FACTORIAL LINEAR MODEL ANALYSIS

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Summary

This thesis develops a general strategy for factorial linear model analysis for experimental and observational studies. It satisfactorily deals with a number of issues that have previously caused problems in such analyses. The strategy developed here is an iterative, four-stage, model comparison procedure as described in Brien (1989); it is a generalization of the approach of Nelder (1965a,b).

The approach is applicable to studies characterized as being structure-balanced, multitiered and based on Tjur structures unless the structure involves variation factors when it must be a regular Tjur structure. It covers a wide range of experiments including multiple-error, change-over, two-phase, superimposed and unbalanced experiments. Examples illustrating this are presented. Inference from the approach is based on linear expectation and variation models and employs an analysis of variance. The sources included in the analysis of variance table is based on the division of the factors, on the basis of the randomization employed in the study, into sets called tiers. The factors are also subdivided into expectation factors and variation factors. From this subdivision models appropriate to the study can be formulated and the expected mean squares based on these models obtained. The terms in the expectation model may be nonorthogonal and the terms in the variation model may exhibit a certain kind of nonorthogonal variation structure. Rules are derived for obtaining the sums of squares, degrees of freedom and expected mean squares for the class of studies covered.

The models used in the approach make it clear that the expected mean squares depend on the subdivision into expectation and variation factors. The approach clarifies the appropriate mean square comparisons for model selection. The analysis of variance table produced with the approach has the advantage that it will reflect all the relevant physical features of the study. A consequence of this is that studies, in which the randomization is such that their confounding patterns differ, will have different analysis of variance tables.

Signed statement

This thesis contains no material which has been accepted for the award of any other degree or diploma in any university and, to the best of my knowledge and belief, the thesis contains no material previously published or written by another person, except where due reference is made in the text of the thesis. The material in chapters 2 and 6, except sections 6.6 and 6.7, is a revised version of that which I have previously published in Brien (1983) and Brien (1989); copies of these two papers are contained in appendices B and C. The material in section 5.2.4 and some of that in section 6.7 is the subject of an unpublished manuscript by Brien and Payne (1989). The analysis for change-over experiments presented in section 4.3.2.4 was originally developed jointly by Mr W B Hall and the author; my contribution to the joint work is detailed in the text.

I consent to the thesis being made available for photocopying and loan if accepted for the award of the degree.

C.J. Brien

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The work in this thesis, being a part-time activity, has been carried out over a long period of time. Once again Ellen, James and Melissa have had to suffer the trials, tribulations and joys of living with a person undertaking such a task. Margaret has also provided support essential to its achievement. Thank you all.

Chapter 1

Factorial linear model analysis: a review

1.1 Introduction

This thesis is concerned with factorial linear model analysis such as is associated with the statistical analysis of designed experiments and surveys. That is, it deals with models in which the independent-variables ($\mathbf{X}$) matrix involves only indicator variables derived from qualitative or quantitative factors or combinations of such factors. Thus, multiple regression models and analysis of covariance models, in which the observed values of the variables are placed in the independent-variable matrix, are excluded from consideration. However, as in the latter situations, the fitting of factorial linear models is achieved using least squares.

In this chapter, the literature on factorial linear model analysis published up until approximately the end of 1984 is reviewed. The review will be conducted by considering the following classes of models in turn:

1) Randomization models

   Linear models in which the stochastic elements are provided by the physical act of randomization:

   1.1 Neyman/Wilk/Kempthorne formulation — linear models with stochastic

indicator variables whose properties are based on randomization;

1.2 Nelder/White/Bailey formulation — covariances derived under randomization and linear contrasts specified for treatment comparisons;

2) General linear models

Linear models for the expectation and variation of the response are specified:

2.1 Fixed effects linear models — linear expectation model and variance known up to a scale factor;

2.2 Mixed linear models — linear expectation and variation model.

1.2 Existing analyses

Central to linear model analysis is the analysis of variance table that is used to summarize the analysis. As Kempthorne (1975a, 1976b) suggests, the analysis of variance can be formulated as an orthogonal decomposition of the data vector such that the *Total* variance is partitioned into components attributable to identifiable causes. That is, an analysis of variance can be obtained from a linear model whose terms have no stochastic properties. Indeed, the analysis of variance can be derived without reference to a model at all; James (1957) describes the derivation of the analysis based on relationship matrices which form an algebra. The work of Nelder (1965a,b) can also be viewed in these terms in that his complete set of binary matrices corresponds to the mutually orthogonal idempotents that generate the ideals of this algebra.

However, in order to interpret the results of an analysis one needs to ascribe stochastic properties to at least some of the terms in the model. That is, the effects for some terms must be able to be regarded as random variables with a finite variance. Two alternative bases for doing this in experiments are the randomization employed in the experiment and hypothesis.

1.2.1 Randomization models

The randomization argument as a basis for statistical inference was first propounded by Fisher (1935b, 1966) when he developed the randomization test as a means of testing hypotheses without making the assumption of normality. However, Scheffé (1959) cites Neyman (1923) as having formulated randomization models for the completely randomized design. Also, Neyman, Iwaskiewicz and Kolodzieczyk (1935) formulated such models for the randomized complete block design.

Since then randomization models of two basic kinds have been developed as a basis for inference in designed experiments. The models of the first kind were developed directly from Neyman *et al.*'s randomization models by Wilk, Kempthorne, Zyskind and White of the Iowa school and by Ogawa and others. Models of the second kind were developed by Nelder (1965a,b) with White (1975) and Bailey (1981) outlining related approaches. This latter kind of model is based on the identification of 'block' and 'treatment' factors and on derivation of the associated null randomization distribution.

1.2.1.1 Neyman/Wilk/Kempthorne formulation

As mentioned above, Scheffé (1959) cites Neyman (1923) as having used randomization models for the completely randomized design. However, the first widely available usage was by Neyman *et al.* (1935) in considering hypotheses about treatment differences for randomized complete block and Latin square experiments; they introduced models for the true yield and considered their properties under randomization. Eden and Yates (1933), Welch (1937), Pitman (1938) and McCarthy (1939) used these concepts but mainly with reference to significance tests for the Latin square and randomized complete block experiments. Kempthorne (1952) formulated models for a wide range of experiments incorporating design random variables that take only the values 0 or 1 and whose stochastic properties are directly based on the randomization employed in the experiment.

Wilk (1955) used a randomization model for the generalized randomized complete block design (each treatment replicated r times in each block) to investigate the in-

ferential properties of randomization models for this design. Wilk and Kempthorne (1955, 1956) did this for factorial experiments. Wilk and Kempthorne (1955) incorporated the effect of complete/incomplete sampling into the models; Wilk and Kempthorne (1956) introduced the idea of expressing the expected mean squares in terms of Σs, the estimable quantities in the analysis. Wilk and Kempthorne (1957) carried out the same exercise for the Latin square and corrected the results of Neyman *et al.* (1935) on the effect of unit-treatment nonadditivity.

Zyskind (1962a) extended the results of Wilk and Kempthorne to regular structures in which, for every term in the structure, the replication of the levels combinations of that term are equal. Rao (1959) and Zyskind (1963) applied randomization models to the balanced incomplete block design, although Rao did not incorporate complete/incomplete sampling considerations. Ogawa has also investigated the inferences under randomization models which are Neyman randomization models, but with the addition of unit-treatment additivity assumptions (Ogawa, 1980).

The approach of these authors will be illustrated using the work of Wilk and Kempthorne (1955, 1956) and Zyskind (1962a) since it represents the most general treatment, the other authors cited above having considered special cases. To illustrate the approach we consider the analysis of the randomized complete block design. Suppose there are B blocks, P plots per block and T treatments available in total and that b blocks, p $(= t)$ plots per block and t treatments are selected for observation. Let

$$Y_{ijk} \quad (i = 1, 2, \ldots, B;\ j = 1, 2, \ldots, P;\ k = 1, 2, \ldots, T)$$

be the true response of the jth plot in the ith block when it receives the kth treatment. Then the population identity, which gives the sum of a number of population components that is identically equal to the true response, for this design would be as follows:

$$\begin{aligned} Y_{ijk} &= \overline{Y}_{...} + (\overline{Y}_{i..} - \overline{Y}_{...}) + (\overline{Y}_{ij.} - \overline{Y}_{i..}) + (\overline{Y}_{..k} - \overline{Y}_{...}) \\ &\qquad + (\overline{Y}_{i.k} - \overline{Y}_{i..} - \overline{Y}_{..k} + \overline{Y}_{...}) + (Y_{ijk} - \overline{Y}_{ij.} - \overline{Y}_{i.k} + \overline{Y}_{i..}) \\ &= \mu + \beta_i + \lambda_{ij} + \tau_k + (\beta\tau)_{ik} + (\lambda\tau)_{ijk} \end{aligned}$$

where

the dot subscript denotes summation over that subscript.

Define population components of variation for each term in this model. That is, σ^2, σ^2_β, σ^2_λ, σ^2_τ, $\sigma^2_{\beta\tau}$ and $\sigma^2_{\lambda\tau}$ with, for example,

$$\sigma^2_\beta = \sum_{i=1}^{B} (\overline{Y}_{i\cdot\cdot} - \overline{Y}_{\cdots})^2 \;/\; (B-1)$$

These components of variation are merely measures of dispersion for the population quantities on which they are defined. Wilk and Kempthorne (1956, 1957) point out that they are not to be confused with components of variance, the latter being the variances of random variables.

Now only bt values, of the BPT in the population, are observed. Let

$$y_{i^\star k^\star} \quad (i^\star = 1, 2, \ldots, b;\ k^\star = 1, 2, \ldots, t)$$

be the observation for the $k^\star$th treatment in the $i^\star$th block. Then the statistical model, that is, the model for the observations, is:

$$\begin{aligned} y_{i^\star k^\star} \;=\; & \mu + \sum_{i=1}^{B} S_i^{i^\star} \beta_i + \sum_{k=1}^{T} S_k^{k^\star} \tau_k + \sum_{i=1}^{B} \sum_{k=1}^{T} S_i^{i^\star} S_k^{k^\star} (\beta\tau)_{ik} \\ & + \sum_{j^\star=1}^{p} D^{k^\star}_{i^\star j^\star} \sum_{i=1}^{B} \sum_{j=1}^{P} S_i^{i^\star} S_{i^\star j}^{i^\star j^\star} \lambda_{ij} \\ & + \sum_{j^\star=1}^{p} D^{k^\star}_{i^\star j^\star} \sum_{i=1}^{B} \sum_{j=1}^{P} \sum_{k=1}^{T} S_i^{i^\star} S_{i^\star j}^{i^\star j^\star} S_k^{k^\star} (\lambda\tau)_{ijk} \end{aligned}$$

where

$$S_i^{i^\star} \;=\; \begin{cases} 1 & \text{if the } i^\star\text{th selected block is the } i\text{th block in the population,} \\ 0 & \text{otherwise} \end{cases}$$

$$S_k^{k^\star} \;=\; \begin{cases} 1 & \text{if the } k^\star\text{th selected treatment is the } k\text{th treatment in the population,} \\ 0 & \text{otherwise} \end{cases}$$

$$S_{i^\star j}^{i^\star j^\star} = \begin{cases} 1 & \text{if the } j^\star\text{th selected plot in the } i^\star \text{ selected block is the } j\text{th plot in the population of plots in the } i^\star\text{th selected block,} \\ 0 & \text{otherwise} \end{cases}$$

$$D_{i^\star j^\star}^{k^\star} = \begin{cases} 1 & \text{if the } k^\star\text{th selected treatment is applied to the } j^\star\text{th selected plot in the } i^\star\text{th selected block,} \\ 0 & \text{otherwise} \end{cases}$$

The $S_i^{i^\star}$, $S_k^{k^\star}$ and $S_{i^\star j}^{i^\star j^\star}$ are termed selection variables in that the values they take reflect the population selection, whereas $D_{i^\star j^\star}^{k^\star}$ is a design variable in that the values it takes reflect the application of treatments to units (Wilk and Kempthorne, 1955). Their distributional properties can be established by considering the probabilities with which they take the values 0 and 1; for example,

$$\mathrm{E}\left[S_i^{i^\star}\right] = \mathrm{E}\left[\left(S_i^{i^\star}\right)^2\right] = \frac{1}{B}; \quad \mathrm{E}\left[S_i^{i^\star} S_{i'}^{i^{\star\prime}}\right] = \frac{1}{B(B-1)} \quad \text{for } i \neq i', i^\star \neq i^{\star\prime}.$$

It can be shown that these variables are all groupwise independent.

Corresponding to this model is an analysis of variance based on the following sample identity:

$$y_{i^\star k^\star} = \overline{y}_{..} + (\overline{y}_{i^\star .} - \overline{y}_{..}) + (\overline{y}_{.k^\star} - \overline{y}_{..}) + (y_{i^\star k^\star} - \overline{y}_{i^\star .} - \overline{y}_{.k^\star} + \overline{y}_{..}).$$

By making use of the properties of the random variables in the statistical model the expected mean squares for the analysis of variance can be obtained and are as given in table 1.1 (Zyskind, 1962a).

1.2.1.2 Nelder/White/Bailey formulation

The Nelder (1965a,b) formulation is based on the null randomization distribution and the division of the factors in an experiment into 'block' and 'treatment' factors. White (1975) and Bailey (1981) outline a slightly different approach from that of Nelder (1965a,b) but one which achieves the same results; White (1975) differs from Bailey

Table 1.1: Analysis of variance table with expected mean squares using the Neyman/Wilk/Kempthorne formulation.

SOURCE	DF	EXPECTED MEAN SQUARES†
Blocks	$b-1$	$\Sigma_{\lambda\tau}+\Sigma_{\lambda}+\Sigma_{\beta\tau}+t\Sigma_{\beta}$
Treatments	$t-1$	$\Sigma_{\lambda\tau}+\Sigma_{\lambda}+\Sigma_{\beta\tau}+b\Sigma_{\tau}$
Residual	$(b-1)(t-1)$	$\Sigma_{\lambda\tau}+\Sigma_{\lambda}+\Sigma_{\beta\tau}$

†The "cap" sigmas, Σs, are the following functions of the population components of variation, σ^2s:

$$\begin{aligned}
\Sigma_{\lambda\tau} &= \sigma^2_{\lambda\tau},\\
\Sigma_{\lambda} &= \sigma^2_{\lambda}-\frac{1}{T}\sigma^2_{\lambda\tau},\\
\Sigma_{\beta\tau} &= \sigma^2_{\beta\tau}-\frac{1}{P}\sigma^2_{\lambda\tau},\\
\Sigma_{\beta} &= \sigma^2_{\beta}-\frac{1}{P}\sigma^2_{\lambda}-\frac{1}{T}\sigma^2_{\beta\tau}+\frac{1}{P}\frac{1}{T}\sigma^2_{\lambda\tau}, \text{ and}\\
\Sigma_{\tau} &= \sigma^2_{\tau}-\frac{1}{B}\sigma^2_{\beta\tau}.
\end{aligned}$$

(1981) and Nelder (1965a,b) in including a component for technical error, although Bailey's (1981) approach can accommodate such a component.

According to Nelder (1965a), the concept of the null randomization distribution appears to have originated with Anscombe (1948). On the other hand, the earliest published record of a block/treatment dichotomization appears to be in the comments made by Fisher (1935a) during the discussion of a paper by Yates, this discussion being cited in this context by Wilk and Kempthorne (1956). Fisher proposed a 'topographical' analysis corresponding to 'blocks' and a 'factorial' analysis corresponding to 'treatments'. Wilk and Kempthorne (1956) assert that the dichotomy is used intuitively by many statisticians and several other writers have emphasized its necessity (Wilk and Kempthorne, 1957; Yates, 1975; Bailey, 1981, 1982a; Preece, 1982; Mead and Curnow, 1983, section 14.1). Yates (1975) suggests that the *failure to distinguish*

between treatment components and block and other local control components [leads] to a confused hotch-potch of interactions. In the same vein, Kempthorne (1955) notes that there is often not a *distinction made between the analysis of randomized blocks and the two-way classification.* That this still occurs is evident from Graybill (1976, chapter 14).

However, the criteria used for classifying factors into block and treatment have not usually been spelt out explicitly by these authors. Although it may be intuitively obvious how to divide the factors into these two classes in many standard agricultural field experiments, this is not so in other areas of experimentation, such as animal, psychological and industrial experiments. In the literature this problem typically arises in the form *Is Sex a block or a treatment factor?* (for example, Preece, 1982, section 6.2). It would appear that Nelder (1965a,b; 1977) intended that the distinction correspond to what will be referred to as the unrandomized/randomized dichotomy of the factors. The unrandomized factors are those factors that would index the observational units if no randomization had been performed, whereas randomized factors are those that are associated with a particular observational unit by a randomization procedure (Brien, 1983). That this correspondence is what Nelder intended is evident from his statement (Nelder, 1977, section 7) that the *treatment structure is imposed on an existing block structure* (by randomization). Bailey (1981, 1982a) follows this line as well. That is, as Fisher began pointing out, the analysis must reflect what was actually done in the experiment, or at least what was intended to be done.

Again, to illustrate the formulation, and to compare it to that of the previous section, the randomized complete block design will be considered. First, the analysis ignoring the fact that treatments have been applied is determined by examining the structure of the observational units under these circumstances. This can be done by identifying the unrandomized factors and the relationships (crossed and nested) between them. The unrandomized factors for the randomized complete block design are *Blocks* and *Plots*, say, and *Plots* are nested within *Blocks* which is written as *Block/Plots*. Let y_{ij} be the observed value for the jth plot in the ith block and $\boldsymbol{y}$ be the vector of these observations ordered lexicographically on *Blocks* then *Plots*.

