda_1, \lambda_2, \dots$  of numbers, one for each association class. Our generalisation carries this idea over to more general block structures than just blocks and plots such as nested BIBDs; Preece (1967).

Let us suppose that the orthogonal block structure of our design arises from a dispersion model based upon an association scheme  $\{A_\alpha\}$  over the set  $I$  of unit labels as described in Section 2.2. That is, the strata projections  $\{S_\alpha\}$  are given by  $S_\alpha = (1/n) \sum_a q_{a\alpha}A_a$  where  $Q = (q_{a\alpha})$  is a matrix of structure constants. The association matrices  $\{A_\alpha\}$  are defined in terms of the strata projections by  $A_\alpha = \sum_a p_{a\alpha}S_a$  where  $P = (p_{a\alpha})$  is the "inverse" matrix of constants:  $PQ = QP = nI$ .

Similarly we suppose—as is customary with PBIBDs—that there is an association scheme  $\{\tilde{B}_b\}$  defined over the set  $\mathcal{X}$  of treatment labels, see Section 2.2, with corresponding orthogonal projectors  $\{\tilde{T}_\beta\}$  given by  $\tilde{T}_\beta = (1/v) \sum_b \tilde{q}_{b\beta}\tilde{B}_b$ , where  $\tilde{Q} = (\tilde{q}_{b\beta})$  and  $\tilde{P} = (\tilde{p}_{\beta b})$  are the appropriate matrices of structure constants.

DEFINITION. A design map  $x:I \rightarrow \mathcal{X}$  is said to be  $(\{A_a\}, \{\tilde{B}_b\})$ -balanced if for all association classes  $a$  over  $I$  and  $b$  over  $\mathcal{X}$  and  $u_1, u_2 \in \mathcal{X}$  with  $\tilde{B}_b(u_1, u_2) = 1$ , the number  $|\{(i, j) \in I \times I : A_a(i, j) = 1, x(i) = u_1, x(j) = u_2\}|$  depends only on  $b$  and not on the pair  $u_1, u_2$  chosen. If we denote the number (of concurrences) in this definition by  $n_{ab}$  then, recalling the design matrix  $X$  introduced in Section 2.1 above, we see that an equivalent form of the definition is: there exists numbers  $n_{ab}$  such that for all  $a$  we have

$$(5.2) \quad X'A_aX = \sum_b n_{ab}B_b.$$

In particular if we consider  $A_e$  and  $\tilde{B}_e$  where  $e$  represents the identity association, we find that  $n_{ee} = r$  defines the common replication number for the treatments of our design.

PROPOSITION 5.1. *An experiment with block structure arising from an association scheme  $\{A_a\}$  over the set  $I$  of units, and having a design map which is  $(\{A_a\}, \{\tilde{B}_b\})$ -balanced with respect to an association scheme  $\{\tilde{B}_b\}$  over the set  $\mathcal{X}$  of treatments, satisfies (GB). In notation introduced above, the treatment decomposition is given by  $\{T_\beta\}$  where  $T_\beta =$*

$r^{-1}X\tilde{T}_\beta X'$ , and the matrix  $\Lambda = (\lambda_{\alpha\beta})$  of efficiency factors is given by

$$\lambda_{\alpha\beta} = (rn)^{-1} \sum_a \sum_b q_{a\alpha} n_{ab} \tilde{p}_{\beta b}$$

where  $\mathbf{n} = (n_{ab})$  is the matrix of concurrences.

**PROOF.** We begin by noting that  $T = r^{-1}XX'$ . Then for all  $\alpha$

$$\begin{aligned} TS_\alpha T &= n^{-1} \sum_a q_{a\alpha} T A_a T && \text{(definition of } S_\alpha) \\ &= (r^2 n)^{-1} \sum_a q_{a\alpha} X(X' A_a X) X' && \text{(definition of } T) \\ &= (r^2 n)^{-1} \sum_a \sum_b q_{a\alpha} n_{ab} X \hat{B}_b X' && \text{(by (5.2))} \\ &= (r^2 n)^{-1} \sum_a \sum_b \sum_\beta q_{a\alpha} n_{ab} \tilde{p}_{\beta b} X \tilde{T}_\beta X' && \text{(definition of } \tilde{T}_\beta) \\ &= \sum_\beta \{(rn)^{-1} \sum_a \sum_b q_{a\alpha} n_{ab} \tilde{p}_{\beta b}\} T_\beta && \text{(definition of } T_\beta) \end{aligned}$$

