MAIN-EFFECT ANALYSIS OF THE GENERAL NON-ORTHOGONAL LAYOUT WITH ANY NUMBER OF FACTORS[1]

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1. Introduction. The analysis of variance of a non-orthogonal two-factor layout is described in detail by Scheffé [6] under the heading "Two-way layout with unequal cell-numbers;" a matrix derivation of the same results was given by Tocher [8]. A method of analysis for a non-orthogonal three-factor layout was given by Freeman and Jeffers [3]. Particular cases of four factor layouts, with some orthogonalities present, were treated e.g. by Pearce [4] and Clarke [1]. Using a different approach, several authors, like Corsten [2] and Stevens [7], have proposed iterative schemes for solving the normal equations.

No general practical method for analyzing a non-orthogonal p-factor layout seems to have been found so far. A survey of the present state of the problem is given by Pearce [5].

The main problem involved in the analysis is how to solve the normal equations i.e. how to project the vector of the observations on the linear hypothesis subspace. For the general p-factor layout, that subspace is the direct sum of a one-dimensional subspace, corresponding to the general mean, and of p subspaces corresponding to the p main-effects vectors. A direct solution of the normal equations requires the inversion of a matrix whose order is roughly equal to the total number of single-factor levels in the layout. Aside from the length of the calculations involved, this puts a definite limitation on the number of factors which can be handled, even by an electronic computer.

In this paper, it is shown (in Sections 4–7) that the normal equations can be solved by a stepwise transformation of the initial $p + 1$ subspaces into a set of $p + 1$ mutually orthogonal subspaces. The procedure, essentially analogous to the Gram-Schmidt method for orthogonalizing a set of vectors, consists of p steps. Each step requires the inversion of a matrix whose order is the number of levels of one of the factors. Therefore, provided the number of levels of each factor does not exceed the maximal order of the matrices which can be handled, there is practically no limitation on the number of factors.

In Section 9, the main-effect analysis based on the normal equations solution is described. In Section 10, it is shown that the analysis can be simplified in the presence of orthogonalities, and some special situations are treated, generalizing results already known for two, three and four factors.

It would, of course, be desirable to extend the method to the general non-orthogonal layout with, say, main-effects and two-factor interactions only.

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Until such an extension is found, it may only be pointed out that for some simple cases, such as the case where only a particular two-factor interaction is suspected, one can treat the level combinations of those two factors as levels of a single artificial factor, and apply the method accordingly.

2. Matrix notation. We consider a general nonorthogonal p-factor layout with h_i levels for the factor $A_i (1 \leqq i \leqq p)$, subject only to the restriction (3.3) which will be explained later. The n observations of the layout are regarded as the coordinates of a column vector $\mathbf{y}$, which is an element of the n-dimensional space V. We define the matrices $\mathbf{X}_i$, $\mathbf{N}_i$ and $\mathbf{N}_{ij}$ $(i, j = 1, 2, \cdots, p)$ as follows.

$\mathbf{X}_i$ is a matrix with h_i rows (corresponding to the h_i levels of A_i) and n columns (corresponding to the n observations). In each column, one of the entries (corresponding to the level of A_i for that observation) is 1; all the other entries are 0.

$\mathbf{N}_i$ is a column vector whose h_i elements are the numbers of observations at the different levels of A_i. $\mathbf{N}_i$ can obviously be supposed to contain no zero elements.

$\mathbf{N}_{ij}$ is an $h_i \times h_j$ matrix, whose elements are the numbers of observations at the $h_i h_j$ combinations of levels of A_i and A_j.

Denote by $\mathbf{1}_s$ the column vector consisting of s unit entries. The following obvious relations hold:

$$\mathbf{1}'_{h_i}\mathbf{X}_i = \mathbf{1}_n'; \qquad \mathbf{X}_i \cdot \mathbf{1}_n = \mathbf{N}_i; \tag{2.1}$$

$$\mathbf{N}_{ij} = \mathbf{X}_i\mathbf{X}_j'; \tag{2.2}$$

and

$$\mathbf{N}_{ij} \cdot \mathbf{1}_{h_j} = \mathbf{N}_i; \qquad \mathbf{1}'_{h_i} \cdot \mathbf{N}_{ij} = \mathbf{N}_j'. \tag{2.3}$$

3. Model and assumptions. In what follows, we shall stick as close as possible to the approach and notation of Scheffé [6].

The n observations are assumed to be independently and normally distributed, with the same variance σ^2, around their respective means. The fixed-effect additive model (without interactions) is considered, i.e. the underlying hypothesis is

$$\omega: E(\mathbf{y}) = \mathbf{n}_\omega = \mathbf{1}_n \cdot \mu + \textstyle\sum_{i=1}^p \mathbf{X}_i'\boldsymbol{\alpha}_i, \qquad \mathbf{N}_i'\boldsymbol{\alpha}_i = 0 \quad (i = 1, 2, \cdots, p), \tag{3.1}$$

where μ is the general mean, and $\boldsymbol{\alpha}_i$ is a column vector whose elements are the main effects of the h_i levels of A_i.

The hypotheses to be tested will be $\omega_i = \omega \cap H_i$, where $H_i : \boldsymbol{\alpha}_i = 0$. Without loss of generality, we shall deal only with H_1.