Corresponding to this structure is the observation identity

$$y_{ij} = \overline{y}_{..} + (\overline{y}_{i.} - \overline{y}_{..}) + (y_{ij} - \overline{y}_{i.})$$

with which can be associated a null analysis of variance. Now any permutation of the values of the suffixes i and j, provided that all the plots in the same block end up with block suffixes being equal, will not alter the sums of squares in this analysis. The population of vectors produced by all permissible permutations of the sample vector defines a multivariate distribution which Nelder (1965a) terms the null randomization distribution. The variance matrix, Var$[\mathbf{Y}]$, of this distribution, for the randomized complete block design, is:

$$\mathbf{V} = \gamma_{Grand\ Mean}\mathbf{K} \otimes \mathbf{J} + \gamma_{Blocks}\mathbf{I} \otimes \mathbf{K} + \gamma_{Blocks.Plots}\mathbf{I} \otimes \mathbf{I}$$

where

$\gamma_{Grand\ Mean}$, γ_{Blocks} and $\gamma_{Blocks.Plots}$ are the covariances under randomization of observations in different blocks, for different plots in the same block, and the same plot, respectively,

$\otimes$ denotes the direct product operator with $\mathbf{A} \otimes \mathbf{B} = \{a_{ij}\mathbf{B}\}$,

$\mathbf{I}$ and $\mathbf{J}$ are the unit matrix and the matrix of ones, respectively,

$\mathbf{K} = \mathbf{J} - \mathbf{I}$, and

the two matrices in each direct product are of order b and t, respectively.

The variance matrix can be re-expressed as follows:

$$\begin{aligned}\mathbf{V} &= \phi_{Grand\ Mean}\mathbf{J} \otimes \mathbf{J} + \phi_{Blocks}\mathbf{I} \otimes \mathbf{J} + \phi_{Blocks.Plots}\mathbf{I} \otimes \mathbf{I} \\ &= \lambda_{Grand\ Mean}\mathbf{G} \otimes \mathbf{G} + \lambda_{Blocks}(\mathbf{I} - \mathbf{G}) \otimes \mathbf{G} + \lambda_{Blocks.Plots}\mathbf{I} \otimes (\mathbf{I} - \mathbf{G})\end{aligned}$$

where

$\phi_{Grand\ Mean}$, ϕ_{Blocks}, and $\phi_{Blocks.Plots}$ are the canonical covariance components measuring, respectively, the basic covariance of 'unrelated' observations, the excess covariance over the basic of observations for different plots in the same block, and the excess of the covariance of same plot over that of observations in the same block,

$\lambda_{Grand\ Mean}$, λ_{Blocks}, and $\lambda_{Blocks.Plots}$ are the spectral components corresponding to the expected mean squares in the analysis of variance, and

$\mathbf{G} = \mathbf{J}/m$ where m is the order of $\mathbf{J}$.

Next, the randomized factors and their relationships are considered. In the case of our example, this is trivial as there is just the one randomized factor, *Treatments*, say. Thus,

$$\mathrm{E}[\,\mathbf{Y}\,] = \mathbf{X}\boldsymbol{t} = \mathbf{X}\boldsymbol{t}^{\star}$$

where

$\mathbf{X}$ is the $bt \times t$ design matrix with rows corresponding to block-plot combinations of the elements of the sample vector and columns to treatments. All its elements will be zero except that, in each row, there will be a one in the column corresponding to the treatment applied to that block-plot combination,

$\boldsymbol{t}$ has elements t_k, t_k being the effect of the kth treatment, and

$\boldsymbol{t}^{\star} = [\mathbf{G} + (\mathbf{I} - \mathbf{G})]\boldsymbol{t}$ and so has elements $\overline{t}_{\cdot} + (t_k - \overline{t}_{\cdot})$.

In general, the analysis of variance is constructed from an investigation of the least squares fit given the expectation and variance presented above. It depends on the relationship between the $\mathbf{X}\boldsymbol{t}$ and the matrices of the spectral form of the variance matrix. For the example, only for $\lambda_{Blocks.Plots}$ is the product of the corresponding matrix and $\mathbf{X}\boldsymbol{t}$ nonzero; that is,

$$\mathbf{I} \otimes (\mathbf{I} - \mathbf{G})\mathbf{X}\boldsymbol{t} \neq 0.$$

This is summarized in the analysis of variance set out as table 1.2.

The sums of squares for this table can be computed using the algorithm described by Wilkinson (1970) and Payne and Wilkinson (1977) and which has been implemented in GENSTAT 4 (Alvey *et al.*, 1977).

Assuming no technical error, Bailey's (1981) and White's (1975) model for the example would be:

Table 1.2: Analysis of variance table with expected mean squares using the Nelder formulation.

SOURCE	DF	EXPECTED MEAN SQUARES Variation contribution
Blocks	$b-1$	$\phi_{BP}+t\phi_B$
Blocks.Plots	$b(t-1)$	
Treatments	$t-1$	ϕ_{BP}
Residual	$(b-1)(t-1)$	ϕ_{BP}

where $\phi_{BP} = \gamma_{BP}$ and
$\phi_B = \gamma_B - \gamma_{BP}$.

$$y_{ij} = t_k + \epsilon_{ij}$$

where

$$t_k \text{ are constants, } \mathrm{E}[\boldsymbol{\epsilon}] = 0 \text{ and } \mathrm{Var}[\boldsymbol{\epsilon}] = \mathbf{V}.$$

The properties of this model are derived directly from the assumption of unit-treatment additivity and the stochastic properties induced by the randomization (White, 1975; Bailey, 1981). The results outlined in this section apply to this model also.

1.2.1.3 Discussion

Following Neyman *et al.* (1935), Wilk (1955) and Wilk and Kempthorne (1957), we would conclude from table 1.1 that in general the test for $\sigma_t^2 = 0$ is biased; it will be unbiased if there is no block-treatment interaction or $B \to \infty$. However, a test for $\Sigma_\tau = 0$ is always available. Cox (1958), Rao (1959) and Nelder (1977) argue that it is the latter hypothesis that is of interest. The Cox hypothesis 'is equivalent to

saying that the treatments do not vary by more than the variation implied by the interaction' (Nelder, 1977). A test of this hypothesis is provided by the ratio of the *Treatment* and *Residual* mean squares.

The appropriate test for treatment differences, according to table 1.2, is also provided by the ratio of the *Treatment* and *Residual* mean squares. That is, the two formulations result in the same mean square comparisons, provided the hypotheses of interest can be expressed in terms of the Σs or, equivalently, the ϕs. However, the underlying models are quite different, with that of the Neyman/Wilk/Kempthorne formulation incorporating complete/incomplete sampling and unit-treatment interactions, whereas those of the Nelder/White/Bailey formulation do not.

Further, the second order parameters associated with the Neyman/Wilk/Kempthorne models are components of variation as discussed above. The second order parameters associated with the Nelder/White/Bailey model are the covariances induced by the randomization. Also, the form of the analysis of variance table is different for the two formulations.

1.2.2 General linear models

Underpinning general linear models is the classification of factors as either fixed or random. Jackson (1939), according to Scheffé (1956), was the first to distinguish explicitly between fixed and random effects in writing down a model. Jackson distinguished between effects for which constancy of performance is expected and those for which variation in performance is expected. Crump (1946) also made this distinction on essentially the same basis, warning that for random terms it has to be assumed that the effects are a random sample from an infinite population. Eisenhart (1947) introduced the terms fixed and random effects and made explicit the distinction between them on the basis of the sampling mechanism employed. Thus, if the levels of a factor are randomly sampled then it is said to be a **random factor**, whereas the levels of **fixed factors** are chosen; consequently the appropriate range of inference differs between the two types of factors.

Fisher (1935b, 1966, section 65), in discussing the analysis of varietal trials in a

randomly selected set of locations, added to section 65 in the sixth edition (1951) of *The Design of Experiments* a discussion of **definite** and **indefinite factors**. The distinction between these two types of factor is essentially the same as that made between fixed and random effects by Jackson (1939) and Crump (1946). Bennett and Franklin (1954) use the same basis as Eisenhart (1947). Wilk and Kempthorne (1955), Cornfield and Tukey (1956), Searle (1971b), Kempthorne (1975a), Nelder (1977) and many other authors use an equivalent basis, namely incomplete versus complete sampling. Eisenhart (1947) also suggests that a parallel basis is whether or not the set of entities (animals, plots or temperatures) associated with the levels of a factor in the current experiment remains unchanged in a repetition of the experiment. Scheffé (1959), Steel and Torrie (1980) and Snedecor and Cochran (1980) also use this prescription. There appears to be universal agreement that fixed terms in a linear model, terms composed only of fixed factors, contribute to the expectation; random terms, terms comprised of at least one random factor, contribute to the variation.

Another direction from which general linear models can be approached, in the context of analysing designed experiments, is given by Nelder (1965a,b), Bailey (1981) and Houtman and Speed (1983). In this approach, one first classifies the factors as either block or treatment factors, as discussed in the *Nelder/White/Bailey* subsection above. The block factors might then be assumed to contribute to the variation, as for random factors, and the treatment factors assumed to contribute to the expectation, as for fixed factors. Even though Houtman and Speed (1983) define the distinction between block/treatment factors in terms of the variation/expectation assumption, and in many agricultural experiments it is the case, it must be emphasized that there is no intrinsic reason for the two classifications to be directly linked.

1.2.2.1 Fixed effects linear models

The analysis to investigate an expectation model for a study, as is done in fixed effects linear model analysis, has developed from least squares regression as used by Gauss from 1795 and formulated independently by Legendre in 1806, Adrain in 1808, and Gauss in 1809 (Seal, 1967; Plackett, 1972; Harter, 1974; Sheynin, 1978). Its

development in the context of factorial linear model analysis derives from Fisher's (1918) introduction of the analysis of variance. However, while Fisher in a note to 'Student' (Gossett, 1923) formulated an additive linear model and Fisher and Mackenzie (1923) formulated a multiplicative model, both to be fitted by least squares, Fisher often discussed the analysis of variance for a study without reference to a linear model. Thus Urquhart, Weeks and Henderson (1973) attribute the introduction of the linear models associated with analysis of variance to Fisher's colleagues.

Allan and Wishart (1930) supplied the first stage by writing a simple model for the randomized complete block design and Irwin (1931) wrote down models of the kind that would be used today for this design, including an error term. Yates (1933a and 1934) is credited with introducing the generally applicable method of 'fitting constants' (Kempthorne, 1955) but Yates (1975) himself recognizes that Fisher had used the fitting of constants in the letter to Gossett (1923), a letter Yates had not seen at the time of writing his 1933 paper. However, Irwin (1934) was the first to give explicit expressions for the elements of the design matrix for the randomized complete block and Latin square designs. Cochran (1934) gave a general presentation based on matrix algebra.

Gauss in 1821 gave an alternative development of the least squares method in which he showed that it leads to what are now called minimum variance linear unbiased estimators (Eisenhart, 1964). A number of authors have subsequently provided proofs of this result; Markov is one whose name became associated with it because, according to Seal (1967), of Neyman's (1934) mistaken attribution of originality. It would appear that the next important development after Gauss was Aitken's (1934) extension of the theorem to cover the case of a nonsingular variance matrix known up to a scale factor. More recent work with a possibly singular variance matrix seems to start with Zyskind (1962b, 1967) on whose work was based the results of Zyskind and Martin (1969), Seely (1970) and Seely and Zyskind (1971). Goldman and Zelen (1964) and Mitra and Rao (1968) have also contributed. A unified and complete theory for estimation and testing under the general Gauss model was developed by Rao (1971, 1972, 1973a) and Rao and Mitra (1971). The theory is outlined by Rao (1973b, chapter 4) and Rao (1978). Kempthorne (1976a) gives an elementary account of the derivation of

the results. The general Gauss model is as follows:

$$\boldsymbol{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

where

$\boldsymbol{y}$ is the vector of n observations,
$\mathbf{X}$ is a known $n \times p$ matrix of rank r $(r \leq p)$,
$\boldsymbol{\beta}$ is a vector of p unknown parameters, and
$\boldsymbol{\epsilon}$ is vector of n errors with $\mathrm{E}[\boldsymbol{\epsilon}] = 0$, $\mathrm{E}[\boldsymbol{\epsilon}\boldsymbol{\epsilon}'] = \mathrm{Var}[\boldsymbol{y}] = \mathbf{V} = \sigma^2\mathbf{D}$, and $\mathbf{D}$ is a known arbitrary, possibly singular, $n \times n$ matrix.

Thus the **fixed-effects linear model** consists of an expectation with multiple parameters, specified by $\mathbf{X}\boldsymbol{\beta}$, and a single error term $\boldsymbol{\epsilon}$. Rao (1973b), and other authors, have called this model the Gauss-Markov setup when the variance matrix is nonsingular and the general Gauss-Markov setup when it can also be singular. In view of the above discussion I shall not include Markov when discussing these models.

Of course, the estimation problem here is to find an estimator of $\boldsymbol{\beta}$. However, in the context of factorial linear models we are often interested in linear functions of $\boldsymbol{\beta}$ and further, as $r < p$ usually, only some linear functions are invariant to the particular estimate of $\boldsymbol{\beta}$; these are termed the **estimable functions** of $\boldsymbol{\beta}$ [a term Scheffé (1959) ascribes to Bose (1944)]. It can be shown that a function $\boldsymbol{q}'\boldsymbol{\beta}$ is estimable if $\boldsymbol{q}'\boldsymbol{\beta} = \boldsymbol{t}'\mathrm{E}[\boldsymbol{y}]$ for some $\boldsymbol{t}'$. The best linear unbiased estimator (BLUE) of an estimable function, $\boldsymbol{q}'\boldsymbol{\beta}$, has been shown (Rao, 1973b) to be $\boldsymbol{q}'\hat{\boldsymbol{\beta}}$ where $\hat{\boldsymbol{\beta}}$ is a stationary value of $(\boldsymbol{y} - \mathbf{X}\boldsymbol{\beta})'\mathbf{M}(\boldsymbol{y} - \mathbf{X}\boldsymbol{\beta})$ if and only if $\mathbf{M} = (\mathbf{D} + \mathbf{X}\mathbf{Z}\mathbf{X}')^-$ for any symmetric g-inverse and where $\mathbf{Z}$ is any symmetric matrix such that $\mathrm{rank}(\mathbf{V}|\mathbf{X}) = \mathrm{rank}(\mathbf{V} + \mathbf{X}\mathbf{Z}\mathbf{X}')$. [$(\mathbf{V}|\mathbf{X})$ is a partitioned matrix.]

Rao (1974) and Rao and Yanai (1979) express these results in terms of projection operators.

In terms of the use of these results in fixed effects models, it is usual to assume that $\mathbf{D} = \mathbf{I}$, in which case somewhat simplified results apply. In particular, it has been proved that $\boldsymbol{q}'\boldsymbol{\beta}$ is estimable and has BLUE $\boldsymbol{q}'\hat{\boldsymbol{\beta}}$ if and only if $\boldsymbol{q}' \in \mathcal{C}(\mathbf{X})$, the column space of $\mathbf{X}$; that is, there exists some $\boldsymbol{t}'$ such that $\boldsymbol{q}' = \boldsymbol{t}'\mathbf{X}$ (Searle, 1971b, section 5.4). It can be shown that

- the elements of $\boldsymbol{\beta}$ are not estimable, in general, and
- any linear function of $\mathbf{X}\boldsymbol{\beta}$ or $\mathbf{X}'\mathbf{X}\boldsymbol{\beta}$ is estimable (Searle, 1971b, section 5.4).

Complementing the concept of estimable functions is that of testable hypotheses, these being hypotheses that can be expressed in terms of estimable functions. A testable hypothesis H: $\mathbf{K}'\boldsymbol{\beta} = \boldsymbol{\mu}$ is taken as one where

$$\mathbf{K}'\boldsymbol{\beta} = \{\boldsymbol{k}_i'\boldsymbol{\beta}\} \quad \text{for} \quad i = 1, 2, \ldots, s$$

such that $\boldsymbol{k}_i'\boldsymbol{\beta}$ is estimable for all i.

For example, consider an experiment involving two crossed factors, Y and Z say, for which there are possibly several observations for each combination of the levels of Y and Z. The usual model for this experiment would be

$$y_{ijk} = \mu + \psi_i + \zeta_j + (\psi\zeta)_{ij} + \epsilon_{ijk}$$

where $\mathrm{E}[\epsilon_{ijk}] = 0$, $\mathrm{Var}[\epsilon_{ijk}] = \sigma^2$, and $\mathrm{Cov}[\epsilon_{ijk}, \epsilon_{i'j'k'}] = 0$ for $(i, j, k) \neq (i', j', k')$. Further, because the model is not of full rank, constraints are often placed on either or both the parameters and the estimates in order to obtain a solution. For the model above, commonly employed constraints are:

$$\sum_i \psi_i = \sum_j \zeta_j = \sum_i (\psi\zeta)_{ij} = \sum_j (\psi\zeta)_{ij} = 0.$$

If constraints are not placed on the parameters, the individual μ, ψ_is, ζ_js and $(\psi\zeta)_{ij}$s in the model are not estimable; however, the $(\mu + \psi_i + \zeta_j + (\psi\zeta)_{ij})$s, and linear combinations of them, are estimable. Note that, in this circumstance, $\psi_i - \psi_{i'}$ is not estimable.

An alternative parametrization of this model is in terms of a cell mean model, namely

$$y_{ijk} = \mu_{ij} + \epsilon_{ijk}.$$

This model is a full rank model and the μ_{ij}s are the basic underlying estimable quantities in that they, and any linear combination of them, are estimable. Thus hypotheses involving linear combinations of the μ_{ij}s are testable.