and the assertion is proved.  $\square$

**EXAMPLE 1.** It is not hard to see that a BIBD is built over an association scheme on its units with associations which can be labeled  $e$  (equality), 1 (same block but different unit) and 2 (different block), whilst its treatments have the trivial association scheme with associations  $e$  (equality) and 1 (inequality). We readily find that  $(rn)^{-1}Q' \mathbf{n} \tilde{P}'$  takes the form

$$(rn)^{-1} \begin{bmatrix} 1 & 1 & 1 \\ b-1 & b-1 & -1 \\ b(k-1) & -b & 0 \end{bmatrix} \begin{bmatrix} r & 0 \\ 0 & \lambda \\ r(r-1) & r^2 - \lambda \end{bmatrix} \begin{bmatrix} 1 & 1 \\ v-1 & -1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 - e \\ 0 & e \end{bmatrix}$$

making use of the relations  $r(k-1) = \lambda(v-1)$  and  $rv = bk = n$ .

**EXAMPLE 2.** Kshirsagar (1957) gave the very interesting  $6 \times 6$  row-column design with 9 treatments A, B, C, D, E, F, G, H, I shown in Table 2. Let us consider the association scheme defined on the treatments by imposing a row-column *pseudo-structure* on them as shown in Table 3. If we let  $e, 1, 2$  and  $3$  denote the associations of equality, same row (but unequal), same column (but unequal) and different row and column for both schemes, then we have what is shown in Table 4, with a similar result holding for  $X' A_3 X$  by differencing, since  $A_1 + A_2 + A_3 = J - I$ , where  $J$  is the matrix of all 1s. These clearly satisfy our balance condition with matrix  $\mathbf{n} = (n_{ab})$  of concurrences, shown in Table 5. With these preliminaries we can readily get  $\tilde{P}$  and  $Q$  and calculate the matrix  $\Lambda = (\lambda_{\alpha\beta})$  of efficiency factors; this turns out to be as given in Table 6.

For many further such designs see Preece (1968, 1976) and Cheng (1981a, b).

TABLE 2  
Treatment allocation to 36 units with a  
 $6 \times 6$  row-column block structure

B	D	H	G	F	C
C	E	G	B	D	I
E	F	C	A	G	H
D	I	A	H	C	E
F	G	I	E	A	B
A	H	B	D	I	F

TABLE 3  
 $3 \times 3$  row-column pseudostructure  
on 9 treatments

A	B	C
D	E	F
G	H	I

TABLE 4

		A	B	C	D	E	F	G	H	I			
$X'A_1X =$	[	0	2	2	2	3	3	2	3	3	]	A	
			0	2	3	2	3	3	2	3		B	
				0	3	3	2	3	3	2		C	
					0	2	2	2	3	3		D	
						0	2	3	2	3		E	
		by symmetry						0	3	3		2	F
									0	2		2	G
										0		2	H
												0	I
		A	B	C	D	E	F	G	H	I			
$X'A_2X =$	[	0	3	3	3	2	2	3	2	2	]	A	
			0	3	2	3	2	2	3	2		B	
				0	2	2	3	2	2	3		C	
					0	3	3	3	2	2		D	
						0	3	2	3	2		E	
		by symmetry						0	2	2		3	F
									0	3		3	G
										0		3	H
												0	I

TABLE 5

		e	1	2	3		
$n =$	[	4	0	0	0	]	e
		0	2	2	3		1
		0	3	3	2		2
		12	11	11	11		3

TABLE 6

<i>Treatment pseudo-factor</i>	gm	r	c	r · c				
$\Lambda =$	[	1	0	0	0	]	Grand mean	
		0	1/8	1/8	0		Rows	<i>Block stratum</i>
		0	0	0	1/8		Columns	
		0	1/8	1/8	1/8		Rows · Columns	