Following the usual method, the analysis of variance will consist of the following steps:

(a) We shall construct the l.s. estimate $\hat{\mathbf{n}}_\omega$ of $\mathbf{n}_\omega$, $\hat{\mathbf{n}}_\omega = \mathbf{1}_n\hat{\mu} + \sum_{i=1}^p \mathbf{X}_i'\hat{\boldsymbol{\alpha}}_i$, i.e. the projection of $\mathbf{y}$ on the subspace V_w of V, where

$$V_\omega = \{\mathbf{n}_\omega = \mathbf{1}_n\mu + \textstyle\sum_{i=1}^p \mathbf{X}_i'\boldsymbol{\alpha}_i \mid \mathbf{N}_i'\boldsymbol{\alpha}_i = 0, \quad i = 1, 2, \cdots, p\}. \tag{3.2}$$

The l.s. estimates $\hat{\mu}$ and $\hat{\boldsymbol{\alpha}}_i$ will be found by solving the normal equations. In order to ensure the existence of the solution, we have to make a single restriction on the generality of the layout. We assume that

$$\text{dimension } (V_\omega) = \textstyle\sum_{i=1}^{p} h_i - p + 1. \tag{3.3}$$

Since

$$\text{dimension } (V_\omega) = \text{rank } (\mathbf{1}_n \vdots \mathbf{X}_1' \vdots \mathbf{X}_2' \vdots \cdots \vdots \mathbf{X}_p'),$$

the verification of (3.3) involves only the determination of the rank of a matrix whose elements are all 0 or 1. Complicated considerations of estimability, which are one of the main difficulties encountered in non-orthogonal experiments, are thus avoided.

Once $\hat{\mathbf{n}}_\omega$ has been found, we can calculate

$$\mathcal{S}_\omega = \|\mathbf{y} - \hat{\mathbf{n}}_\omega\|^2 = \|\mathbf{y}\|^2 - \mathbf{y}'\hat{\mathbf{n}}_\omega . \tag{3.4}$$

(b) Analogously, we shall construct l.s. estimates of μ and $\boldsymbol{\alpha}_i (i \geqq 2)$ under the hypothesis ω_1, obtaining the projection $\hat{\mathbf{n}}_{\omega_1}$ of $\mathbf{y}$ on the subspace

$$V_{\omega_1} = \{\mathbf{n}_{\omega_1} = \mathbf{1}_n\mu + \textstyle\sum_{i=2}^{p} \mathbf{X}_i'\boldsymbol{\alpha}_i \mid \mathbf{N}_i'\boldsymbol{\alpha}_i = 0, \quad i = 2, \cdots, p\}.$$

It follows immediately from (3.3) that the dimension of V_{ω_1} is $\sum_{i=2}^{p} h_i - p + 2$.

(c) The sums of squares SS_e and SS_{A_1}, for error and for A_1 respectively will be computed, where

$$SS_e = \mathcal{S}_\omega = \sigma^2\chi^2_{\nu_e}(\nu_e = n - \textstyle\sum_{i=1}^{p} h_i + p - 1) \qquad \text{under } \omega,$$

and

$$SS_{A_1} = \mathcal{S}_{\omega_1} - \mathcal{S}_\omega = \sigma^2\chi^2_{h_1-1} \qquad \text{under } \omega_1 .$$

The ratio $\mathfrak{F} = MS_{A_1}/MS_e$ of the corresponding mean squares is distributed as a central F_{h_1-1,ν_e} variable under ω_1 and can be used to test ω_1.

4. The first step. To solve the normal equations, we shall not use directly the matrices $\mathbf{X}_i$ but other matrices which will be constructed step by step. At each stage new matrices $\mathbf{X}_i^{(k)}$, and new parameters $\boldsymbol{\alpha}_i^{(k)}$, will be introduced. For the sake of convenience, the "stage index" k will take on values in descending order; the first step will correspond to $k = p$, and the last to $k = 1$.

At the first step, or, as we shall say, at the pth stage, we define

$$\mathbf{X}_i^{(p)} = \mathbf{X}_i - \mathbf{N}_i \cdot \mathbf{1}_n'/n \quad \text{and} \quad \boldsymbol{\alpha}_i^{(p)} = \boldsymbol{\alpha}_i \quad (i = 1, 2, \cdots, p). \tag{4.1}$$

Expressing (3.1) in terms of $\mathbf{X}_i^{(p)}$ and $\boldsymbol{\alpha}_i^{(p)}$, and remembering that $\mathbf{N}_i'\boldsymbol{\alpha}_i = 0$, we obtain

$$\mathbf{n}_\omega = \mathbf{1}_n\mu + \textstyle\sum_{i=1}^{p} \mathbf{X}_i^{(p)\prime}\boldsymbol{\alpha}_i^{(p)}, \qquad \mathbf{N}_i'\boldsymbol{\alpha}_i^{(p)} = 0 \quad (i = 1, 2, \cdots, p);$$

and similarly

$$V_\omega = \{\mathbf{n}_\omega = \mathbf{1}_n\mu + \textstyle\sum_{i=1}^{p} \mathbf{X}_i^{(p)\prime}\boldsymbol{\alpha}_i^{(p)} \mid \mathbf{N}_i'\boldsymbol{\alpha}_i^{(p)} = 0, \quad i = 1, 2, \cdots, p\}$$

where, again, $\boldsymbol{\alpha}_i^{(p)}$ is a column vector. It may be seen easily that $\mathbf{X}_i^{(p)} \cdot \mathbf{1}_n = 0$, $\mathbf{1}_{h_i}' \cdot \mathbf{X}_i^{(p)} = 0$.