Analyses based on these two models have been termed, respectively, the **model comparison** and **parametric interpretation** approaches by Burdick and Herr (1980). In the model comparison approach a series of models is fitted and the simplest model not contradicted by the data is selected. In the parametric interpretation approach a single maximal model is fitted and the pattern in the data investigated by testing hypotheses specified in terms of linear parametric functions.

The first approach consists of comparing a sequence of models. It appears that there is agreement that the models should observe the marginality (Nelder, 1977 and 1982) or containment (Goodnight, 1980) relationships between terms in the study (see for example Burdick and Herr, 1980). However, there is much divergence of opinion surrounding the sequencing and parametrization of models. There is still debate over whether main effects should be tested in the presence of interaction (Appelbaum and Cramer, 1974; Nelder, 1977 and 1982; Aitkin, 1978; and Hocking, Speed and Coleman, 1980). In terms of parametrization, should one use

- models not of full rank with nonestimable constraints to obtain a solution (Speed and Hocking, 1976), or
- full rank models reparametrized using restrictions placed on parameters (Speed and Hocking, 1976; Aitkin, 1978; and Searle, Speed and Henderson, 1981)?

The advantages of the model comparison approach are that one can produce an orthogonal analysis of variance and that it can be used for studies involving more than one random term. A disadvantage is that the issues of sequencing and parametrization outlined above arise. A number of authors also assert that a further disadvantage is that the hypotheses to be tested involve the observed cell frequencies (see Hocking and Speed, 1975; Speed and Hocking, 1976; Urquhart and Weeks, 1978; Speed, Hocking and Hackney, 1978; Burdick and Herr, 1980; Goodnight, 1980; Hocking, Speed and Coleman, 1980; and Searle, Speed and Henderson, 1981) and so are not readily interpretable (see for example Burdick and Herr, 1980). However, Nelder (1982) suggests that when seen from an information viewpoint there is no problem; the unequal cell frequencies just reflect the differences in information available on the various contrasts of the parameter space.

The second approach is implicit in the writings of Yates (1934), Eisenhart (1947) and Elston and Bush (1964). However, it was explicitly reintroduced by Urquhart, Weeks and Henderson (1973) and Hocking and Speed (1975) and its use advocated in a host of subsequent papers. Goodnight (1980) gives an equivalent procedure in which the overparametrized model is fitted and tests based on estimable functions of the parameters in this model are carried out. The appropriate function (Type III in his notation) yields the same tests as those of the cell means approach.

Proponents of this method claim that it has the advantage that all linear functions of the parameters are estimable and the hypotheses being tested are interpretable as they are analogous to the tests used in the balanced case and do not involve the observed cell frequencies (see for example Speed, Hocking and Hackney, 1978; Burdick and Herr, 1980; Goodnight, 1980; and Searle, Speed and Henderson, 1981). Further, it is asserted that the essence of many studies is the comparison of several populations, based on random samples from them, and cell means models reflect this (Urquhart, Weeks and Henderson, 1973; and Hocking, Speed and Coleman, 1980). A disadvantage is the nonadditivity of sums of squares for the set of hypotheses (see for example Burdick and Herr, 1980; Goodnight, 1980; and Hocking, Speed and Coleman, 1980) and this may result in significant effects going undetected (Burdick and Herr, 1980). Steinhorst (1982) also draws attention to the inadequacy of the cell means models for experiments involving more than a single random term (for example the randomized complete block and split-plot experiments).

1.2.2.2 Mixed linear models

The mixed linear model extends the fixed-effects linear model to represent the variation in the data by including terms in the model that specify random variables assumed to be independently distributed and to have finite variance. Thus, whereas models that have only one such term are called fixed-effects linear models and those composed solely of such terms except for the general mean term are called **random effects** or **variance components** models, models involving several of both kinds of terms are called **mixed linear** models [see for example Scheffé (1956)].

Variance component analysis, although first used by Airy (1861) and Chauvenet (1863) (Scheffé, 1956; Anderson, 1979), seems not to have come into general usage until after Fisher's (1918) development of analysis of variance. It received great impetus from Eisenhart's (1947) much cited paper. Tippett (1929) calculated expected mean squares for variance component models. He was the first (Tippett, 1931) to incorporate them into the analysis of variance table, although Irwin (1960) and Anderson (1979) credit Daniels (1939) with the introduction of the term component of variance. Mixed models appear to have been first employed, implicitly, by Fisher (1925, 1970) in developing the split-plot analysis and Fisher (1935b, 1966) in analysing an experiment involving the testing of varieties at several locations. Yates (1975) describes this as a major extension of Gaussian least squares, involving as it did multiple error terms. However, Scheffé (1956) suggests that the first explicit mixed model was given by Jackson (1939); random interaction effects were introduced by Crump (1946). Eisenhart (1947) introduced the terms model I and model II and it was his article that was highly influential in the development of mixed model analysis.

Since then the field has been reviewed by Eisenhart (1947), Crump (1951) and Plackett (1960); recent expository articles are by Harville (1977) and Searle (1968, 1971a, 1974). Sahai (1979) has published an extensive bibliography on variance components which is relevant to mixed models also. Searle (1971b) and Graybill (1976) are textbooks with considerable coverage of mixed models.

Mixed linear models form a subclass of the general linear model, the general linear model (Graybill, 1976) being:

$$\boldsymbol{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\epsilon}$$

where $\boldsymbol{y}$, $\mathbf{X}$ and $\boldsymbol{\beta}$ are as for the fixed model, and $\boldsymbol{\epsilon}$ is such that $\mathrm{E}[\boldsymbol{\epsilon}] = 0$ and $\mathrm{Cov}[\boldsymbol{\epsilon}] = \Sigma$.

Mixed linear models are then that subclass of models that can be written in the following form (Hartley and Rao, 1967; Harville, 1977; Smith and Hocking, 1978; Miller, 1977; Searle and Henderson, 1979; Szatrowski and Miller, 1980):

$$\mathbf{y} = \sum_{i=1}^{p} \boldsymbol{x}_i \beta_i + \sum_{j=1}^{m} \mathbf{Z}_j \boldsymbol{\eta}_j$$

with $\mathrm{E}[\boldsymbol{y}] = \mathbf{X}\boldsymbol{\beta} = (\boldsymbol{x}_1\boldsymbol{x}_2 \ldots \boldsymbol{x}_p)(\beta_1\beta_2 \ldots \beta_p)'$, $\mathbf{Z}_j$ being a design matrix for the jth random term and of order $n \times m_j$, m_j being the number of effects in the jth term, $\boldsymbol{\eta}_j$ an $m_j \times 1$ vector of random effects and $\boldsymbol{\eta}_j \sim (\mathbf{o}, \phi_j\mathbf{I})$, and $m_m = n$ and $\mathbf{Z}_m = \mathbf{I}$, so that $\mathrm{Var}[\boldsymbol{y}] = \mathbf{V} = \sum_{j=1}^{m} \phi_j\mathbf{S}_j = \sum_{j=1}^{m} \phi_j\mathbf{Z}_j\mathbf{Z}_j'$.

Nelder (1977), following Smith (1955), has called the ϕs canonical components of excess variation, or just canonical components. They correspond to the Σ quantities of Wilk and Kempthorne (1956) and Zyskind (1962a) and the ϕs of Nelder (1965a). As Nelder (1977) and Harville (1978) discuss, they can be interpreted as classical variance components (Searle, 1971b, section 9.5a; Searle and Henderson, 1979), variance components corresponding to the formulations of Graybill (1961) or Scheffé (1959) or covariances of the observations (Nelder, 1977). As Harville (1978) details, the differences between these formulations lie in their parameter spaces and the interpretation of the random effects and their variances. Thus, in terms of classical variance components, the random effects are uncorrelated and their variances, given by the canonical components, are nonnegative. In terms of covariances, the effects for a particular term will have equal, possibly negative, covariance and the canonical components measure excess covariation which may also be negative but restricted so that the variance matrix remains nonnegative definite. The advantages of the canonical components are that they have the same interpretation in respect of the variance matrix of the observations for all formulations of the model, albeit with different restrictions on the parameter spaces, and they are the quantities which will be estimated and tested in the analysis of variance.

Thus, a mixed model for the two-way experiment described in the previous section would again be based on the following model:

$$y_{ijk} = \mu + \psi_i + \zeta_j + (\psi\zeta)_{ij} + \epsilon_{ijk}$$

In terms of the classical variance components approach, the mixed model might involve the following conditions and assumptions:

$$\sum_i \psi_i = 0,$$

$$\mathrm{E}[\zeta_j] = \mathrm{E}[(\psi\zeta)_{ij}] = \mathrm{E}[\epsilon_{ijk}] = 0,$$

$$\mathrm{Var}[\zeta_j] = \phi_Z \geq 0, \mathrm{Var}[(\psi\zeta)_{ij}] = \phi_{YZ} \geq 0, \mathrm{Var}[\epsilon_{ijk}] = \phi_\epsilon \geq 0,$$

$$\mathrm{Cov}[\zeta_j, \zeta_{j'}] = \mathrm{Cov}[(\psi\zeta)_{ij}, (\psi\zeta)_{i'j'}] = \mathrm{Cov}[\epsilon_{ijk}, \epsilon_{i'j'k'}] = 0$$

$$\text{for } i' \neq i, j' \neq j \text{ or } k' \neq k, \text{ and}$$

$$\mathrm{Cov}[\zeta_j, (\psi\zeta)_{i'j'}] = \mathrm{Cov}[\zeta_j, \epsilon_{i'j'k'}] = \mathrm{Cov}[(\psi\zeta)_{ij}, \epsilon_{ijk}] = 0$$

$$\text{for all } i, i', j, j', k \text{ and } k'.$$

On the other hand, in terms of a covariance interpretation, parallel assumptions are:

$$\begin{aligned}
\mathrm{Cov}[y_{ijk}, y_{i'j'k'}] &= \gamma, && \text{if} \quad j' \neq j, \\
\mathrm{Cov}[y_{ijk}, y_{i'j'k'}] &= \gamma_Z, && \text{if} \quad i' \neq i, j' = j, \\
\mathrm{Cov}[y_{ijk}, y_{i'j'k'}] &= \gamma_{YZ}, && \text{if} \quad i' = i, j' = j, k' \neq k, \text{ and} \\
\mathrm{Cov}[y_{ijk}, y_{i'j'k'}] &= \gamma_\epsilon, && \text{if} \quad i' = i, j' = j, k' = k.
\end{aligned}$$

Then, the quantities μ, ζ_j, $(\psi\zeta)_{ij}$ and ϵ_{ijk} are assumed independent and with variances ϕ, ϕ_Z, ϕ_{YZ} and ϕ_ϵ, respectively, where

$$\begin{aligned}
\phi &= \gamma, \\
\phi_Z &= \gamma_Z - \gamma, \\
\phi_{YZ} &= \gamma_{YZ} - \gamma_Z, \quad \text{and} \\
\phi_\epsilon &= \gamma_\epsilon - \gamma_{YZ}.
\end{aligned}$$

For the covariance interpretation in the regular case ($i = 1, \ldots, a$; $j = 1, \ldots, b$; $k = 1, \ldots, r$), rather than requiring the ϕs to be nonnegative, the following conditions on the ϕs must be satisfied:

$$\phi_\epsilon > 0, \quad \phi_{YZ} \geq -\phi_\epsilon / r, \quad \phi_Z \geq -(\phi_\epsilon + r\phi_{YZ}) \,/\, (ra), \text{ and}$$

$$\phi \geq -(\phi_\epsilon + r\phi_{YZ} + ra\phi_Z) \,/\, (rab).$$

Clearly, a mixed model involves both an expectation vector and a variance matrix based on multiple parameters and so does not in general come under the general Gauss umbrella. However, in some situations mixed models can be transformed so that they come under the umbrella. This prompts one to ask under what conditions this will be true.

To answer this question requires an examination of the relationship between the fixed and random parts of mixed models. This can be reduced to a study of the relationship between the column space of the fixed-effects design matrix, that is $\mathcal{C}(\mathbf{X})$, and the eigenspaces of $\mathbf{V}$. This research was originally begun in the context of linear regression analysis with an examination of the conditions under which simple least squares estimators (SLSEs) are BLUEs. That is, when estimators which are a solution of the simple normal equations $\mathbf{X}'\mathbf{X}\widehat{\boldsymbol{\beta}} = \mathbf{X}'\boldsymbol{y}$ are BLUEs.

Papers on this topic include those by Anderson (1948), Watson (1955, 1967, 1972), Grenander (1954), Grenander and Rosenblatt (1957), Magness and McGuire (1962), Zyskind (1962b, 1967), Kruskal (1968), Rao (1967, 1968), Thomas (1968), Mitra and Rao (1969), Seely and Zyskind (1971), Mitra and Moore (1973) and Szatrowski (1980). These authors have established a number of equivalent conditions for which the SLSEs are BLUEs when the variance matrix is arbitrary nonnegative definite, thereby extending the Gauss BLUE property of the simple least squares estimator from $\mathbf{V} = \sigma^2\mathbf{I}$ to $\mathbf{V}$ arbitrary. The generalized condition is that the linear function $\boldsymbol{w}'\boldsymbol{y}$ is both a SLSE and a BLUE if and only if for every vector $\boldsymbol{w} \in \mathcal{C}(\mathbf{X})$ the vector $\mathbf{V}\boldsymbol{w} \in \mathcal{C}(\mathbf{X})$ (Zyskind, 1967, 1975); this simplifies to just $\boldsymbol{w} \in \mathcal{C}(\mathbf{X})$ for $\mathbf{V} = \sigma^2\mathbf{I}$. An equivalent general condition is that, if the rank of $\mathcal{C}(\mathbf{X})$ is r, then there must be r eigenvectors of $\mathbf{V}$ that form a basis of $\mathcal{C}(\mathbf{X})$, or that the column space of each idempotent, $\mathbf{P}_i$, of the spectral representation of $\mathbf{V}$ can be expressed as a direct sum of a subspace belonging to $\mathcal{C}(\mathbf{X})$ and one belonging to $C^{\perp}(\mathbf{X})$ (Zyskind, 1967). The implication of this for designed experiments is that the experiment must be orthogonal for the SLSEs to be BLUEs.

A number of authors have considered the relationship between $\mathcal{C}(\mathbf{X})$ and $\mathbf{V}$ specifically in the context of designed experiments. It appears that Box and Muller (1959) and Muller and Watson (1959) were the first to do so, their investigation being for the randomized complete block design. Morley Jones (1959) carried out a detailed examination for block designs in general. Subsequent papers in this area then include: Kurkjian and Zelen (1963); Zelen and Federer (1964); Nelder (1965a,b); James and Wilkinson (1971); Pearce, Caliński and Marshall (1974); Corsten (1976); Houtman and Speed (1983). Here the concern has not been with establishing the equality of SLSEs and BLUEs, since for many useful designs (for example, incomplete block designs) orthogonality does not obtain and so simple least squares estimates are not appropriate. However, some simplification obtains when the model for the variation structure has **orthogonal variation structure** (OVS); that is, an analysis based on an hypothesized variance matrix $\mathbf{V}$ can be written as a linear combination of a known complete set of mutually orthogonal idempotent matrices:

$$\mathbf{V} = \sum_i \lambda_i \mathbf{P}_i,$$

where

$$\lambda_i \geq 0 \text{ for all } i, \text{ and}$$
$$\textstyle\sum_i \mathbf{P}_i = \mathbf{I},\ \mathbf{P}_i\mathbf{P}_{i'} = \delta_{ii'}\mathbf{P}_i \text{ and } \delta_{ii'} = \begin{cases} 1 & \text{for } i = i' \\ 0 & \text{for } i \neq i' \end{cases}.$$

The great majority of experimental designs used in practice have OVS (Nelder, 1965a,b; Bailey, 1982a; Houtman and Speed, 1983). They include any study with what Bailey (1984) termed an orthogonal block structure and for which all the 'block' factors are assumed to contribute to the variation; thus, they include experiments with Nelder's (1965a) simple orthogonal block structure, provided all the 'block' factors are assumed to contribute to variation.

As Nelder (1965b) points out, in an analysis based on OVS, one can obtain the generalized least squares estimators of $\boldsymbol{\beta}$ by performing a least squares fit for each $\mathbf{P}_i$, that is, by solving the following set of normal equations:

$$(\mathbf{X}'\mathbf{P}_i\mathbf{X})\widehat{\boldsymbol{\beta}} = \mathbf{X}'\mathbf{P}_i\boldsymbol{y}.$$

These can be conveniently reparametrized by letting $\boldsymbol{\mu} = \mathbf{X}\boldsymbol{\beta}$ and $\mathrm{E}[\boldsymbol{y}] = \mathbf{M}\boldsymbol{\mu}$, where $\mathbf{M}$ is the projection operator on $\mathcal{C}(\mathbf{X})$; the normal equations for a particular $\mathbf{P}_i$ become

$$\mathbf{M}\mathbf{P}_i\mathbf{M}\hat{\boldsymbol{\mu}} = \mathbf{M}\mathbf{P}_i\boldsymbol{y}.$$

The study of the relationship between $\mathcal{C}(\mathbf{X})$ and the eigenspaces of $\mathbf{V}$ now becomes an investigation of the spectral decomposition of $\mathbf{M}\mathbf{P}_i\mathbf{M}$. For suppose the spectral form of $\mathbf{M}\mathbf{P}_i\mathbf{M}$ is given by

$$\mathbf{M}\mathbf{P}_i\mathbf{M} = \sum_j e_{ij}\mathbf{Q}_{ij},$$

then the solution to the normal equations becomes

$$\hat{\boldsymbol{\mu}}_i^\star = (\sum_j e_{ij}^{-1}\mathbf{Q}_{ij})\mathbf{M}\mathbf{P}_i\boldsymbol{y}.$$

This particular solution is obtainable for any experiment satisfying OVS. However, the eigenspaces corresponding to a particular $\mathbf{Q}_{ij}$ are not always obvious; in some cases they will correspond to contrasts of scientific interest, while in others they will not. It is therefore often useful to ask, 'Does a particular fixed-effect decomposition correspond to the spectral form of the normal equations?'. If it does, the experiment is said to be **generally balanced** *with respect to that fixed-effect decomposition*. That is, suppose that corresponding to the projection operator $\mathbf{M}$, there is an orthogonal decomposition $\sum_j \mathbf{M}_j^\star = \mathbf{M}$ with $\mathbf{M}_j^\star\mathbf{M}_{j'}^\star = \delta_{jj'}\mathbf{M}_j^\star$. Then an experiment is generally balanced with respect to this fixed effect decomposition if

$$\mathbf{M}\mathbf{P}_i\mathbf{M} = \sum_j e_{ij}\mathbf{M}_j^\star, \text{ for all } i \text{ and } j$$

(Nelder, 1965b, 1968).