5.3. *Supplemented balance and related notions.* Pearce (1960) described a class of block designs possessing what he termed *supplemented balance*, and later Pearce (1963) extended the notion to row-column and more general designs. A typical example is a BIBD consisting of  $b$  blocks of  $k$  plots each and a standard balanced allocation of  $v$  treatments, which is supplemented by the addition of an extra plot to each block to which a *control* is applied. The resulting block design has  $b$  blocks each of  $k + 1$  plots and  $v + 1$  "treatments", but is readily found to satisfy (GB) for the "treatment" decomposition

$$(5.3) \quad \mathcal{T} = \mathcal{S} \oplus \mathcal{T}_* \oplus \mathcal{T}_c$$

where  $\mathcal{S} = \mathcal{R}(G)$ ,  $\mathcal{T}_*$  is the  $(v - 1)$ -dimensional space of contrasts amongst the  $v$  original treatments, and  $\mathcal{T}_c$  is the 1-dimensional subspace spanned by the contrast comparing the control to the average of the original treatments. This contrast is estimated with efficiency 1 in the intra-block stratum, whilst the contrasts in  $\mathcal{T}_*$  are estimated intra-block with

efficiency  $e^*$  where  $1 - e^* = k(k + 1)^{-1}(1 - e)$ ,  $e$  being the efficiency factor of the original BIBD.

A similar analysis holds for block designs which only satisfy (GB) with more complicated treatment decompositions, and also for row-column and other designs with supplemented balance: in these cases  $\mathcal{T}_*$  is replaced by the direct sum of the terms relative to which the original (unsupplemented) design satisfied (GB).

Pearce's block designs with supplemented balance are a special case of a class of block designs introduced by Nair and Rao (1942), which are themselves a variant on those described in the previous sub-section. They are analogous to PBIBDs with group-divisible association schemes defined on the treatments, but do not necessarily have equal group sizes, in which case they do not define an association scheme. Despite this fact, even when the group sizes are unequal the line of argument used in Proposition 5.1 carries over. We illustrate the results with the case of two groups, as discussed in Nair and Rao (1942), supposing that there are  $v_1$  "rare" treatments each replicated  $r_1$  times, and  $v_2$  "frequent" treatments each replicated  $r_2$  times. Each pair of "rare" (resp. "frequent") treatments occurs together in the same block  $n_{11}$  (resp.  $n_{22}$ ) times, whilst pairs of treatments one of which is "rare" and the other "frequent" occur together in a block  $n_{12} = n_{21}$  times. It is easy to establish that such designs are balanced with respect to the treatment decomposition

$$\mathcal{T} = \mathcal{G} \oplus \mathcal{T}_1 \oplus \mathcal{T}_2 \oplus \mathcal{T}_c$$

where  $\mathcal{T}_1$  (resp.  $\mathcal{T}_2$ ) is the space of dimension  $n_1 - 1$  (resp.  $n_2 - 1$ ) spanned by contrasts between the "rare" (resp. "frequent") treatments, and  $\mathcal{T}_c$  is spanned by the single d.f. contrast comparing the average of the "rare" treatments with the average of the "frequent" treatments. The array of efficiency factors is shown in Table 7.

5.4. *Designs satisfying (GB).* Nelder (1965) observed that most of the common designs in use satisfied his definition of general balance. With our extension (GB) to designs in which treatments are not necessarily equally replicated, we can go further and assert that *all* block designs (with equal block sizes, and the usual dispersion model) satisfy (GB), since it is quite obvious that  $TGT$ ,  $T(B - G)T$  and  $T(I - B)T$  all commute. All row and column designs which we have seen in the literature satisfy (GB), see Kshirsagar (1957), Pearce (1963, 1975), Zelen and Federer (1964a) for examples, and so also do all designs known to us with orthogonal block structure having three or more strata.

Knowing that a block design must satisfy (GB) is one thing; having explicit expressions for the orthogonal projections  $\{T_\beta\}$  is quite another matter. There are a very large number of types of PBIBDs, and although it is generally not difficult to describe the structure of their Bose-Mesner algebra, see MacWilliams and Sloane (1978, Chapter 21), and hence obtain the  $\{T_\beta\}$ , most writers in statistics have not taken this viewpoint. Corsten (1976) is an exception.

For classes of block designs which are not PBIBDs, other methods must be used; the details concerning rectangular lattice designs, linked block and a number of other classes

TABLE 7

Treatment term:	gm	1	2	c	Stratum:
	1	0	0	0	grand mean
$\Lambda =$	0	$\frac{r_1 - n_{11}}{kr_1}$	$\frac{r_2 - n_{22}}{kr_2}$	$\frac{r_1 r_2 - bn_{12}}{r_1 r_2}$	blocks
	0	$\frac{r_1(k - 1) + n_{11}}{kr_1}$	$\frac{r_2(k - 1) + n_{22}}{kr_2}$	$\frac{bn_{12}}{r_1 r_2}$	plots

are available on request. Recently the class of  $\alpha$ -designs was introduced, Patterson and Williams (1976), these being obtained in a particularly simple way from a basic generating array. This class seems to be so large, including BIBDs, PBIBDs, square and rectangular lattice designs as well as many others, that it does not seem to be possible to give a general description of the subspaces  $\{\mathcal{T}_\beta\}$  relative to which the designs satisfy (GB). However this should be regarded as a challenging unsolved problem.