We define also the matrices

$$\mathbf{N}_{ij}^{(p)} = \mathbf{X}_i^{(p)}\mathbf{X}_j^{(p)\prime} + \mathbf{N}_i\mathbf{N}_j^{\prime}/n.$$

Since direct computation shows that $\mathbf{N}_{ij}^{(p)} = \mathbf{N}_{ij}$, it follows that the matrices $\mathbf{N}_{ij}^{(p)}$ may trivially be substituted for $\mathbf{N}_{ij}$ in (2.1–3), and that $\mathbf{N}_{ii}^{(p)}$ are nonsingular.

5. Description of the kth stage. Let us now suppose that we have, at the kth stage, a set of matrices $\mathbf{X}_i^{(k)}$ and a set of parameter column vectors $\boldsymbol{\alpha}_i^{(k)}$ ($i = 1, 2, \cdots, p$) with the following properties.

(i) The mean $\mathbf{n}_\omega$, defined by (3.1), can be expressed as

$$\mathbf{n}_\omega = \mathbf{1}_n\mu + \textstyle\sum_{i=1}^{p} \mathbf{X}_i^{(k)\prime}\boldsymbol{\alpha}_i^{(k)}; \qquad \mathbf{N}_i^{\prime}\boldsymbol{\alpha}_i^{(k)} = 0 \quad (i = 1, 2, \cdots, p); \tag{5.1}$$

and the subspace V_ω, defined by (3.2), as

$$V_\omega = \{\mathbf{n}_\omega = \mathbf{1}_n\mu + \textstyle\sum_{i=1}^{p} \mathbf{X}_i^{(k)\prime}\boldsymbol{\alpha}_i^{(k)} \mid \mathbf{N}_i^{\prime}\boldsymbol{\alpha}_i^{(k)} = 0, \quad i = 1, 2, \cdots, p\} \tag{5.2}$$

(ii) The matrices $\mathbf{X}_i^{(k)}$ satisfy

$$\mathbf{1}_{h_i}^{\prime}\mathbf{X}_i^{(k)} = 0; \tag{5.3}$$

$$\mathbf{X}_i^{(k)}\cdot\mathbf{1}_n = 0; \tag{5.4}$$

and

$$\mathbf{X}_i^{(k)}\mathbf{X}_j^{(k)\prime} = 0 \qquad \text{if} \qquad i \neq j \tag{5.5}$$

and at least one of the two subscripts is greater than k.

To complete the kth stage, we define the matrices $\mathbf{N}_{ij}^{(k)}$ by means of

$$\mathbf{N}_{ij}^{(k)} = \mathbf{X}_i^{(k)}\mathbf{X}_j^{(k)\prime} + \mathbf{N}_i\mathbf{N}_j^{\prime}/n \qquad (i, j = 1, 2, \cdots, p). \tag{5.6}$$

These matrices, which are a generalization of the matrix $\boldsymbol{\Omega}^{-1}$ of Tocher [8], are easily seen to satisfy

$$\mathbf{N}_{ij}^{(k)\prime} = \mathbf{N}_{ji}^{(k)}; \tag{5.7}$$

$$\mathbf{N}_{ij}^{(k)} = \mathbf{N}_i\mathbf{N}_j^{\prime}/n \quad \text{if} \quad i \neq j \tag{5.8}$$

and at least one of the two subscripts is greater than k; and

$$\mathbf{1}_{h_i}^{\prime}\cdot\mathbf{N}_{ij}^{(k)} = \mathbf{N}_j^{\prime}; \qquad \mathbf{N}_{ij}^{(k)}\cdot\mathbf{1}_{h_j} = \mathbf{N}_i\,. \tag{5.9}$$

We now prove that

$$\operatorname{rank} \mathbf{N}_{ii}^{(k)} = \mathbf{h}_i \qquad (i = 1, 2, \cdots, p), \tag{5.10}$$

i.e. the matrices $\mathbf{N}_{ii}^{(k)}$ are nonsingular. The relation (5.3) implies that the rank of $\mathbf{X}_i^{(k)}$ does not exceed $h_i - 1$. But, by (5.2), $\mathbf{1}_n$ and the columns of $\mathbf{X}_i^{(k)}$ ($i = 1, 2, \cdots, p$) generate the whole space V_ω. If the rank of $\mathbf{X}_i^{(k)}$ were smaller than $h_i - 1$ for some i we would have dimension $(V_\omega) < \sum_{i=1}^{p} h_i - p + 1$, contradicting the assumption (3.3). Therefore, the rank of $\mathbf{X}_i^{(k)}$ is $h_i - 1$ for all i. It follows that no linear combination of the rows of $\mathbf{X}_i^{(k)}$, except for multiples of (5.3), can vanish. Hence, if $\mathbf{a}$ is any column vector with $\mathbf{h}_i$ elements whose sum is not zero, the rank of the augmented matrix $(\mathbf{X}_i^{(k)} \vdots \mathbf{a})$ is h_i. In particular, this is true for the matrix

$$\mathbf{U} = (\mathbf{X}_i^{(k)} \vdots \mathbf{N}_i / n^{\frac{1}{2}}).$$

Since rank $(\mathbf{UU}')$ = rank $\mathbf{U}$, and $\mathbf{N}_{ii}^{(k)} = \mathbf{UU}'$, it follows that $\mathbf{N}_{ii}^{(k)}$ is nonsingular.