The Houtman and Speed (1983) definition of general balance differs from this Nelder definition in as much as, rather than requiring the above condition be met in respect of a specified fixed-effect decomposition, it requires only that some fixed-effect decomposition satisfying the above decomposition can be found. Consequently, Houtman and Speed (1983) can 'assert that *all* block designs (with equal block sizes, and the usual dispersion model) satisfy' general balance. On the other hand, whether or not

partially balanced block designs satisfy Nelder's (1965b, 1968) definition of general balance depends on what decomposition of the treatment subspace is specified. I will use the term **structure balance** to mean general balance in the sense defined by Nelder (1965b, 1968)

James and Wilkinson (1971) also refer to generally balanced designs as designs for which each factor in the fixed-effects model has associated with it a single efficiency factor. However, this does not require that the fixed-effects decomposition is orthogonal as is the case for the other definitions. To avoid confusion, I will use James and Wilkinson's (1971) alternative nomenclature and refer to experiments satisfying their condition as being **first-order balanced**. That is, the set of projection operators $\mathbf{M}_j^\star$, with $\mathbf{M}\mathbf{M}_j^\star = \mathbf{M}_j^\star$ and $\mathbf{M}_j^\star\mathbf{M}_{j'}^\star\mathbf{M}_j^\star = e_{jj'}^\star\mathbf{M}_j^\star$ for all j and j', is first-order balanced if

$$\mathbf{M}_j^\star\mathbf{P}_i\mathbf{M}_j^\star = e_{ij}\mathbf{M}_j^\star, \text{ for all } i \text{ and } j.$$

Note that first-order balance differs from structure balance in that the specified fixed-effect decomposition does not have to be orthogonal for first-order balance, and from the Houtman and Speed (1983) definition of general balance in that for Houtman and Speed's (1983) definition there merely has to exist some orthogonal fixed-effect decomposition for which the above condition is true. Thus, the set of structure-balanced designs is a subset of those that are first-order balanced and of those satisfying the Houtman and Speed (1983) definition of general balance.

If the design is generally balanced, the normal equations for a particular $\mathbf{P}_i$ have solution

$$\hat{\boldsymbol{\mu}}_i^\star = (\sum_j e_{ij}^{-1}\mathbf{M}_j^\star)\mathbf{P}_i\boldsymbol{y}.$$

The combined BLUE of $\boldsymbol{\mu}$, when the λ_is are known, is the weighted sum of the individual estimators and is given by

$$\hat{\boldsymbol{\mu}} = \sum_i \sum_j e_{ij}\lambda_i^{-1}\left(\sum_i e_{ij}\lambda_i^{-1}\right)^{-1} e_{ij}^{-1}\mathbf{M}_j^\star\mathbf{P}_i\boldsymbol{y}$$

(Nelder, 1968; Houtman and Speed, 1983).

The difficulties begin when one turns to examine the situation in which the ϕ_is are unknown; that is, the ϕ_is must be estimated from the data. There are several estima-

tion methods available: analysis of variance (ANOVA), maximum likelihood (ML), residual maximum likelihood (REML), minimum norm quadratic unbiased estimation (MINQUE) and minimum variance quadratic unbiased estimation (MIVQUE). ANOVA estimators are those obtained by equating mean squares in an ANOVA table to their expectations. It is well known that the ANOVA estimators are equivalent to REML, MINQUE and MIVQUE estimators for orthogonal analyses, provided the nonnegativity constraints on the variance components do not come into play. They have the desirable properties that they are location invariant, unbiased, minimum variance amongst all unbiased quadratic estimators and, under normality, minimum variance amongst all unbiased estimators (Searle, 1971b, section 9.8a). However, they may lead to negative parameter estimates which may be outside the parameter space. In comparison, ML estimators, while biased because they do not take into account degrees of freedom lost in estimating the model's fixed effects and require heavy computations, are always well-defined. Furthermore, nonnegativity constraints can be imposed, if desired. REML estimators, as well as enjoying the advantages of M L estimators, overcome the ML loss of degrees of freedom problem and, as noted above, are the same as ANOVA estimators provided the nonnegativity constraints on the variance components do not come into play. (Harville, 1977).

On the other hand, for nonorthogonal cases, the equivalence between ANOVA and other estimators does not hold. The only advantage ANOVA(-like) estimators (estimators yielded by Henderson's (1953) methods 1, 2 and 3) retain in this situation, other than that they are analogous to the procedure for orthogonal analyses, is that they are location-invariant and quadratic unbiased (Harville, 1977). Thus the disadvantages exhibited by ANOVA estimators in nonorthogonal experiments include that they are not available for terms totally confounded with fixed-effects (they are not well-defined) and may not have minimum variance. Harville (1977) suggests that REML or approximate REML procedures are to be preferred to Henderson estimators.

Searle (1979b) outlines the relationships between REML, MINQUE and MIVQUE estimators, the details being presented in Searle (1979a). He argues that there are only two distinctly different methods of maximum likelihood and minimum variance estimation of variance components: ML and REML. A number of simulation stud-

ies (Hocking and Kutner, 1975; Corbeil and Searle, 1976; Harville, 1978) comparing ML and REML estimators have shown that, although ML estimates are biased, they often have smaller mean-squared-error than REML estimates even in orthogonal experiments. Harville (1977) suggests that there is unlikely to be a 'clear-cut winner' between REML and ML. Thus, the preferred estimator is likely to depend on such considerations as the importance of bias, the likely values of the variance components, the size of the experiment and the ease of computation.

In the context of generally balanced experiments, Nelder (1968) and Houtman and Speed (1983) give an iterative ANOVA-like method for simultaneously estimating the fixed effects and variance components. The estimation of the variance components is essentially equivalent to REML (Harville, 1977; Houtman and Speed, 1983).

1.2.2.3 Fixed versus random factors

A number of authors believe the fixed/random dichotomy of factors to be unnecessary. Yates (1965, 1970, 1975, 1977) has consistently argued that the dichotomy is 'a distinction without a difference' (Yates, 1975). Yates (1965, p. 783) argues, as does Barnard (1960), that

> whether the factor levels are a random selection from some defined set ..., or are deliberately chosen by the experimenter, does not affect the logical basis of the formal analysis of variance .... Once the selection or choice has been made the levels are known, and the two cases are indistinguishable as far as the actual experiment is concerned.

Notwithstanding this argument, many textbooks make the distinction between fixed and random factors in their presentation of the analysis of variance. Consequently, the expected mean squares for a particular analysis depend on the categorization of the factors in the study into fixed and random factors (for example, Bennett and Franklin, 1954; Kempthorne and Folks, 1971; Snedecor and Cochran, 1980; Steel and Torrie, 1980). Yates (1965) argues that the differences in mean squares arising from differences in the classification of factors as fixed or random are the result of imposing constraints on the parameters for fixed terms which are not imposed on those of random terms. As Nelder (1977) acknowledges, Wilkinson would say 'that a

transfer of variance results from the imposition of constraints'. Also, it appears that the expected mean squares depend on the proportion of the population sampled (see, for example, Bennett and Franklin, 1954). However, Nelder (1977) has demonstrated that, if the expected mean squares are formulated in terms of the canonical covariance components, they are independent of the proportion of the population sampled (see table 1.2); that is, they are the same no matter what fixed/random dichotomy is used.

Yates (1970, p.285) asserts:

> The real distinction is ... between factors for which the interaction components in the model can be specified not too unreasonably as random uncorrelated values with the same variance ... and factors for which this assumption is patently false.

Thus, while the endpoint of some factors contributing to the expectation and others to the variation would seem to be acceptable, the route by which one reaches this endpoint is subject to debate.

1.3 Randomization versus general linear models

There is much discussion about the role of randomization *vis à vis* general linear models. The most popular arguments favouring the use of randomization models as a basis for inference are:

1. the assumptions required are less restrictive than for general linear models and
2. inferences are based on the population actually sampled, that is the given set of units and the set of possible repetitions under randomization of the experiment

(Kempthorne, 1955, 1966, 1975b; Scheffé, 1959, chapters 4 and 9; Easterling,1975).

The fundamental assumption underlying randomization-based inference is that of unit-treatment additivity (Kempthorne, 1955, 1966, 1975b; Wilk and Kempthorne, 1957; Nelder, 1965b; White, 1975; Bailey, 1981). This assumption is required so that constant treatment effects can be defined and hence ensure that the treatment effects are independent of the particular randomization employed in the experiment.

Kempthorne (1975b, *pp.* 314, 323) goes so far as to assert that an approach based on general linear models, combined with the assumption of normality, is irrelevant in the context of comparative experiments, except as providing approximations to the randomization distribution. Similarly, Easterling (1975, *p.* 729) maintains that, for most experiments, normal model-based analysis only has a role in providing descriptive, not statistical, inferences and that a serious defect of normal model-based analysis is that not all the available information is incorporated into the model, namely the randomization employed. Rubin (1980) quotes Brillinger, Jones and Tukey (1978) as saying that the appropriate role of general linear models seems to be confined to assistance in selection of a test statistic. However, Wilkinson, Eckert, Hancock and Mayo (1983, *p.*205) contend that, even in a randomization-based analysis, general linear models play an essential role in that they determine the appropriate test statistic and the relevant reference set of randomized designs.

That general linear models are not essential for determining a test statistic becomes apparent when it is realized that, as has been described in section 1.2.1 above, a model can be derived purely on the basis of the randomization employed in the experiment and some assumptions about the scale, for example additive versus multiplicative scale, on which the analysis is to be performed. A test statistic can be then determined on the basis of the randomization model. As for the relevant reference set, this is defined in terms of the target population from which our sample of one is chosen; that is, it is defined by the sampling process employed, which in this case is randomization.

A number of authors, such as Fisher (1935b, 1966, section 21.1), Cox and Hinkley (1979) and Hinkley (1980) are of the view that the role of the randomization test lies in establishing the robustness of the tests based on a general linear model. That is, randomization tests are an adjunct to tests based on an hypothesized model. Fisher (1935b, 1966) declares that knowledge of the behaviour of the experimental material should be incorporated into the analysis in the form of an hypothesized model.

Basu (1980) argues even more extremely that (pre)randomization-based inference must be rejected because it leads to manifestly absurd conclusions in experiments employing weighted randomization and because the randomized design actually employed in the experiment becomes an ancillary statistic to be conditioned on in an

analysis of the experiment. The first point is further exemplified by Lindley (1980) but argued against by Hinkley (1980) and Kempthorne (1980) in the discussion of Basu's paper. Hinkley (1980) suggests that if one is prepared to use a biased coin it is likely that 'Nature has done the randomization for us' and Kempthorne (1980) argues that the conclusions are not absurd but a direct consequence of the operating characteristics of the investigation. The second of Basu's points is similar to Harville's (1975) argument that 'conditional on the realized ... [randomization], the randomization model is no more appropriate if the design were chosen by randomization than if it were chosen arbitrarily. In respect of determining the relevant reference set, Cox and Hinkley (1979) state:

> we are here [in the randomization test] interpreting data from a given design by hypothetical repetitions over a set of possible designs. In accordance with general ideas on conditionality, this interpretation is sensible provided that the design actually used does not belong to a subset of designs with recognizably different properties from the whole set.

Thus, it would appear that one is not only to condition on the particular design employed in the experiment, but on all possible designs containing the same amount of information as the design used. In an experiment which satisfies OVS and in which the hypothesized variance matrix is related to the block structure as described in section 1.2.2, the 'design' ancillaries are the block relations.

Rubin (1980) also draws attention to the fact that randomization tests are inadequate for complicated questions such as adjusting for covariates and generalizing the results to other units.

The conclusion to be made here is that, while a model may be necessary to determine a test statistic, general linear and randomization models are equally suitable. The close ties between randomization and general linear models noted by Wilkinson *et al.* (1983) are related to the fact that the covariance component of the general linear model is of the same form as that generated by randomization in many instances. However, since the test statistics and relevant reference sets can be established without recourse to hypothetical models, I do not agree with Wilkinson *et al.* (1983, p. 205) that an hypothesized model is required to establish the inferential validity of a randomization test.

1.4 Unresolved problems

Steinhorst (1982) outlines a number of unresolved issues associated with analysis of factorial linear models. These and a number of others arose in the discussion contained in sections 1.2 and 1.3. Issues that would need to be dealt with adequately if a strategy for analysing factorial linear models is to be adjudged as satisfactory include:

1. application to as wide a range of studies as possible including multiple-error, two-phase (McIntyre, 1955, 1956; Curnow, 1959) and unbalanced experiments,
2. the basis for inference as in randomization versus general linear models
3. factor categorizations, such as fixed/random and block/treatment, and the consequences of this for expected mean squares,
4. model composition and the role of constraints on parameters,
5. appropriate mean square comparisons in model selection,
6. the form of the analysis of variance table, and
7. the appropriate partition of the *Total* sum of squares for a particular study.

It is the purpose of this thesis to develop an approach to factorial linear model analysis which satisfactorily treats these issues.

Chapter 2

The elements of the approach to linear model analysis

2.1 Introduction

This chapter summarizes for the purposes of this thesis an approach to linear model analysis that has been published elsewhere by the author (Brien, 1983 and 1989); the full texts of these publications have been incorporated into the thesis as appendices B and C. The purpose of this approach is to provide a paradigm for linear model analysis that facilitates the formulation of the analysis and which is applicable to as wide a range of situations as possible. As outlined in Brien (1989), the overall analysis is a four-stage process in which the three stages of model identification, model fitting and model testing, jointly referred to as model selection, are repeated until the simplest model not contradicted by the data is selected. In the final stage the selected model is used for prediction. In this thesis, I concentrate on model identification.

The essential steps in applying the model selection component of the approach are:

Observational unit and factors: Identify the unit on which individual measurements are taken (Federer, 1975) and specify the factors in the study.

Tiers: Divide the factors into disjoint, randomization-based sets, called tiers.

Expectation and variation factors Also divide the factors into expectation

and variation factors.

Structure set: Determine the structure set for the study based on the tiers.

Analysis of variance table: Derive the analysis table for the study from the structure set (table 2.1) and compute the degrees of freedom (table 2.2), sums of squares (table 2.3) and mean squares.

Expectation and variation models: Categorize the terms derived from the structure set, as summarized in the analysis table, as expectation or variation. Form maximal expectation and variation models (table 2.5) and the lattices of expectation and variation models.

Expected mean squares: Compute expected mean square for each source in the analysis table for the maximal expectation and variation models (table 2.8).

Model fitting/testing: In model fitting, the currently model is fitted to the data to yield the fitted values for the expectation model and their estimated variances. Then, based on the expected mean squares, carry out model testing to see if the expectation and variation models can be reduced to simpler models not contradicted by the data. If it can, repeat the model selection cycle.

All of these steps, except the last, are concerned with model identification.

The approach to be proposed is closely allied to that advocated by Fisher (1935), Wilk and Kempthorne (1957), Nelder (1965a,b), Yates (1975), Bailey (1981, 1982a), and Preece (1982). Their approach has been described in section 1.2.1.2; it involves dividing the factors in the experiment into 'block' and 'treatment' factors. White (1975) has made a similar proposal in which the 'design units' ('treatment' factors) and the 'experimental units' ('block' factors) are determined. The proposed approach also has features in common with the approach of Tjur (1984). However, Tjur's (1984) approach only covers orthogonal studies and the analysis is specified using a single structure.

The novel features of the approach are that:

- more than two randomization-based categories, or tiers, of factors are possible;
- terms involving factors from different tiers are allowed;
- while the factors are classified into tiers on the basis of their randomization, inference utilizes general linear models rather than randomization models;
- the designation of factors as expectation/variation factors is independent of their classification into tiers;
- for any one of a study's expectation models, the model does not contain terms marginal to others in the model; this is not the case for the variation models.

It is candidly acknowledged that a satisfactory analysis for many studies can be formulated without utilizing the proposed paradigm. However, there are experiments (section 5.2.4) whose full analysis can only be achieved with it. In addition, as the advocates of related approaches suggest, the employment of the paradigm will assist in the formulation of analyses of variance, particularly for complex experiments (see chapters 4, 5 and 6). In particular, the division of the factors into tiers ensures that all relevant sources are included in the analysis and that the analysis reflects, through its display of the confounding relationships, the design and purpose of the study (see section 6.6).

2.2 The elements of the approach

An experiment is now introduced which will be used throughout this section to illustrate the approach.

> **Example 2.1:** The experiment (adapted from Steel and Torrie, 1980, section 16.3) was conducted to investigate the yields of 4 varieties of oats and the effect on yield of the treatment of seeds either by spraying them or leaving them unsprayed. The seeds were sown according to a split-plot design. The seeds from the varieties were assigned to whole plots according to a Latin square design by choosing a square at random from those given in Cochran and Cox (1957, plan 4.1) and the rows and columns of the selected square randomized. The assignment of seed treatments to the subplots was randomized. The field layout and yields are given in figure 2.1. [To be continued.]