#### 5.5. Designs not satisfying (GB).

*A black sheep.* Although all block designs satisfy (GB) this is not necessarily the case for row-column designs as the following  $4 \times 4$  example with four equally-replicated treatments is shown in Table 8. To see that (GB) fails, one simply notes that the contrast which compares treatment 1 with the average of treatments 2, 3 and 4 is an eigenvector of  $T(C - G)T$  (notation as in Section 2 above) and *not* of  $T(R - G)T$ .

*Other designs.* Some designs in common use which may not satisfy (GB) are those in which repeated measures are taken on a number of units, when both time (e.g. periods) and subjects (say) are assumed to contribute to the dispersion model, i.e. are regarded as "random effects", and "residual" as well as "direct" treatment effects are included in the model, see Cochran and Cox (1957) for a general discussion. The problem here is that there are no residual effects applying to the first period. In general both time and subjects are regarded as "fixed", in which case no problems arise because the dispersion model is then trivial.

Another class of designs whose structure and accepted analysis does not satisfy (GB) is the class of so-called *two-phase experiments*, McIntyre (1955, 1956), Curnow (1959). The explanation here appears to be simply the amount of structure in the experiment.

5.6. *Concluding discussion.* Throughout this paper we have discussed the notion of balance and its generalisations from a purely theoretical point of view, focusing upon contrasts with particular mathematical properties. It has not been our concern whether these contrasts are natural, or of possible scientific interest, although this is clearly the case in many common examples.

The designer of an experiment has a quite different perspective. Amongst other things, he tries to ensure that contrasts of primary interest are estimated with as high a precision as possible, subject to the constraints imposed by the experimental material. It by no means follows that he should always design his experiment so that such contrasts are eigenvectors of all the  $\{TS_\alpha T\}$  of Section 4.1; indeed in many cases this is impossible.

If a designed experiment with orthogonal block structure satisfies (GB), then the coarsest decomposition  $\mathcal{T} = \oplus \mathcal{T}_\beta$  with respect to which it does so is uniquely defined by the design. Other decompositions of  $\mathcal{T}$  which satisfy (GB) can only arise by further decomposition of the individual  $\{\mathcal{T}_\beta\}$  in the coarsest one. When the designer is able to arrange that all of the subspaces  $\{\mathcal{T}_\beta\}$  consist of contrasts of interest, the analysis of data from the experiment and the display of the results will be particularly straightforward; examples here include BIBDs and the designs of Section 5.3. In general, however, not all

TABLE 8  
*Design not satisfying (GB).*

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2	1	1	1
1	3	3	2
2	2	4	3
4	4	4	3

---

contrasts of interest will belong to one of the  $\mathcal{T}_\beta$ , and it will be necessary in the analysis to use the more complicated formula (4.2) involving the projections  $\{T_\beta\}$ ; examples here include unbalanced lattice designs.

A final point concerning the subspaces  $\{\mathcal{T}_\beta\}$  in (GB) is worth making. Even when they do not consist of contrasts of scientific interest, they are frequently recognisable as arising from a pseudo-structure on the treatments, i.e. an artificial view of the treatments relative to which the  $\{\mathcal{T}_\beta\}$  are natural or interpretable. Examples here include many PBIBDs, most lattice designs and Example 2 of Section 5.2. The most general design satisfying (GB)—and we need go no further than block  $\alpha$ -designs to find examples—involves a decomposition of  $\mathcal{T}$  into subspaces  $\{\mathcal{T}_\beta\}$  which have neither scientific interest nor any natural or interpretable structure, however we care to view the treatments. Our general theory applies to such designs, although it may be an affront to some to describe them as balanced in any sense. We hope that our readers will appreciate the value of tracing the path from balance in BIBDs through to the notion of general balance, and conclude that the unity of outlook achieved outweighs any terminological problems met along the way.

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