6. The iteration procedure. In order to pass to the $(k-1)$st stage, we define the matrices $\mathbf{X}_i^{(k-1)}$ by

$$(6.1) \qquad \begin{aligned} \mathbf{X}_i^{(k-1)} &= \mathbf{X}_i^{(k)} - \mathbf{N}_{ik}^{(k)}[\mathbf{N}_{kk}^{(k)}]^{-1}\mathbf{X}_k^{(k)} \qquad &\text{if} \quad i < k \\ &= \mathbf{X}_i^{(k)} \qquad &\text{if} \quad i \geqq k, \end{aligned}$$

and the parameters $\boldsymbol{\alpha}_i^{(k-1)}$ by

$$(6.2) \qquad \begin{aligned} \boldsymbol{\alpha}_i^{(k-1)} &= \boldsymbol{\alpha}_i^{(k)} \qquad \text{if} \quad i \neq k \\ \boldsymbol{\alpha}_k^{(k-1)} &= \boldsymbol{\alpha}_k^{(k)} + [\mathbf{N}_{kk}^{(k)}]^{-1} \textstyle\sum_{j<k} \mathbf{N}_{kj}^{(k)} \boldsymbol{\alpha}_j^{(k)}. \end{aligned}$$

We now prove that the Properties (i) and (ii) of Section 5 hold when k is replaced by $k-1$.

(i) The representation $\boldsymbol{\eta}_\omega = \mathbf{1}_n\mu + \sum_{i=1}^{p} \mathbf{X}_i^{(k-1)\prime}\boldsymbol{\alpha}_i^{(k-1)}$ follows immediately from (5.1), and it remains to show that $\mathbf{N}_i'\boldsymbol{\alpha}_i^{(k-1)} = 0$ $(i = 1, 2, \cdots, p)$. This is immediate for $i \neq k$. For $i = k$ and $j < k$ we have, by (5.9),

$$\mathbf{N}_k'[\mathbf{N}_{kk}^{(k)}]^{-1}\mathbf{N}_{kj}^{(k)} = \mathbf{1}_{h_k}'[\mathbf{N}_{kk}^{(k)}][\mathbf{N}_{kk}^{(k)}]^{-1}\mathbf{N}_{kj}^{(k)} = \mathbf{1}_{h_k}'\mathbf{N}_{kj}^{(k)} = \mathbf{N}_j',$$

and hence, by (6.2), $\mathbf{N}_k'\boldsymbol{\alpha}_k^{(k-1)} = \mathbf{N}_k'\boldsymbol{\alpha}_k^{(k)} + \sum_{j<k} \mathbf{N}_j'\boldsymbol{\alpha}_j^{(k)} = 0$.

(ii) We have to prove that

$$\mathbf{1}_{h_i}'\mathbf{X}_i^{(k-1)} = 0, \qquad \mathbf{X}_i^{(k-1)} \cdot \mathbf{1}_n = 0 \quad \text{and} \quad \mathbf{X}_i^{(k-1)}\mathbf{X}_j^{(k-1)\prime} = \mathbf{0}$$

if $i \neq j$ and at least one of the subscripts is greater than $k-1$. This is immediate except for the first two relations with $i < k$, and for the last one with $i < k$ and $j = k$. The proof for these remaining cases consists of expressing $\mathbf{X}_i^{(k-1)}$ in terms of $\mathbf{X}_i^{(k)}$ following (6.1), and using (5.3–5) and (5.9).

To complete the $(k-1)$st stage, we proceed like in Section 5, defining the matrices $\mathbf{N}_{ij}^{(k-1)}$ by

$$\mathbf{N}_{ij}^{(k-1)} = \mathbf{X}_i^{(k-1)}\mathbf{X}_j^{(k-1)\prime} + \mathbf{N}_i\mathbf{N}_j'/n \quad (i, j = 1, 2, \cdots, p).$$

The following two properties should be pointed out here.

(a) For any $i, j > k-1$,

$$(6.3) \qquad \mathbf{N}_{ij}^{(k-1)} = \mathbf{N}_{ij}^{(k)},$$

and in particular $\mathbf{N}_{ii}^{(k-1)} = \mathbf{N}_{ii}^{(k)} (i \geqq k)$. This property is obvious.