Figure 2.1: Field layout and yields of oats for split-plot experiment

U	S	S	U	S	U	S	U
V1		CL		V2		BR	
42.9	53.8	63.4	62.3	57.6	53.3	70.3	75.4
U	S	U	S	U	S	S	U
CL		BR		V1		V2	
58.5	50.4	65.6	67.3	41.6	58.5	69.6	69.6
U	S	U	S	U	S	U	S
V2		V1		BR		CL	
45.4	42.4	28.9	43.9	54.0	57.6	44.6	45.0
U	S	U	S	S	U	S	U
BR		V2		CL		V1	
52.7	58.5	35.1	51.9	46.7	50.3	46.3	30.8

2.2.1 Observational unit and factors

The first step in obtaining the quantities required in an analysis-of-variance-based linear model analysis is to identify the **observational unit**, this being the unit on which individual measurements are taken (Federer, 1975).

Also the factors in the study have to be specified. A **factor** is a variable observed for each observational unit and corresponding to a possible source of differences in the response variable between observational units. Unlike a term (see section 2.2.4), a single factor may not represent a meaningful partition of the observational units. The **levels of the factor** are the values the factor takes.

> **Example 2.1 (cont'd):** The observational unit is a subplot. The factors are *Rows*, *Columns*, *Subplots*, *Varieties* and *Treatments*. [To be continued.]

2.2.2 Tiers

The factors identified in the first step of the approach are now divided into tiers on the basis of the randomization employed in the study.

In the following discussion, the term **levels combination** will be used. A levels combination of a set of factors is the combination of one level from each of the factors in the set; that is, an element from the set of observed combinations of the levels of the factors in a set.

A **tier** is a set of factors having the same randomization status; a particular factor can occur in one and only one tier. The first tier will consist of **unrandomized factors**, or, in other words factors innate to the observational unit; these factors will uniquely index the observational units. The second tier consists of the factors whose levels combinations are randomized to those of the factors in the first tier, and subsequent tiers the factors whose levels combinations are randomized to those of the factors in a previous, in the great majority of cases the immediately preceding, tier.

A further property of the factors in different tiers is that it is physically impossible to assign simultaneously more than one of the levels combinations of the factors in one tier to one of the levels combinations of the factors in a lower tier.

These properties result in the tiers being unique for a particular situation. Provided that the levels combinations of factors are randomized to those of the factors in the immediately preceding tier, the properties also uniquely define the order of the tiers. The only examples in this thesis where they are not are the superimposed experiments in section 5.3 and the animal experiment in section 5.4.2. However, the order of the tiers is clear-cut in the case of the superimposed experiments, but not for the animal experiment.

The essential distinction between unrandomized and randomized factors is that the latter have to be allocated to observational units whereas the former are innate. Of course, randomization is only one method of achieving this allocation. However, as discussed in section 6.2, good experimental technique dictates that randomization be used in allocating the factors; it has the advantage that it provides insurance against bias in the allocation process. Because of this, the use of randomization is almost

universal and we will restrict our attention to studies in which it is the method of allocation. That is not to say that the approach cannot be applied to studies involving nonrandom allocation. Clearly, the factors can be divided into tiers based on their allocation status; however, the advantage mentioned above may not apply.

A randomization is to be distinguished from randomization in the sense of the act of randomizing (Bailey, 1981). **A randomization** is a random permutation of the factors in a tier that respects the structure derived from that tier. **Randomization** is the allocation of levels combinations of factors in one tier to those of the factors in a previous, usually the immediately preceding, tier. That is, while the unrandomized factors may be permuted to achieve the randomization, it is the randomized factors whose levels are being allocated at random. Of course, applying a randomization is not the only way of randomizing; another method is the random selection from a set of plans (Preece, Bailey and Patterson, 1978).

> **Example 2.1 (cont'd):** Of the factors specified for the example, *Rows*, *Columns* and *Subplots* are innate to the subplots (the observational units). Hence, they are the unrandomized factors and would be called 'block' factors by Nelder (1965a) and Alvey *et al.* (1977). They are then the set of factors comprising the bottom tier. It is the only possible set of factors for the bottom tier for this experiment.
>
> The levels combinations of the set of factors *Varieties* and *Treatments* were randomized to the levels combinations of the unrandomized factors. Further, only one combination of *Varieties* and *Treatments* is physically observable with each levels combination of the unrandomized factors, that is on each subplot. Thus, *Varieties* and *Treatments* are the randomized factors and are called 'treatment' factors by Nelder (1965b) and Alvey *et al.* (1977). Again, they form the only possible set of factors for the second tier. [To be continued.]

The term tier has been chosen to reflect the building up of the sets, one on another in an order defined by the randomization; it is intended to be distinct from any terms previously used in the literature. In particular, it is not a substitute for stratum which is a particular type of source in an analysis of variance table. There is no restriction placed on the number of tiers that can occur in an experiment, although in practice it would be extremely unusual for there to be more than three. An experiment requiring more than two tiers will be referred to as a **multitiered experiment**. A sample survey involves only one tier as no randomization is involved.

2.2.3 Expectation and variation factors

Classification of factors as expectation or variation factors is based on both the type of inference it is desired to draw about the factors and the anticipated behaviour of the factors. Factors are designated as **expectation factors** when it is considered most appropriate or desirable to make inferences about the relative performance of individual levels. **Variation factors** are more relevant when the performance of the set of levels as a whole is potentially informative; in such cases, the performance of a particular level is inferentially uninformative. Hence, for expectation factors, inference would be based on location summary measures ('means') and, for variation factors, on dispersion summary measures ('variances' and 'covariances'). Alternative names for this dichotomy are systematic/random and location/dispersion.

A point to be borne in mind when categorizing factors as expectation/variation factors is that, for a factor to be classified as a variation factor, an assumption of symmetry must have some justification whereas this is not required of expectation factors. This symmetry has to do with the property that labelling of the levels of variation factors is inferentially inconsequential because arbitrary permutations of the levels of a factor do not affect the inferences to be drawn. This implies that, as Yates (1965; 1970, p. 283-285) recognized, the levels of a variation factor must not be able to be partitioned into inferentially meaningful subclasses on the basis of the anticipated performance of the observational units. For example, if in a field trial it is expected that there will be gradients in a particular direction across the experimental material, the homogeneity required for *Blocks* to be regarded as a variation factor would not obtain and it should be designated as an expectation factor. Another situation in which it would be inappropriate to classify *Blocks* as a variation factor is where it is expected that an identifiable group of the blocks will be low yielding while another group will be high yielding. One consequence of the difference in the symmetry properties of expectation and variation factors is that inferences about the effects of an expectation factor will necessarily be restricted to the levels observed in a study.

We here note that it is not uncommon for the division of the factors into expectation/variation classes to yield exactly the same sets of factors as the tiers. This is the usual case for field trials where all the unrandomized factors (that is, first tier factors) are often categorized as variation factors and all the randomized factors (that is, second tier factors) as expectation factors. However, it is not always the case that the two dichotomies are equivalent as is discussed in more detail in section 6.3.

> **Example 2.1 (cont'd):** It is likely that the expectation/variation classes will correspond to the tiers in this example. That is, *Rows*, *Columns* and *Subplots* will be categorized as variation factors and *Varieties* and *Treatments* as expectation factors.
>
> However, this is not the only possible classification for the example. For example, one can envisage situations where it would be appropriate to classify *Varieties* as a variation factor and/or *Rows* as an expectation factor. [To be continued.]

2.2.4 Structure set

The **structure set for a study** consists of a set of structures, usually only one for each tier of factors, ordered in the same way as the tiers. Each **structure** summarizes the relationships between the factors in a tier and, perhaps, between the factors in a tier and those from lower tiers; it may include pseudofactors. A structure is labelled according to the tier from which it is primarily derived in that it is the relationships between all the factors in that tier that are specified in the structure. Clearly, the set of factors in a structure may not be the same as the set of factors in a tier as the set of factors in a structure may include factors from more than one tier.

The structure set for a study is derived from the tiers by:

1. determining the relationships between the factors in the first tier, expressing them in notation of Wilkinson and Rogers (1973); and
2. for each of the remaining tiers determine the structure by specifying the relationships, possibly including pseudofactor relationships,
   (a) between all factors in a tier, and
   (b) between factors from a tier and from the tiers below it.

In the notation of Wilkinson and Rogers (1973) the crossed relationship is denoted by an asterisk ($*$), the nested relationship by a slash ($/$), the additive operator by a plus ($+$) and the compound operator by a dot (.); the pseudofactor operator is denoted by two slashes ($//$) (Alvey *et al.*, 1977). A **pseudofactor** is a factor included in a structure for the study which has no scientific meaning but which aids in the analysis (Wilkinson and Rogers, 1973).

In addition to containing the factors and their relationships, the order of each factor will precede the factor's name in the lowest structure in which it appears. However, to be able to define the order of a factor, definitions are required of the properties of terms; the terms are derived, as outlined in section 2.2.5, from the structures in the structure set. The associated definitions are illustrated by example in that section.

A **term** is a set of factors which might contribute, in combination, to differences between observational units. Note that pseudofactors lead to **pseudoterms**, a pseudoterm being a term whose factors include at least one pseudofactor. As for pseudofactors, pseudoterms are included only to aid in the analysis; for example, their inclusion may result in a structure-balanced study as in the case of the example 3.1 presented in chapter 3.

A term is written as a list of factors or letters, separated by full stops. The list of letters for a term is formed by taking one letter, usually the first, from each factor's name; on occasion, to economize on space, the full stops will be omitted from the list of letters. A term is, in some ways, equivalent to a factor as defined by Tjur (1984) and Bailey (1984). It obviously is when the term consists of only one of the factors from the original set of factors making up the tiers; when a term involves more than one factor from the original set, it can be thought of as defining a new factor whose levels correspond to the levels combinations of the original factors. However, I reserve the name factor for those in the original set.

The **summation matrix** for a term is the $n \times n$ matrix whose elements are ones and zeros with an element equal to one if the observation corresponding to the row of the matrix has the same levels combinations of the factors in the term as the observation corresponding to the column (James, 1957, 1982; Speed, 1986). The **model space** of a term is the subspace of the observation space, $\mathbf{R}^n$, which is the range of the

summation matrix for the term. One term is said to be **marginal** to another if its model space is a subspace of the model space of another term from the same structure, this being the case because of the innate relationship between the levels combinations of the two terms and being independent of the replication of the levels combination of the two terms (Nelder, 1977). The marginality relationships between terms are displayed in Hasse diagrams of term marginalities as described in section 2.2.5. One term (A) is said to be **immediately marginal** to another (B) if A is marginal to B but not marginal to any other term marginal to B. A **nesting term for a nested factor** is a term that does not contain the nested factor but which is immediately marginal to a term that does. An **observational-unit subset for a term** is a subset consisting of all those observational units that have the same levels combination of the factors in the term. The **replication of a levels combination** for the factors in a term is the number of elements in the corresponding observational-unit subset.

The **order of a factor**, that is not nested within another factor, is its number of levels; the order of a nested factor is the maximum number of different levels of the factor that occurs in the observational-unit subsets of the nesting term(s) from the structure for the tier to which the factor belongs.

The crossing and nesting relationships between factors are usually thought of as being innate to the observational units (Nelder, 1965a; Millman and Glass, 1967; White, 1975). However, it is desirable that the particular relationships which are finally used in the structure set for a study depend upon the randomization employed.

To illustrate, consider a field trial in which the plots are actually arranged in a rectangular array. The plots could be indexed by two factors, one (*Rows*) corresponding to the rows and the other (*Position*) to the position of the plots along the rows. The two factors are clearly crossed since plots in different rows but in the same position along the row are connected by being in the same position. However, suppose a randomized complete block design is to be superimposed on the plots, with treatments being randomized to the plots within each row. Because of this randomization, it is no longer feasible to estimate both overall *Position* and *Treatment* effects as they are not orthogonal. Thus, rather than giving the relationship as crossed (the relationship innate to the observational units), it is usual to regard *Rows* as nesting *Position*. The

decision to randomize, without restriction, the treatments to plots within each row makes it impractical to estimate the effects of *Position*.

Thus the structure set for a particular study depends on the innate physical structure and the randomization employed. It is clear that a structure so based incorporates the procedures used in setting up the study. Because of this, one might be tempted to conclude that, like the division of the factors into tiers, the structures in the structure set for the study are fixed. However, a further influence on the structure set for a study is the subjective assumptions made about the occurrence (or not) of terms. For example, as in the analyses presented in chapters 4 and 5, we may or may not decide to assume that there is intertier additivity. Thus, in general there is not a unique analysis to be employed for a particular study.

When writing out the structure, relationships between factors within a tier should usually be specified before the intertier relationships. This is because a structure formula is read from left to right and fitted in this order when a sequential fitting procedure is used. As terms arising in the current tier are confounded with terms from lower tiers, rule 5 of table 2.1 may result in terms being incorrectly deleted if intratier terms are not fitted first.

The rules for deriving the structure set for a study and associated analysis of variance table, given in this section and table 2.1, apply to a very wide range of studies. However, the steps that will be given for computing the degrees of freedom, the sums of squares and expected mean squares apply to a restricted class of studies. In particular, structure sets for studies that are covered by the approach put forward in this thesis may be comprised of a combination of simple orthogonal, regular (or balanced) Tjur and Tjur structures.

Before giving the conditions to be met by structures of these types, definitions are provided of terms used in these conditions. A **simple factor** is one that is not nested in any other factor or a nested factor for which the same number of different levels of the factor occurs in the observational-unit subsets of its nesting term(s); this number is the order of the factor. A **regular term** is a term for which there is the same number of elements in the subsets of the observational units, a subset being formed by taking all those observational units with the same levels combinations of the factors in the

term. The **minimum of a set of terms** is the term whose model space corresponds to the intersection of the model spaces of the terms. Two terms are **orthogonal** if, in their model spaces, the orthogonal complements of their intersection subspace are orthogonal (Wilkinson, 1970; Tjur, 1984, section 3.2).

A **simple orthogonal structure** (Nelder, 1965a) is one for which:

1. all the factors are simple;
2. all relationships between factors are specified to be either crossed or nested; and
3. either the product of the order of the factors in the structure equals the number of observational units or the replications of the levels combinations of the factors in the structure are equal.

A **Tjur structure** (Tjur, 1984, section 4.1; Bailey, 1984) is one for which:

1. there is a term derived from the structure that is equivalent to the term derived by combining all the factors in the structure, or there is a **maximal term** derived from the structure to which all other terms derived from the structure are marginal;
2. any two terms from the structure are orthogonal; and
3. the set of terms in the structure is closed under the formation of minima.

A **regular Tjur structure** is a Tjur structure in which all the terms are regular.

Thus, a Tjur structure can involve, in addition to the nesting and crossing operators, operators such as the additive and pseudofactor operators, described by Wilkinson and Rogers (1973). Further, the terms do not have to be regular; however, as outlined by Tjur (1984, section 3.2), to ensure that terms are orthogonal, the terms from a structure do have to meet a proportionality condition in respect of the replications of levels combinations of terms.

As Bailey (1984) has outlined, simple orthogonal structures are a subset of regular Tjur structures which, in turn, are a subset of Tjur structures. Note that all the terms derived from a simple orthogonal structure are regular.

Example 2.1 (cont'd): The structure set is:

Tier	Structure
1	*(v Rows∗v Columns)/t Subplots*
2	*v Varieties∗t Treatments*

That *Rows* and *Columns* are crossed and *Subplots* nested within these two factors in the bottom tier structure is a consequence of the randomization that was employed; that is, these relationships are appropriate because a Latin square design was employed in assigning whole-plot treatments and subplot treatments were randomized within each whole plot.

The structures in both sets are simple orthogonal structures:

1. all the factors are simple;
2. in any structure, the only relationships are crossing and nesting relationships; and
3. the product of the orders of the factors in the first structure is v^2t which equals the number of observational units and the replication of the levels combinations of *Varieties* and *Treatments* is v for all combinations.

[To be continued.]

2.2.5 Analysis of variance table

In this step, the analysis table for the study is derived from the structure set (table 2.1) and the degrees of freedom (table 2.2), sums of squares (table 2.3) and mean squares are computed.

To obtain the analysis of variance table, the structure set for a study has to be combined with the layout. The conventions for doing this are given in table 2.1. From rule 1 we obtain a set of terms for each structure and from these derive the sets of sources for the analysis of variance table. Each **source** is a subspace of the sample space, the whole of which is identified as arising from a particular set of terms. A source will either correspond to a term (called the **defining term**) or be a residual source, the latter being the remainder for a source once terms confounded with it have been removed. A residual source takes its defining term from the highest nonresidual source with which it is confounded, highest meaning from the highest structure. The sources with which a source is confounded are not cited specifically if no ambiguity

Table 2.1: Rules for deriving the analysis of variance table from the structure set

Rule 1:	Having determined the structure set as described in section 2.2.4, expand each structure, using the rules described in Wilkinson and Rogers (1973), to obtain a set of terms including a grand mean term (G) and, perhaps, some pseudoterms for each structure.
Rule 2:	All the terms from the structure for the bottom tier will have a source in the table and these sources will all begin in the same column.
Rule 3:	Sources for terms from higher structures will be included in the table under the source(s) from the structures below, with which they are confounded. They will be indented so that sources from the same structure all start in the same column, there being a different starting column for each structure.
Rule 4:	Terms that occur in the sets derived from two consecutive structures will not have a source entered for the higher of the structures.
Rule 5:	Terms totally aliased with terms occurring previously in the same structure will not be included in the table. A note of such terms will be made underneath the table.
Rule 6:	For a source which has other terms from higher structures confounded with it, a residual source is included along with sources for other terms from the closest, usually the next, structure if there is any information in excess of these latter terms.

will result. A **confounded source** is one whose defining term is in a higher structure than that of the source with which it is confounded and the subspaces for the two sources are not orthogonal. This is in contrast to a **marginal source** which is a source whose defining term is marginal to that for the other source. An **aliased source** is a source that is neither orthogonal nor marginal to sources and whose defining terms arise from the same structure as its own. The aliasing may be **partial** or **total**, depending on whether a part or none of the information is available for the aliased source; for partial aliasing, the efficiency factor for the aliased source is strictly between zero and one whereas, for total aliasing, the efficiency factor is zero. Also, the confounding may be either **partial** or **total** depending on whether only part or all of the information about a confounded term is estimable from a single source; that

is, for partial confounding, the efficiency factor for the confounded term is strictly between zero and one whereas, for total confounding, it is one.