(b) For $i, j \leqq k-1$, we have *the recurrence formula*

$$(6.4) \qquad \mathbf{N}_{ij}^{(k-1)} = \mathbf{N}_{ij}^{(k)} - \mathbf{N}_{ik}^{(k)}[\mathbf{N}_{kk}^{(k)}]^{-1}\mathbf{N}_{kj}^{(k)} + \mathbf{N}_i\mathbf{N}_j'/n.$$

This can be proved by expressing $\mathbf{X}_i^{(k-1)}$ in terms of $\mathbf{X}_i^{(k)}$ and expanding

$\mathbf{X}_i^{(k-1)}\mathbf{X}_j^{(k-1)\prime}$; using (5.3–5) and (5.9), we get

$$\mathbf{X}_i^{(k-1)}\mathbf{X}_j^{(k-1)\prime} = \mathbf{N}_{ij}^{(k-1)} - \mathbf{N}_{ik}^{(k)}[\mathbf{N}_{kk}^{(k)}]^{-1}\mathbf{N}_{kj}^{(k)},$$

and hence (6.4).

7. Solution of normal equations. After p steps, we obtain a set of matrices $\mathbf{X}_i^{(1)}$, $\mathbf{N}_{ii}^{(1)}$ $(i = 1, 2, \cdots, p)$ such that

$$(7.1) \qquad \mathbf{X}_i^{(1)}\cdot\mathbf{1}_n = 0, \qquad \mathbf{X}_i^{(1)}\mathbf{X}_j^{(1)\prime} = 0 \quad \text{for} \quad i \neq j$$

and

$$(7.2) \qquad \mathbf{N}_{ii}^{(1)} \text{ is nonsingular } (i = 1, 2, \cdots, p).$$

The linear hypothesis (3.1) can be expressed as

$$(7.3) \qquad \mathfrak{n}_\omega = \mathbf{1}_n\mu + \textstyle\sum_{i=1}^{p} \mathbf{X}_i^{(1)\prime}\boldsymbol{\alpha}_i^{(1)}, \qquad \mathbf{N}_i'\boldsymbol{\alpha}_i^{(1)} = 0 \quad (i = 1, 2, \cdots, p),$$

and the corresponding subspace (3.2) as

$$(7.4) \qquad V_\omega = \{\mathfrak{n}_\omega = \mathbf{1}_n\mu + \textstyle\sum_{i=1}^{p} \mathbf{X}_i^{(1)\prime}\boldsymbol{\alpha}_i^{(1)} \mid \mathbf{N}_i'\boldsymbol{\alpha}_i^{(1)} = 0, \ i = 1, 2, \cdots, p\}.$$

Owing to (7.1), the normal equations are now reduced to the simple form

$$(7.5) \qquad \begin{aligned} n\hat{\mu} &= \mathbf{1}_n'\mathbf{y} \\ \mathbf{X}_i^{(1)}\mathbf{X}_i^{(1)\prime}\hat{\boldsymbol{\alpha}}_i^{(1)} &= \mathbf{X}_i^{(1)}\mathbf{y} \qquad (i = 1, 2, \cdots, p) \end{aligned}$$

with the supplementary conditions

$$(7.6) \qquad \mathbf{N}_i'\boldsymbol{\alpha}_i^{(1)} = 0 \qquad (i = 1, 2, \cdots, p).$$

From (7.5) and (7.6) we obtain

$$[\mathbf{X}_i^{(1)}\mathbf{X}_i^{(1)\prime} + b\mathbf{X}_i\mathbf{X}_i']\hat{\boldsymbol{\alpha}}_i^{(1)} = \mathbf{X}_i^{(1)}\mathbf{y} \quad (i = 1, 2, \cdots, p; \ b \neq 0)$$

or, choosing for convenience the value $1/n$ for b,

$$(7.7) \qquad \mathbf{N}_{ii}^{(1)}\hat{\boldsymbol{\alpha}}_i^{(1)} = \mathbf{X}_i^{(1)}\mathbf{y} \qquad (i = 1, 2, \cdots, p).$$

Now, it follows from (6.1) and (6.3) that $\mathbf{X}_i^{(1)} = \mathbf{X}_i^{(i)}$, $\mathbf{N}_{ii}^{(1)} = \mathbf{N}_{ii}^{(i)}$, $(i = 1, 2, \cdots, p)$, and hence we obtain

$$(7.8) \qquad \mathbf{N}_{ii}^{(i)}\hat{\boldsymbol{\alpha}}_i^{(1)} = \mathbf{X}_i^{(i)}\mathbf{y}.$$

If we introduce the notations

$$(7.9) \qquad Y = \mathbf{1}_n'\cdot\mathbf{y}; \qquad \mathbf{Y}_i^{(k)} = \mathbf{X}_i^{(k)}\mathbf{y}; \qquad \mathbf{Y}_i = \mathbf{X}_i\mathbf{y}; \qquad (i = 1, 2, \cdots, p),$$

we obtain the formulae

$$(7.10) \qquad \hat{\mu} = (Y/n), \qquad \hat{\boldsymbol{\alpha}}_i^{(1)} = [\mathbf{N}_{ii}^{(i)}]^{-1}\mathbf{Y}_i^{(i)} \qquad (i = 1, 2, \cdots, p)$$

and

$$(7.11) \qquad \hat{\mathfrak{n}}_\omega = \mathbf{1}_n(Y/n) + \textstyle\sum_{i=1}^{p} \mathbf{X}_i^{(i)\prime}[\mathbf{N}_{ii}^{(i)}]^{-1}\mathbf{Y}_i^{(i)}$$

for the l.s. estimates of the parameters μ and $\boldsymbol{\alpha}_i^{(1)}$, and of the mean $\mathfrak{n}_\omega$.

8. Recapitulation. We now summarize the construction described above, and outline the extent of the computations involved. Starting from the set of matrices $\mathbf{X}_i^{(p)}$, $\mathbf{Y}_i^{(p)}$, $\mathbf{N}_{ij}^{(p)}$ $(i, j = 1, 2, \cdots, p)$, the construction consists of p successive steps. The $(k-1)$st stage, i.e. the $(p-k+2)$nd step, requires the inversion of a matrix $\mathbf{N}_{kk}^{(k)}$ whose order is h_k, followed by the construction of $(k-1)^2$ matrices $\mathbf{N}_{ij}^{(k-1)} = \mathbf{N}_{ij}^{(k)} - \mathbf{N}_{ik}^{(k)}[\mathbf{N}_{kk}^{(k)}]^{-1}\mathbf{N}_{kj}^{(k)} + \mathbf{N}_i\mathbf{N}_j'/n$, $(i, j = 1, 2, \cdots, k-1)$, of $k-1$ matrices $\mathbf{X}_i^{(k-1)} = \mathbf{X}_i^{(k)} - \mathbf{N}_{ik}^{(k)}[\mathbf{N}_{kk}^{(k)}]^{-1}\mathbf{X}_k^{(k)}$, $(i = 1, 2, \cdots, k-1)$, and of $k-1$ column vectors $\mathbf{Y}_i^{(k-1)} = \mathbf{Y}_i^{(k)} - \mathbf{N}_{ik}^{(k)}[\mathbf{N}_{kk}^{(k)}]^{-1}\mathbf{Y}_k^{(k)}$, $(i = 1, 2, \cdots, k-1)$. From these elements, the estimates (7.10) and (7.11) can be computed.

The estimates obtained are expressed in terms of the parameters $\boldsymbol{\alpha}_i^{(1)}$. Using (6.2), we can relate these parameters to the initial parameters $\boldsymbol{\alpha}_i$ by

$$\boldsymbol{\alpha}_k^{(1)} = \boldsymbol{\alpha}_k + [\mathbf{N}_{kk}^{(k)}]^{-1}\textstyle\sum_{1=j<k}\mathbf{N}_{kj}^{(k)}\boldsymbol{\alpha}_j \quad (k = 1, 2, \cdots, p). \tag{8.1}$$

In particular $\boldsymbol{\alpha}_1^{(1)} = \boldsymbol{\alpha}_1$. The relations (8.1) allow the $\boldsymbol{\alpha}_i$ to be expressed stepwise in terms of $\boldsymbol{\alpha}_i^{(1)}$, though general formulae do not seem to be too easy to establish.

9. Analysis of variance. Substituting in (3.4) the expression (7.11) for $\hat{\mathbf{n}}_\omega$, we obtain $\mathcal{S}_\omega = \|\mathbf{y}\|^2 - (\mathbf{Y}^2/n) - \sum_{i=1}^p \mathbf{Y}_i^{(i)\prime}[\mathbf{N}_{ii}^{(i)}]^{-1}\mathbf{Y}_i^{(i)\prime}$. We now introduce the notations

$$SS_{\text{total}} = \|\mathbf{y}\|^2 - (\mathbf{Y}^2/n) \quad \text{and} \quad SS_i = \mathbf{Y}_i^{(i)\prime}[\mathbf{N}_{ii}^{(i)}]^{-1}\mathbf{Y}_i^{(i)}, \tag{9.1}$$

obtaining

$$\mathcal{S}_\omega = SS_{\text{total}} - \textstyle\sum_{i=1}^p SS_i. \tag{9.2}$$

Considering the problem under the hypothesis $\omega_1 = \omega \cap H_1$, the situation corresponds to a modified layout, in which only the factors $A_2, A_3, \cdots, A_p$ appear, while A_1 is ignored. The same stepwise construction may be applied to the modified layout, involving $k-1$ steps. However, as is readily seen, we obtain at each stage $(k = 2, 3, \cdots, p)$ the same matrices $\mathbf{X}_i^{(k)}$, $\mathbf{Y}_i^{(k)}$, $\mathbf{N}_{ij}^{(j)}$, $(i, j = 2, 3, \cdots, p)$, as in the case of the full layout, except of course the matrices with either $i = 1$ or $j = 1$. It follows that $\mathcal{S}_{\omega_1} = SS_{\text{total}} - \sum_{i=2}^p SS_i$ and hence

$$SS_{A_1} = \mathcal{S}_{\omega_1} - \mathcal{S}_\omega = SS_1. \tag{9.3}$$

Thus, SS_1 is the sum of squares due to the factor A_1, calculated "eliminating $A_2, \cdots, A_p$". As noted in Section 3, it can be used to test ω_1 under the underlying hypothesis ω.