The form of the analysis of variance table produced as described in this section is the same as the table produced by GENSTAT 4 (Alvey *et al.*, 1977). The interpretation of the sources in the analysis is described by Wilkinson and Rogers (1973). Central to determining this table are the marginality, aliasing and confounding inherent in a study. These three phenomena are similar in that they all refer to cases in which the model subspaces for two different sources from a study are nonorthogonal. However, the circumstances leading to their being nonorthogonal are different in each case.

Marginality, as defined above, is an innate relationship between the model spaces of different terms, being independent of the actual levels combinations included in the study and the manner in which they are replicated. This relationship extends to sources in that a source is marginal to another if its defining term is marginal to that of the other source.

For example, for a study involving two factors A and B which are crossed, the model subspace for A is marginal to that for $A.B$ in that the model subspace for A is a subspace of that for $A.B$. This is true irrespective of which combinations of the levels of A and B are included and how they are replicated. Thus, sources with defining term A are marginal to those with defining term $A.B$.

On the other hand, aliasing arises when it is decided to replicate disproportionately the levels combinations of at least some factors, possibly excluding some levels combinations altogether. That is, the complete set of levels combinations is theoretically observable in equal numbers but one chooses to observe them disproportionately. Thus, aliasing occurs in connection with the fractional and nonorthogonal factorial designs but not the balanced incomplete block designs.

Confounding occurs as a result of the need to associate one and only one levels combination of one set of factors with a levels combination of a set of factors from a lower tier. This is necessary because it is impossible to observe more than one levels combination from the first set with a levels combination from the second set.

For example, in a completely randomized experiment we wish to associate one and only one of the t treatments with each of the p plots. The underlying conceptual

population is the set of pt observations that would be obtained if all t treatments were observed on each of the p plots (see Kempthorne, 1952, section 7.5; Nelder, 1977, sections 7.1 and 7.2)). It is clearly impossible to observe all treatment-plot combinations; we observe only a fraction. Consequently, the model subspace for the *Treatments* source is a subspace of that for the *Plots* source.

A major difference between aliasing and confounding is that all randomized experiments necessarily involve confounding but often do not involve aliasing. Further, with total aliasing, it is usually assumed that the term associated with the totally aliased source does not contribute to differences between the observational units while with confounding it is recognized that the associated terms will both contribute to such differences. Thus a totally aliased source is redundant and is omitted from the analysis while a confounded source remains relevant and should be retained in the analysis.

The steps for computing the degrees of freedom and sums of squares for the sources in this analysis table are given in tables 2.2 and 2.3. These steps rely on identifying marginal terms and obtaining means and effects vectors. The marginality relationships between terms are displayed in a **Hasse diagram of term marginalities** by linking, with descending lines,terms that are immediately marginal; the marginal term is placed above the term to which it is marginal. This diagram is called the Hasse diagram for ancestral subsets by Bailey (1982a, 1984) and the factor structure diagram by Tjur (1984). The **means vector** for a particular term is obtained by computing the mean for each observational unit from all observations with the same levels combination of the factors in the term as the unit for which the mean is being calculated; this is denoted by $\overline{\boldsymbol{y}}$ subscripted with the name of the term. The **effects vector** for a particular term is a linear form in the means vectors for terms marginal to that term.

The steps given in tables 2.2 and 2.3 apply to studies in which the structure set is comprised of Tjur structures and the relationship between terms from different structures is such that the analysis for the study is orthogonal. However, more general expressions for the degrees of freedom and sums of squares, in terms of projection operators, are given in theorems 3.14 and 3.15 of section 3.3.1. Further, conditions under which the steps for computing the expected mean squares, given in table 2.8,

Table 2.2: Steps for computing the degrees of freedom for the analysis of variance

Step 1:	First, for each simple orthogonal structure in the structure set, obtain the degrees of freedom for the terms in the structure. Define the component for each factor in a term to be the factor's order minus one if the factor does not nest other factors in the term, otherwise the component is the order. The degrees of freedom of the term is the product of this set of components. More generally, the degrees of freedom for the terms in a Tjur structure can be obtained using the Hasse diagram of term marginalities (Tjur, 1984). Each term in the Hasse diagram has to its left the number of levels combinations of the factors comprising that term for which there are observations. To the right of the term is the degrees of freedom which is computed by taking the difference between the number to the left of that term and the sum of the degrees of freedom to the right of all terms marginal to that term.
Step 2:	Compute the degrees of freedom for each source in the analysis table. They will be either the degrees of freedom computed for the term or, for residual sources, they will be computed as the difference between the degrees of freedom of the term for which it is the residual and the sum of the degrees of freedom of all sources confounded with that term which have no sources confounded with them.

can be applied will affect the range of studies covered by the approach being outlined. Overall, the approach can be applied to studies for which:

1. a structure involving only expectation factors is a Tjur structure;
2. a structure involving variation factors is a regular Tjur structure;
3. the maximal term for Tier 1 is a **unit term**; that is, a term for which each of its levels combinations is associated with one and only one observational unit;
4. expectation and variation factors are randomized only to variation factors; and
5. all terms in the analysis display structure balance as outlined in section 3.3.1.

The structure-balance condition above can be relaxed to become: the terms in the study must exhibit structure balance after those involving only expectation factors

Table 2.3: Steps for computing the sums of squares for the analysis of variance in orthogonal studies

Step 1: Firstly, for each simple orthogonal structure in the structure set, obtain expressions for the sums of squares. To do this write down the algebraic expression for the degrees of freedom in terms of the components given in step 1 of table 2.2; use symbols for the order of the factors, not the observed numbers. Expand this expression and replace each product of orders of the factors in this expression by the means vector for the same set of factors. The effects vector for the term is this linear form in the means vectors. The sum of squares for the term is then the sum of squares of the elements of the effects vector.

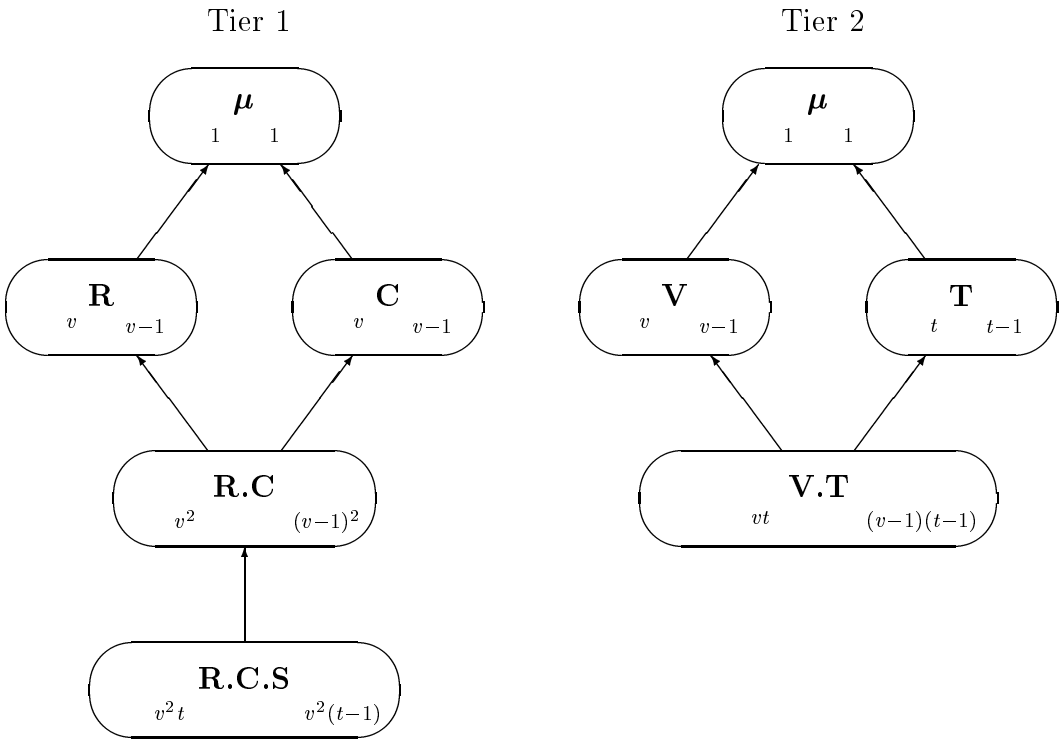
More generally, the expressions for the sums of squares for the terms in a Tjur structure can be obtained using the Hasse diagram of term marginalities (Tjur, 1984). For each term in the Hasse diagram there is to the left the mean vector for the set of factors in the term. To the right of the term is the effects vector which, for a term, is computed by taking the difference between the mean vector to the left of that term and the sum of the effects vectors to the right of all terms marginal to that term. Again the sum of squares for a term is then the sum of squares of the elements in the effects vector.

Step 2: Compute the sum of squares for each source in the analysis table. The sum of squares for a source in the table, other than a residual source, will be the sum of squares computed for the term. For residual sources, the sum of squares will be computed as the difference between the sum of squares of the term for which the source is residual and the sums of the sums of squares of all sources confounded with that term which have no sources confounded with them.

have been omitted. Thus, the approach outlined can also be employed with experiments whose expectation terms exhibit first-order balance such as the carry-over experiment of section 4.3.2.4, or those with completely nonorthogonal expectation models such as the two-factor completely randomized design with unequal replication presented in section 4.2.2.

Example 2.1 (cont'd): The Hasse diagrams of term marginalities giving the terms derived from the structure set are shown in figures 2.2 and 2.3. In the set of terms derived from the first structure, *Rows.Columns*, but not

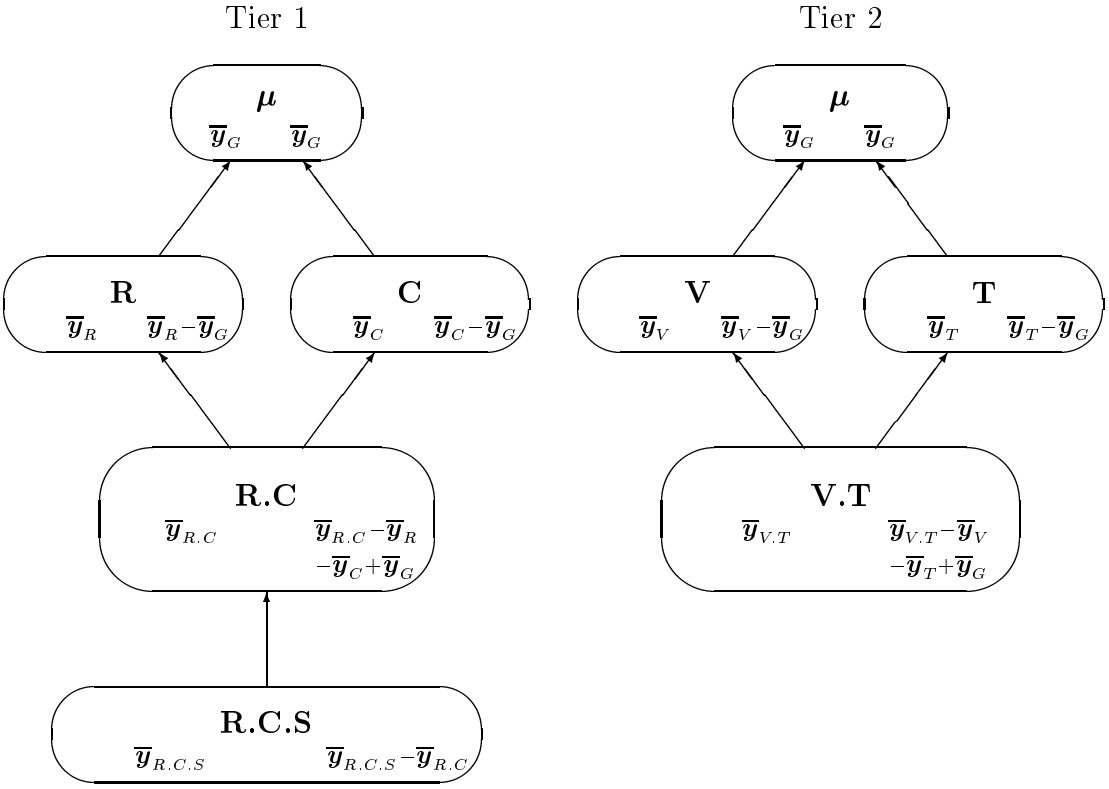
Figure 2.2: Hasse Diagram of term marginalities for a split-plot experiment with degrees of freedom



Rows, is immediately marginal to *Rows.Columns.Subplots*; *Rows*, *Columns* and *Rows.Columns* are the terms immediately marginal to *Rows.Columns*. *G*, denoted by $\boldsymbol{\mu}$ in figures 2.2 and 2.3, is the minimum of *Rows* and *Columns*; *Rows.Columns* is the minimum of *Rows.Columns* and *Rows.Columns.Subplots* . *Rows.Columns.Subplots* is a unit term. *Rows.Columns* is the only nesting term in the structure, being the nesting term for the factor *Subplots*.

The degrees of freedom of the terms, derived using step 1 of table 2.2, are given in figure 2.2; expressions for the effects vectors in terms of means vectors, derived using step 1 of table 2.3, are given in figure 2.3.

Figure 2.3: Hasse diagram of term marginalities for a split-plot experiment with effects vectors



The analysis of variance table, derived from the structure set given in section 2.2.4 as described in tables 2.1–2.3, is given in table 2.4. The sums of squares are based on the above effects vectors as described in step 2 of table 2.3.

The interpretation of the sources in the analysis of variance table is as follows:

- *Rows*, which is derived from the first structure and so is not confounded with any other source, represents the overall *Rows* effects;
- *Rows.Columns* represents the interactions of *Rows* and *Columns*;
- *Rows.Columns.Subplots* represents the differences between subplots within each row-column combination as the sources *Rows*, *Columns* and *Rows.Columns* have been excluded;
- *Varieties*, confounded with *Rows.Columns*, represents the overall *Varieties* effects; the confounding is epitomised by the indentation of *Varieties* under *Rows.Columns*;

- *Varieties.Treatments*, confounded with *Rows.Columns.Subplots*, represents the interaction of *Varieties* and *Treatments*. in this case, the confounding is epitomised by the indentation of *Varieties.Treatments* under *Rows.Columns.Subplots*.
- The *Residual* sources correspond to the unconfounded *Rows.Columns* and *Rows.Columns.Subplots* subspaces, respectively; they have defining terms *Rows.Columns* and *Rows.Columns.Subplots*, respectively.

[To be continued.]

Table 2.4: Analysis of variance table for a split-plot experiment with main plots in a Latin square design

Source	DF	MSq
Rows	3	534.43
Columns	3	49.50
Rows.Columns	9	
Varieties	3	498.91
Residual	6	40.38
Rows.Columns.Subplots	16	
Treatments	1	162.90
Varieties.Treatments	3	106.81
Residual	12	15.34
Total	31	

2.2.6 Expectation and variation models

At this stage, the terms derived from the structure set, as summarized in the analysis table, are categorized as expectation or variation terms. The maximal expectation and variation models are derived from these terms (table 2.5).

Then the sets of alternative models that might be considered are obtained with the aid of Hasse diagrams of models, one each for expectation and variation. These Hasse diagrams of models differ from the Hasse diagrams of term marginalities of Bailey (1982a, 1984) and Tjur (1984) which have been used earlier in this chapter.

2.2.6.1 Generating the maximal expectation and variation models

The steps to be performed in generating the maximal expectation and variation models are given in table 2.5.

In order to specify the maximal expectation and variation models, one begins by nominating which of the terms, obtained from the structure set for a study, influences each aspect. These terms, together with their interrelationships, have been conveniently summarized in an analysis of variance table, derived from the structure set for a study as described in section 2.2.5. Determination of which terms contribute to the expectation model and which to the variation model utilizes the expectation/variation dichotomy of the factors. As detailed in table 2.5, expectation terms are those that include only expectation factors; variation terms are those that include at least one variation factor. A consequence of this is that a factor nested within a variation factor must also be capable of being regarded as a variation factor; this is because any term involving the nested factor will also involving the nesting factor and hence will be a variation term.

Having classified the terms on which the analysis of variance table is based, our next aim is to define the maximal expectation model. A model's **minimal set of marginal terms** for a particular set of expectation terms is the smallest set whose model space is the same as that of the full set; that is, the set obtained after all marginal terms (section 2.2.5) have been deleted. The **maximal expectation model** is the sum of terms in the minimal set of marginal terms for the full set of expectation terms.