To elucidate the meaning of SS_i for $i \geqq 2$, let H_i be the hypothesis $\boldsymbol{\alpha}_i = 0$, and ω_i^* the hypothesis $\omega \cap H_1 \cap \cdots \cap H_i$. An argument similar to that used in the derivation of $\mathcal{S}_{\omega_1}$, gives $SS_i = \mathcal{S}_{\omega_i^*} - \mathcal{S}_{\omega_{i-1}^*}$. Hence SS_i is the sum of squares due to A_i in the reduced layout in which the factors $A_i, A_{i+1}, \cdots, A_p$ are considered and $A_1, \cdots, A_{i-1}$ ignored, i.e. the sum of squares due to A_i calculated "ignoring $A_1, \cdots, A_{i-1}$" and "eliminating $A_{i+1}, \cdots, A_p$". It can be compared with $\mathcal{S}_{\omega_{i-1}^*}$, obtaining a test of the hypothesis ω_i^* under the assumption of ω_{i-1}^* as underlying hypothesis. But under ω as underlying hypothesis, the expressions SS_i, (for $i \geqq 2$) are formal sums of squares, to be used only for computing the error sum of squares.

Estimates for the variances of the components of the vector $\hat{\boldsymbol{\alpha}}_1$, and of linear contrasts in these components, may be obtained easily. Let $\mathbf{V}(\hat{\boldsymbol{\alpha}}_1)$ be the variance covariance matrix of $\hat{\boldsymbol{\alpha}}_1$. Since, according to (7.10), $\hat{\boldsymbol{\alpha}}_1 = [\mathbf{N}_{11}^{(1)}]^{-1}\mathbf{X}_1^{(1)}\mathbf{y}$, a direct calculation, using (5.6) and (5.9), gives

$$\mathbf{V}(\hat{\boldsymbol{\alpha}}_1) = \sigma^2[[\mathbf{N}_{11}^{(1)}]^{-1} - \mathbf{1}_{h_1}\cdot\mathbf{1}_{h_1}'/n]. \tag{9.4}$$

Also, if $\psi = \mathbf{C}'\boldsymbol{\alpha}_1$, $\mathbf{1}_{h_1}'\cdot\mathbf{C} = 0$ is a contrast in the main effects of A_1, and $\hat{\psi} = \mathbf{C}'\hat{\boldsymbol{\alpha}}_1$ its l.s. estimate, it follows from (9.4) that the variance of $\hat{\psi}$ is

$$V(\hat{\psi}) = \sigma^2\mathbf{C}'[\mathbf{N}_{11}^{(1)}]^{-1}\mathbf{C}. \tag{9.5}$$

Unbiased estimates $\hat{\mathbf{V}}(\hat{\boldsymbol{\alpha}}_1)$ and $\hat{\mathbf{V}}(\hat{\psi})$ are, of course, obtained by substituting $\hat{\sigma}^2$ for σ^2, where $\hat{\sigma}^2 = \mathcal{S}_\omega/[n - \sum_{i=1}^{p} h_i + p - 1]$. The formulae (9.4) and (9.5) are known for the particular cases treated in the literature; see Pearce [5].

10. Some layouts with orthogonalities present. Two factors A_i, A_j, $i \neq j$, are said to be orthogonal if the subspaces $\{\mathbf{X}_i'\boldsymbol{\alpha}_i \mid \mathbf{N}_i'\boldsymbol{\alpha}_i = 0\}$ and $\{\mathbf{X}_j'\boldsymbol{\alpha}_j \mid \mathbf{N}_j'\boldsymbol{\alpha}_j = 0\}$ are orthogonal. A necessary and sufficient condition for this is rank $\mathbf{N}_{ij} = 1$, or, in the form given by Scheffé [6],

$$\mathbf{N}_{ij} = \mathbf{N}_i\mathbf{N}_j'/n, \tag{10.1}$$

i.e. "proportional frequencies".

Two simple remarks will be useful.

(a) If for some $i < k$, $\mathbf{N}_{ik}^{(k)} = \mathbf{N}_i\mathbf{N}_k'/n$, then, by (5.9) and (6.1), $\mathbf{X}_i^{(k-1)} = \mathbf{X}_i^{(k)}$.

(b) If for some $i, j < k$ at least one of the relations $\mathbf{N}_{ik}^{(k)} = \mathbf{N}_i\mathbf{N}_k'/n$, $\mathbf{N}_{jk}^{(k)} = \mathbf{N}_j\mathbf{N}_k'/n$ holds, then, by (5.6) and (5.9), $\mathbf{N}_{ij}^{(k-1)} = \mathbf{N}_{ij}^{(k)}$.

We now consider two important cases of simplified analysis in the presence of orthogonalities.

CASE 1. *A_i, A_j are orthogonal for all $i, j \geqq 2$*, i.e.

$$\mathbf{N}_{ij} = \mathbf{N}_i\mathbf{N}_j'/n \qquad (i, j \geqq 2, \quad i \neq j).$$

This situation arises whenever a new classification A_1 is added to an orthogonal layout with the factors $A_2, \cdots, A_p$.

From the remarks (a) and (b) of this section it follows that $\mathbf{X}_i^{(k)}$ and $\mathbf{N}_{ij}^{(k)}$ $(i, j \geqq 2, k = 1, 2, \cdots, p)$ remain unchanged throughout our stepwise construction, i.e.

$$\mathbf{X}_i^{(k-1)} = \mathbf{X}_i^{(k)}, \qquad \mathbf{N}_{ij}^{(k-1)} = \mathbf{N}_{ij}^{(k)} \quad (i, j \geqq 2, \quad k = 2, \cdots, p); \tag{10.2}$$

and hence

$$\begin{aligned} \mathbf{X}_i^{(i)} &= \mathbf{X}_i^{(p)} = \mathbf{X}_i - \mathbf{N}_i \cdot \mathbf{1}_n'/n \\ \mathbf{N}_{ii}^{(i)} &= \mathbf{N}_{ii} \end{aligned} \qquad \text{for } i \geqq 2. \tag{10.3}$$

The matrices $\mathbf{N}_{1j}^{(k)}$ for $2 \leqq j < k$ (and, of course, also $\mathbf{N}_{i1}^{(k)} = \mathbf{N}_{1i}^{(k)\prime}$ for $2 \leqq i < k$) are also not affected, i.e.

$$\mathbf{N}_{1j}^{(k-1)} = \mathbf{N}_{1j}^{(k)} \qquad (2 \leqq j < k), \tag{10.4}$$

and hence

$$\mathbf{N}_{1j}^{(k)} = \mathbf{N}_{1j} \quad \text{for} \quad 2 \leqq j < k + 1 \leqq p. \tag{10.5}$$

As for $\mathbf{X}_1^{(k)}$ and $\mathbf{N}_{11}^{(k)}$, they are changed at each step; from (6.1) and (6.4), using (10.3–5), we obtain

$$\begin{aligned} \mathbf{X}_1^{(k-1)} &= \mathbf{X}_1^{(k)} - \mathbf{N}_{1k}\mathbf{N}_{kk}^{-1}\mathbf{X}_k + \mathbf{N}_1 \cdot \mathbf{1}_n'/n, \\ \mathbf{N}_{11}^{(k-1)} &= \mathbf{N}_{11}^{(k)} - \mathbf{N}_{1k}\mathbf{N}_{kk}^{-1}\mathbf{N}_{k1} + \mathbf{N}_1\mathbf{N}_1'/n; \end{aligned} \tag{10.6}$$

and iteration of (10.6) gives

$$\mathbf{X}_1^{(1)} = \mathbf{X}_1 - \textstyle\sum_{k=2}^{p} \mathbf{N}_{1k}\mathbf{N}_{kk}^{-1}\mathbf{X}_k + (p-2)\mathbf{N}_1 \cdot \mathbf{1}_n'/n \tag{10.7}$$

and

$$\mathbf{N}_{11}^{(1)} = \mathbf{N}_{11} - \textstyle\sum_{k=2}^{p} \mathbf{N}_{1k}\mathbf{N}_{kk}^{-1}\mathbf{N}_{k1} + (p-1)\,\mathbf{N}_1\mathbf{N}_1'/n. \tag{10.8}$$

Finally, from (10.7) we obtain

$$\mathbf{Y}_1^{(1)} = \mathbf{Y}_1 - \textstyle\sum_{k=2}^{p} \mathbf{N}_{1k}\mathbf{N}_{kk}^{-1}\mathbf{Y}_k + (p-2)\,\mathbf{N}_1 \cdot Y/n, \tag{10.9}$$

Since the layout obtained ignoring A_1 is orthogonal, the sums of squares SS_i are $SS_i = \mathbf{Y}_i'\mathbf{N}_{ii}^{-1}\mathbf{Y}_i - (Y^2/n)$ for $i \geqq 2$. Thus, the only matrix inversion in the whole analysis is that of $\mathbf{N}_{11}^{(1)}$, which is necessary in order to compute SS_1.

CASE 2. *The set of factors consists of two classes, such that every factor in one class is orthogonal to every factor of the other class, i.e.* $\mathbf{N}_{ij} = \mathbf{N}_i\mathbf{N}_j'/n$ if $1 \leqq i \leqq m$; $m + 1 \leqq j \leqq p$.

From the remarks (a) and (b) of this section, it follows that $\mathbf{X}_i^{(k)} = \mathbf{X}_i^{(p)}$ and $\mathbf{N}_{ij}^{(k)} = \mathbf{N}_{ij}$ $(i, j = 1, 2, \cdots, m; k = m + 1, \cdots, p)$, i.e. they remain unchanged as the stages from $k = p$ through $k = m + 1$ of the stepwise construction are carried out, while the analysis involving the factors $A_{m+1}, \cdots, A_p$ is completed. The stages from $k = m$ through $k = 1$, on the other hand, are equivalent to a complete analysis involving only the factors $A_1, \cdots, A_m$. This means that we may apply the stepwise construction separately to the class $(A_1, \cdots, A_m)$ and to the class $(A_{m+1}, \cdots, A_p)$, obtaining the sums of squares $SS_1, \cdots, SS_m$; $SS_{m+1}, \cdots, SS_p$. As before, SS_1 is the sum of squares due to A_1, and may be used to test the hypothesis ω_1. But now also SS_{m+1} is the sum of squares due to A_{m+1}, and may be used to test the hypothesis ω_{m+1}.

This can, of course, be generalized to the case when the set of factors consists of several classes such that any two factors belonging to different classes are orthogonal.

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