Table 2.5: Steps for determining the maximal expectation and variation models

Step 1:	Classify as expectation factors those factors for which inference is to be based on location summary measures and as variation factors those for which it is to be based on dispersion summary measures.
Step 2:	Designate as **expectation terms** those terms consisting of only expectation factors and as **variation terms** those comprising at least one variation factor.
Step 3:	The maximal expectation model is the sum of terms in the minimal set of marginal terms for the full set of expectation terms (see page 53 for more detailed description). The maximal variation model is the sum of several variance matrices, one for each structure in the study. Each variance matrix is the linear combination of the summation matrices for the variation terms from the structure; the coefficient of a summation matrix in the linear combination is the canonical covariance components for the corresponding variation term. The variation model can be expressed symbolically as the sum of the variation terms for the study.

The maximal expectation model represents the most complex model for the mechanism by which the expectation factors might affect the expectation of the response variable. We note that other parametrizations of the expectation are possible. The parametrization of the expectation is not unique (see section 6.4). It could in fact be expressed in terms of polynomial functions on the levels of quantitative factors with appropriate deviations and interactions with qualitative factors; or a set of orthogonal subspaces on the levels of factors might be specified. For the initial cycle, such alternative parametrizations must cover the same model space as the saturated model described above, since this will ensure that the estimates of variation model parameters are uncontaminated by expectation parameters. As the differences between these parametrizations are inconsequential in the present context, we will consider explicitly only the parametrization based on the minimal set of marginal terms for the full set of expectation terms. It has the advantage that it relates directly to the mechanism by which the expectation factors might affect the expectation of the response variable.

The **maximal variation model** represents an hypothesized structure for the variance matrix of the observations. As outlined in table 2.5, the variance matrix is expressed as the sum of several variance matrices, one for each structure in the study. Each of these matrices is the linear combination of the summation matrices for the variation terms from the structure. For experiments in which the variation factors occur in only simple orthogonal structures, the summation matrices are the direct product of **I** (the unit matrix) and **J** (the matrix of ones) matrices, premultiplied by the permutation matrix for the structure and postmultiplied by its transpose; the **permutation matrix for a structure** specifies the association between the observed levels combinations of the factors in the structure and the observational units (see section 3.2). The coefficients of the terms in the linear combination are **canonical covariance components** which measure the covariation, between the observational units, contributed by a particular term in excess of that of marginal terms (Nelder, 1965a and 1977). That is, of possible interpretations outlined in section 1.2.2.2, I will use the covariance interpretation so that estimates of the canonical components may be negative. The canonical covariance components are the quantities that will be estimated and tested for in the analysis.

Example 2.1 (cont'd): Given the terms obtained by expanding the structures and contained in the analysis of variance table given in table 2.4, the maximal expectation model is $\mathrm{E}[Y] = V.T$; that is, an element of $\boldsymbol{\mu}$ is:

$$\mathrm{E}\left[y_{(ij)klm}\right] = (\zeta\tau)_{ij}$$

where

$y_{(ij)klm}$ is an observation with klm indicating the levels of the factors *Rows*, *Columns*, and *Subplots*, respectively, for that observation, and

$(\zeta\tau)_{ij}$ is the expected response when the response depends on the combination of *Variety* and *Treatment* with ij being the levels combination of the respective factors which is associated with observation klm.

The maximal model for the variation is

$$\mathrm{Var}[Y] = G + R + C + R.C + R.C.S$$

and the variance matrix for this model is given by the following expression (Nelder, 1965a),

$$\begin{aligned}\mathrm{Var}[\boldsymbol{y}] &= \mathbf{V} \\ &= \phi_G \mathbf{J}\otimes\mathbf{J}\otimes\mathbf{J} + \phi_R \mathbf{I}\otimes\mathbf{J}\otimes\mathbf{J} + \phi_C \mathbf{J}\otimes\mathbf{I}\otimes\mathbf{J} \\ &\quad + \phi_{RC}\mathbf{I}\otimes\mathbf{I}\otimes\mathbf{J} + \phi_{RCS}\mathbf{I}\otimes\mathbf{I}\otimes\mathbf{I}\end{aligned}$$

where

ϕ_j is the canonical covariance component arising from the factor combination of the factor set j, and

the three matrices in the direct products correspond to *Rows*, *Columns* and *Subplots*, respectively, and so are of orders v, v and t.

The canonical covariance component ϕ_G is the basic covariance of observations in the study, ϕ_R (or ϕ_C) is the excess covariance of observations in the same row (or column) over the basic, ϕ_{RC} is the excess covariance of observations in the same row-column combination over that of those in the same row or the same column, and ϕ_{RCS} is the excess covariance of identical observations over that of those in the same row-column combination. [To be continued.]

2.2.6.2 Generating the lattices of expectation and variation models

The expectation and variation lattices, which contains all possible expectation and variation models, are constructed as described in table 2.6. Models in such lattices are either mutually exclusive or marginal to each other. A model is **marginal** to another if the terms in the first model are either contained in, or marginal (section 2.2.5) to, those in the second model.

The expectation models correspond to alternative hypotheses concerning the mechanisms by which the expectation factors might operate, and are based on the terms derived from the structure set for the study. However, we do not follow the traditional practice of parametrizing our models so that the parameters in a model are either a subset or superset of those in another model, for reasons discussed in section 6.4. Hence, the expectation lattice is based on the marginality relationships between terms in the different models.

In the case of the variation models, it is prescribed that the unit terms are always included as there is usually variation between individual observations. Similarly with

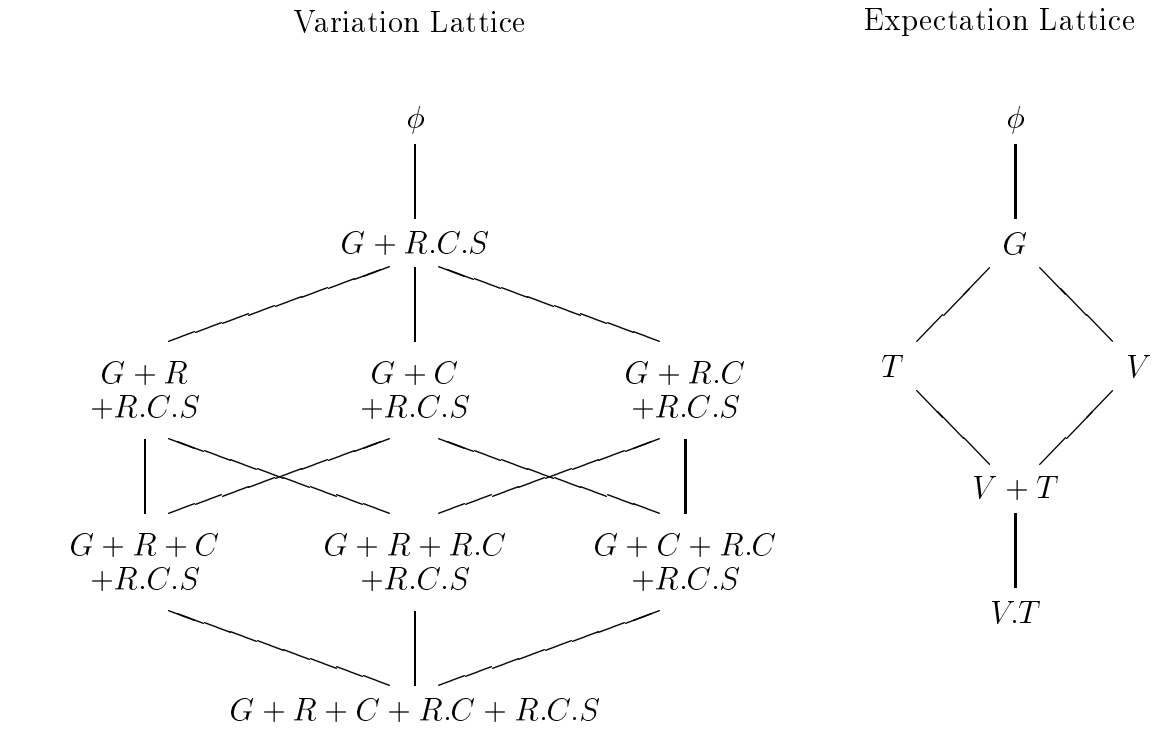
the grand mean term G, because we are unable to distinguish between variation models with and without the term; except in the unusual circumstance that the expectation is hypothesized to be zero, the expected mean square for the source associated with G will involve both a variation and an expectation contribution.

The variation lattice is based on the inclusion relationships between the sets of terms in the models for the variation. The models themselves correspond to alternative hypotheses concerning the origin of variation in the study; that is, the models correspond to alternative models for the variance matrix.

Table 2.6: Generating the expectation and variation lattices of models

Step 1:	Form all possible minimal sets of marginal terms from the expectation terms. The expectation model corresponds to the sum of the terms in one of these sets.
Step 2:	To construct the Hasse diagram of the expectation model lattice we must determine the relationships between the expectation models. A model's minimal set of marginal models is obtained by listing all models marginal to it and deleting those models marginal to another model in the list. Two models in the lattice are linked if one is in the minimal set of marginal models of the other; the marginal model is placed above the other model.
Step 3:	The Hasse diagram of the variation lattice is constructed by taking the sums of all possible combinations of variation terms in the study, subject to the restriction that the unit term(s) and the term G are included. Again, the Hasse diagram of the variation model lattice is obtained by drawing downwards links to a model from the models in its minimal set of marginal models.

Figure 2.4: Lattices of models for a split-plot experiment in which the main plots are arranged in a Latin square design



Example 2.1 (cont'd): The Hasse diagram of expectation models is shown in figure 2.4. The details of these models are as follows:

$\mathrm{E}[Y] = V.T$ This is the maximal model for the expectation since $\{V.T\}$ is the smallest set of terms that has the same model space as the full set of terms. The formal expression for this model, given in section 2.2.6.1, is $\mathrm{E}[y_{(ij)klm}] = (\zeta\tau)_{ij}$ which in vector notation is written $\boldsymbol{\mu} = \boldsymbol{\mu}_{VT}$. The underlying mechanism for this model is that the effect of V depends on the level of T.

$\mathrm{E}[Y] = V + T$ The formal expressions are $\mathrm{E}[y_{(ij)klm}] = \zeta_i + \tau_j$ and, in vector notation, $\boldsymbol{\mu} = \boldsymbol{\mu}_{V+T} = \boldsymbol{\mu}_V + \boldsymbol{\mu}_T$. This model, which is immediately marginal to $\mathrm{E}[Y] = V.T$, corresponds to a mechanism in which the two factors are (additively) independent.

$\mathrm{E}[Y] = V$ The formal expressions are $\mathrm{E}[y_{(ij)klm}] = \zeta_i$ and, in vector notation, $\boldsymbol{\mu} = \boldsymbol{\mu}_V$. This model corresponds to V only having an

effect. It is immediately marginal to $\mathrm{E}[Y] = V + T$ and mutually exclusive to $\mathrm{E}[Y] = T$.

$\mathrm{E}[Y] = T$ The formal expressions are $\mathrm{E}[y_{(ij)klm}] = \tau_j$ and, in vector notation, $\boldsymbol{\mu} = \boldsymbol{\mu}_T$. This model corresponds to T only having an effect. It is immediately marginal to $\mathrm{E}[Y] = V + T$ and mutually exclusive to $\mathrm{E}[Y] = V$.

$\mathrm{E}[Y] = G$ The formal expressions are $\mathrm{E}[y_{(ij)klm}] = \mu$ and, in vector notation, $\boldsymbol{\mu} = \boldsymbol{\mu}_G$. This model is the constant expectation model and is immediately marginal to both the models $\mathrm{E}[Y] = V$ and $\mathrm{E}[Y] = T$.

$\mathrm{E}[Y] = \phi$ A formal expression is $\mathrm{E}[y_{(ij)klm}] = 0$. It is the zero model and is immediately marginal to the model $\mathrm{E}[Y] = G$.

That the models are distinct is established by considering the estimators for each model. For example, the estimators under the model $\mathrm{E}[Y] = V + T$ are $\overline{y}_V + \overline{y}_T - \overline{y}_G$ and under $\mathrm{E}[Y] = V$ are $\overline{y}_V$ where $\overline{y}$s are vectors of means for the levels combinations of the subscripted factors.

The set of variation models is derived by taking the highest order variation term, $R.C.S$, and the term G in combination with all possible subsets of the other terms. The Hasse diagram of the variation model is shown in figure 2.4 and the covariance-based interpretation of these variation models is given in table 2.7. The model involving the highest order term, $R.C.S$, and G is now the simplest model, other than the no variation model (ϕ) which is included only for completeness. [To be continued.]

Table 2.7: Interpretation of variation models for a split-plot experiment with main plots in a Latin square design

Model	Interpretation
$G + R.C.S$	All observations have the same covariance.
$G + R + R.C.S$	Observations from the same row are more alike than observations from different rows.
$G + R + C + R.C.S$	A pair of observations from different columns are more alike if they are from the same row.
$G + R.C + R.C.S$	Observations from the same row-column combination are more alike than those from different row-column combinations. Observations from different row-column combinations are equally alike irrespective of the row-column combinations involved
$G + R + R.C + R.C.S$	Observations from different row-column combinations are more alike if they come from the same row.
$G + R + C + R.C + R.C.S$	Observations from either the same row or the same column are more similar than observations that differ in both their row and column.

2.2.7 Expected mean squares

The expected mean squares, based on the maximal expectation and variation models, are computed for the sources in the analysis table as outlined in table 2.8. In order for these steps to be applied the study should satisfy the conditions outlined in section 2.2.5. Having computed the expected mean squares, one should then pool pseudoterms, if any, with the term(s) to which they are linked. If only pseudoterms, and not the term(s) to which they are linked, are confounded with a particular source, then pseudoterms linked to the same term should be pooled together and labelled with the name of that term (see example 3.1 in section 3.1).

Table 2.8: Steps for determining the expected mean squares for the maximal expectation and variation models

Step 1: Write down a canonical covariance component for each variation term that is not a pseudoterm;

Step 2: Determine the coefficient for each canonical covariance component. For a particular component, provided the term corresponding to it is regular, it is the replication for its term; for a simple orthogonal structure, it is the product of the orders of the factors not in its term.

Step 3: For each canonical covariance component, write the product of the component with its coefficient against any source in the table that:

- has a defining term marginal to the component's term;
- is confounded with, and hence indented under, a source marginal to the component's term;

In the expression for the expected mean square for any source which is nonorthogonal but structure-balanced, multiply the coefficients of all components arising in the same structure as it by its efficiency factor That is, multiply the coefficients of all variation terms to which it is marginal.

Step 4: For each source in the table that corresponds to an expectation term, include an expectation component which is the same quadratic form, in the expectation of the variable, as is the mean square, in the observations (Searle, 1971b).

Example 2.1 (cont'd) The expected mean squares have been derived, using the steps given in table 2.8 thereby extending table 2.4 to table 2.9. [To be continued.]

Table 2.9: Analysis of variance table for a split-plot experiment with main plots in a Latin square design.

SOURCE	DF	EXPECTED MEAN SQUARES Variation Contribution - Coefficients of $\phi_{R.C.S}$	ϕ_{RC}	ϕ_R	ϕ_C	Expectation Contribution† - function of $\boldsymbol{\mu}$
Rows	3	1	2	8		
Columns	3	1	2		8	
Rows.Columns	9					
V	3	1	2			$f_V(\boldsymbol{\mu})$
Residual	6	1	2			
Rows.Columns.Subplots	16					
T	1	1				$f_T(\boldsymbol{\mu})$
V.T	3	1				$f_{VT}(\boldsymbol{\mu})$
Residual	12	1				
Total	31					

†The functions giving the expectation contribution under the maximal expectation model are as follows:

$$\begin{aligned} f_V(\boldsymbol{\mu}) &= 8\Sigma((\overline{\zeta\tau})_{i.} - (\overline{\zeta\tau})_{..})^2/3; \\ f_T(\boldsymbol{\mu}) &= 16\Sigma((\overline{\zeta\tau})_{.j} - (\overline{\zeta\tau})_{..})^2; \\ f_{VT}(\boldsymbol{\mu}) &= 4\Sigma\Sigma((\zeta\tau)_{ij} - (\overline{\zeta\tau})_{i.} - (\overline{\zeta\tau})_{.j} + (\overline{\zeta\tau})_{..})^2/3; \end{aligned}$$

where the dot subscript denotes summation over that subscript.

2.2.8 Model fitting/testing

Model testing and fitting, based on the analysis of variance method, have been discussed by Brien (1989). The purpose of model testing is to see if the expectation and variation models can be reduced to more parsimonious models that still adequately describe the data. The purpose of model fitting is to obtain the fitted values, and their variances, for a particular expectation model.

Basic to model testing and fitting are the stratum components. A **stratum** is a source in an analysis of variance table whose expected mean square includes canonical covariance components but not functions of the expectation vector. That is, a source whose defining term is a variation term. The **stratum component** is then the covariance associated with a stratum which is expressible as the linear combination of canonical covariance components corresponding to the expected mean square for the stratum. This usage of stratum differs from that of Nelder (1965a,b) who uses it to mean a source in the null analysis of variance; that is, an analysis for two-tiered experiments involving only unrandomized factors.

In carrying out model fitting and testing, estimates of the stratum components are obtained by calculating mean squares from the data. The expectation parameters are estimated from linear contrasts on the data and their variances from the stratum components.

To determine if a model can be reduced, testing is carried out in steps such that the current model, initially the maximal model, is compared to a reduced model immediately above it in the lattice of models for the study. The models are compared, following traditional practice, by taking the ratio of two (linear combinations of) mean squares. The mean squares involved are such that the difference between the expected values of the numerator and the denominator is a function only of parameters for the terms by which the two models differ. Expected mean squares under reduced models are obtained by setting the omitted canonical covariance components to zero and deriving the formula for the quadratic form in the expectation vector for a reduced expectation model. One way in which the proposed model selection method differs from traditional practice arises when such ratios are used to test hypotheses

about canonical covariance components; when the canonical covariance components are being interpreted as covariances, as in this thesis, the tests will be two-sided to allow for negative components (as in Smith and Murray, 1984).

For the purposes of the thesis, we will perform model testing without the pooling of nonsignificant mean squares. This is because, as Cox (1984) suggests, there is likely to be little difference in the conclusions from tests with and without pooling when there are sufficient degrees of freedom. Further the occurrence of Type II errors will lead to biased estimates of stratum components. However, estimation will be based on the selected model and, as discussed in section 3.4, will employ generalized linear models.

Variation model selection precedes expectation model selection because, in the choice between variation models, the expected mean squares will involve only canonical covariance components. On the other hand, in choosing between expectation models, the expected mean squares will include a single expectation component and one or more variation terms. This is because, for orthogonal studies at least, the variation contribution to the expected mean square for a particular source in the analysis involves only the source's and confounded sources' defining terms and terms marginal to these defining terms; any term which has a variation term marginal to it is also a variation term and it is desirable that any term that has another term confounded with it be a variation term.

2.2.8.1 Selecting the variation model

As there is to be no pooling in selecting the variation model, the order of testing is of no consequence. One merely carries out the significance tests for all terms based on the expected mean squares under the maximal variation model.

> **Example 2.1 (cont'd):** The F-ratios, when there is to be no pooling, are given in table 2.10. Based on two-sided tests, the selected variation model is
>
> $$\mathrm{Var}[Y] = G + R + R.C.S.$$
>
> The estimated canonical covariance components, obtained using generalized linear models as described in section 3.4, are
>
> $$\phi_R = 63.4 \text{ and } \phi_{RCS} = 27.4.$$

Table 2.10: Analysis of variance table for a split-plot experiment with main plots in a Latin square design.

		EXPECTED MEAN SQUARES									
		Variation Contribution – Coefficients of				Expectation Contribution† under Models					
SOURCE	DF	$\phi_{R.C.S}$	ϕ_{RC}	ϕ_R	ϕ_C	V	T	$V+T$	$V.T$	MSq	F
Rows	3	1	2	8						534.43	13.24
Columns	3	1	2		8					49.50	1.23
Rows.Columns	9										
V	3	1	2			$f_V(\boldsymbol{\mu}_V)$	–	$f_V(\boldsymbol{\mu}_V)$	$f_V(\boldsymbol{\mu}_{VT})$	498.91	
Residual	6	1	2							40.38	2.63
Rows.Columns.Subplots	16										
T	1	1				–	$f_T(\boldsymbol{\mu}_T)$	$f_T(\boldsymbol{\mu}_T)$	$f_T(\boldsymbol{\mu}_{VT})$	162.90	
$V.T$	3	1				–	–	–	$f_{VT}(\boldsymbol{\mu}_{VT})$	106.81	6.96
Residual	12	1								15.34	
Total	31										

†The functions given in the expectation contribution are as follows:

$$f_V(\boldsymbol{\mu}_{VT}) = 8\Sigma((\overline{\zeta\tau})_{i.} - (\overline{\zeta\tau})_{..})^2/3; \qquad f_V(\boldsymbol{\mu}_V) = 8\Sigma(\zeta_i - \overline{\zeta}_{.})^2/3;$$
$$f_T(\boldsymbol{\mu}_{VT}) = 16\Sigma((\overline{\zeta\tau})_{.j} - (\overline{\zeta\tau})_{..})^2; \qquad f_T(\boldsymbol{\mu}_T) = 16\Sigma(\tau_j - \overline{\tau}_{.})^2;$$
$$f_{VT}(\boldsymbol{\mu}_{VT}) = 4\Sigma\Sigma((\zeta\tau)_{ij} - (\overline{\zeta\tau})_{i.} - (\overline{\zeta\tau})_{.j} + (\overline{\zeta\tau})_{..})^2/3;$$

where the dot subscript denotes summation over that subscript.

These are exactly the same as obtained by pooling nonsignificant mean squares. The estimated canonical covariance components, without pooling, are

$$\phi_R = (534.43 - 40.38)/8 = 61.76 \text{ and } \phi_{RCS} = 15.34.$$

That is, there is a substantial difference between the two estimates for ϕ_{RCS}. [To be continued.]

2.2.8.2 Selecting the expectation model

Having settled on an appropriate variation model, one then chooses the expectation model. However, there is a marked contrast between variation and expectation model selection in the treatment of terms that are marginal to significant terms. For variation models the marginal terms are considered, whereas for expectation models they are ignored. *To examine main effects which are marginal to significant interactions is, in the context of the proposed approach, seen to be inappropriate; to do so would be to attempt to fit two different models to the same data.* The situation here parallels that when choosing between linear and quadratic models where, once significance of the quadratic term is established, the test for a linear term is inappropriate; the linear term should always be included in the model. Thus, for orthogonal expectation factors, model selection simply means testing the mean squares for expectation terms, provided they are not marginal to significant expectation terms. This is a consequence of employing a backward elimination procedure.

Because of this difference in the treatment of expectation and variation terms, significance testing may depend on the division of the factors into expectation/variation classes.

Example 2.1 (cont'd): To choose between the models

$$\mathrm{E}[Y] = V.T \text{ and } \mathrm{E}[Y] = V + T,$$

the $V.T$ mean square is appropriate since it is the only mean square whose expectation does not involve models marginal to $\mathrm{E}[Y] = V.T$ (table 2.10); to obtain the expectation contribution under reduced models one merely applies step 3 of table 2.8 to the expectation vector for the reduced model. The $V.T$ mean square is compared to the *Rows.Columns.Subplots Residual* mean square.

If $\mathrm{E}[Y] = V.T$ is selected as the appropriate model then there is no need to go further at this stage. We have determined our expectation model.

If $\mathrm{E}[Y] = V.T$ is rejected, then choosing between the models

$$\mathrm{E}[Y] = G,\ \mathrm{E}[Y] = V,\ \mathrm{E}[Y] = T \text{ and } \mathrm{E}[Y] = V + T$$

is based on the V and T mean squares. The appropriate denominator for testing the T mean square, when nonsignificant terms are not pooled, would be the *Rows.Columns.Subplots Residual* mean square; the *Rows.Columns Residual* mean square would be used to test the V mean square.

If both the V and T mean squares are significant, the model $\mathrm{E}[Y] = V + T$ is appropriate. If only one of V or T is significant, a model involving the

significant term is sufficient. Otherwise, if neither is significant, $\mathrm{E}[Y] = G$ is the appropriate model.

If V and T had been designated as variation factors then the tests about terms involving these factors would differ from those just described. A test for T would be performed irrespective of whether $V.T$ was significant and, further, would have $V.T$ as the denominator rather than the *Rows.Columns.Subplots Residual* source.

In fact, V and T are clearly expectation factors and the $V.T$ term is significant so that the interaction model is required to describe the data adequately. The estimates of the expectation parameters are the means given in table 2.11. An examination of this table reveals the differential response of Vicland (1) and the other varieties to the treatments.

Table 2.11: Estimates of expectation parameters for a split-plot experiment with main plots in a Latin square design.

	Treatment	
Variety	Check	Ceresan M
Vicland (1)	36.0	50.6
Vicland (2)	50.8	55.4
Clinton	53.9	51.5
Branch	61.9	63.4

Chapter 3

Analysis of variance quantities

3.1 Introduction

In chapter 2 a method of linear model analysis based on comparing alternative models was outlined. Central to this method is computation of an analysis of variance table which guides the comparison of mean squares based on their expectation under the various models.

It is the purpose of this chapter to provide the justification of the rules given in chapter 2 for obtaining the important quantities in such tables, namely the degrees of freedom, sums of squares and expected mean squares. The rules will be established for the maximal models from multitiered studies (section 2.2.2; Brien, 1983) in which the structures, derived from the tiers that contain variation factors, are regular. Further, attention is restricted to structure-balanced experiments in a sense similar to that described in section 1.2.2.2 and elucidated in section 3.3.1. Results for this class of experiments have not been supplied previously.

The rules given in chapter 2 rely on the degrees of freedom, sums of squares and expected mean squares for a single structure. Thus, we shall first outline, in section 3.2, the algebraic analysis of a single structure. This will provide a basis from which the results for a whole analysis of variance for a multitiered study can be assembled in section 3.3.

The derivation of the expressions for quantities for a single structure is achieved via an analysis of the algebra generated by the summation matrices for a structure (James, 1957, 1982; Speed and Bailey, 1982). This analysis involves establishing the connection between the three types of matrices fundamental to an analysis of variance (Speed and Bailey, 1982; Brien, Venables, James and Mayo, 1984; Tjur, 1984; Speed, 1986), namely incidence matrices ($\mathbf{W}$), summation/relationship matrices ($\mathbf{S}$) and orthogonal idempotent operators ($\mathbf{E}$). The role for the incidence matrices is to provide a basis for the specification of the variation model in terms of the covariance components (γs), that, in some circumstances, are the covariances between pairs of observations. Three roles for the summation matrices are to specify the relationships between the observations and so provide a basis for the relationship algebra for a structure (James, 1957, 1982; Speed and Bailey, 1982), to obtain expressions for the sums of squares that are convenient for calculation purposes and to provide a basis for specifying the model for the variance matrix in terms of the canonical covariance components (ϕs) (Nelder, 1965a and 1977). The idempotents are the mutually orthogonal idempotents of the relationship algebra, the matrices of the sums-of-squares quadratic forms, and a basis for specifying the model for the variance matrix in terms of the spectral components (λs). Expressions for the expected mean squares, in terms of these latter quantities, are particularly simple as we shall see.

Having separately obtained the quantities for the structures in the study, the results are merged to produce the final analysis. This is done by identifying for a structure, the ith say, a set of projection operators that specify an orthogonal decomposition of the sample space taking into account the terms in the first i structures. The ith set of projection operators is obtained by taking the projection operators from the $(i-1)$th structure and the set of terms from the ith structure. The set of projection operators from the $(i-1)$th structure that have terms from the ith structure estimated from their range will be partitioned to yield the projection operators for the ith structure. A term will be estimated from the range of a projection operator from the $(i-1)$th structure if the term is confounded with the source corresponding to the projection operator.

The confounding relationships between sources will be illustrated using a **decom-**

position tree, this tree also depicting the analysis of variance decomposition. Its root is the sample space or uncorrected *Total* source. Connected directly to the root are the sources arising from the first structure. The sources arising from the second structure are connected to the sources from the first structure with which they are confounded; sources from the third structure, if any, are similarly connected to sources from the second and so on. For examples, see figures 3.3, 3.6 and 3.5.

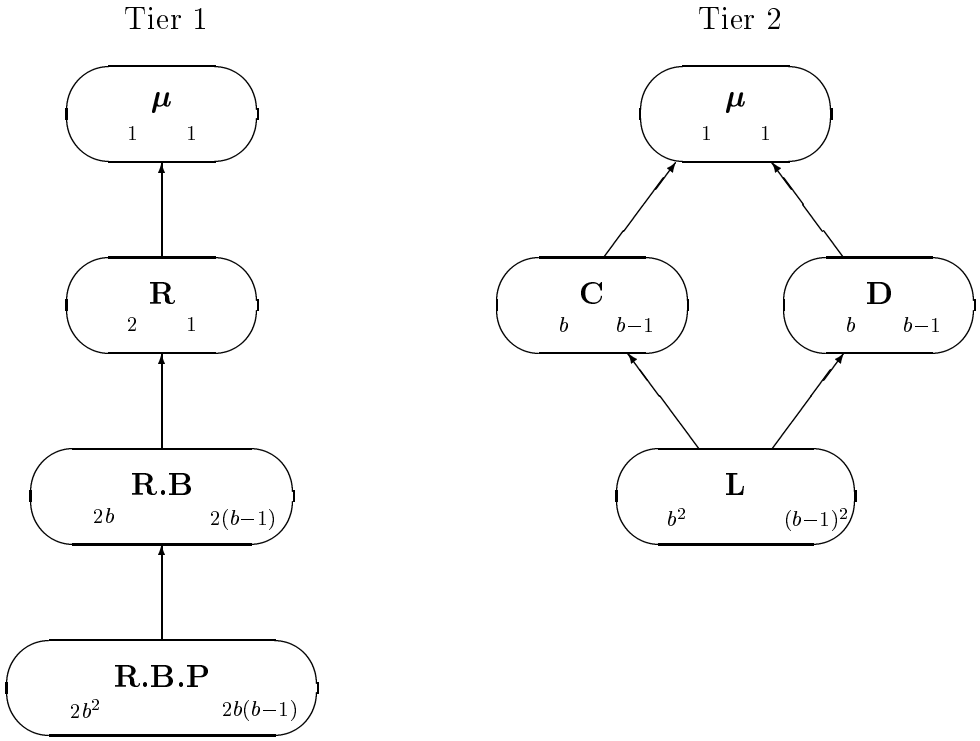
Before proceeding to the derivation of the expressions, we introduce a simple nonorthogonal example to be used, as a supplement to the orthogonal experiment presented in chapter 2, in demonstrating the application of the results.

Figure 3.1: Field layout and yields for a simple lattice experiment

		Replicates					
		I			II		
Block		1	2	3	1	2	3
	1	1 18	5 19	3 21	1 23	5 21	9 17
Plot	2	4 13	2 18	6 22	2 25	4 23	8 20
	3	7 11	8 14	9 26	3 27	6 25	7 17

Example 3.1: In an experiment, different lines of a plant are randomized according to a simple lattice design (Cochran and Cox, 1957, section 10.21). This involves the association of two pseudofactors (Wilkinson and Rogers, 1973), C and D say, with the levels of *Lines*. The levels of one of the *Lines* pseudofactors, C say, is randomized within the blocks of the first replicate and between the blocks of the second replicate; the complementary between-block and within-block randomizations are performed for the other pseudofactor, D. The factors in the first tier are *Reps*, *Blocks*, and *Plots* and the factors in the second tier are *Lines*. The field layout and yields (from Wilkinson, 1970) are given in figure 3.1.

Figure 3.2: Hasse diagram of term marginalities for a simple lattice experiment



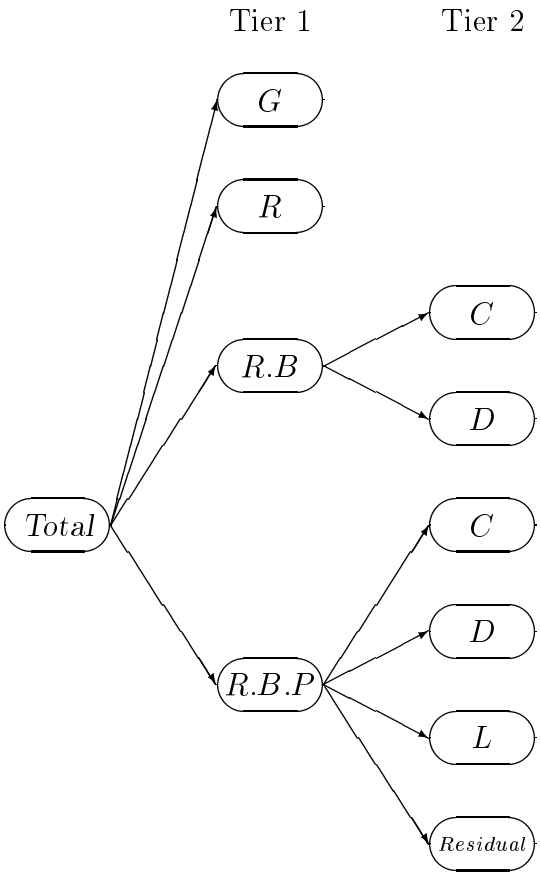
The structure set is as follows:

Tier	Structure
1	*2 Reps/3 Blocks/3 Plots*
2	*9 Lines//(3 C+3 D)*

It is necessary to include the pseudofactors C and D in the structure derived from tier 2 to obtain a set of structure-balanced terms.

The Hasse diagrams of term marginalities, giving the terms and their degrees of freedom, are shown in figure 3.2 and the decomposition tree is given in figure 3.3.

Figure 3.3: Decomposition tree for a simple lattice experiment



If the factors in both tiers of the experiment are classified as being variation factors, then the maximal expectation and variation models are expressed symbolically as follows:

$$\mathrm{E}[\boldsymbol{y}] = G \qquad \text{and} \qquad \mathrm{Var}[\boldsymbol{y}] = G + R + R.B + R.B.P + L.$$

The analysis table and expected mean squares for the experiment are shown in table 3.1; general expressions for the contents of this table are given in table 3.4. In testing for *Lines*, the pseudoterms and *Lines* sources confounded with the same source are usually pooled as the individual terms are of no scientific interest *per se*. [To be continued.]

Table 3.1: Analysis of variance table for a simple lattice experiment

SOURCE	DF	EXPECTED MEAN SQUARES Coefficients of ϕ_{RBP}	ϕ_{RB}	ϕ_R	ϕ_L	MSq	Pooled MSq	F
Reps	1	1	3	9		72.0	72.0	
Reps.Blocks	4							
$C^\dagger$	2	1	3		$\frac{1}{2}2$	39.0		
$D^\dagger$	2	1	3		$\frac{1}{2}2$	63.0		
Lines‡	4	1	3		$\frac{1}{2}2$		51.0	
Reps.Blocks.Plots	12							
$C^\dagger$	2	1			$\frac{1}{2}2$	3.0		
$D^\dagger$	2	1			$\frac{1}{2}2$	3.0		
Lines	4	1			2	2.0		
Lines‡	8	1			$\frac{3}{2}$		2.5	0.18
Residual	4	1				14.0	14.0	

†These sources are partially confounded with efficiency $\frac{1}{2}$.
‡These lines are obtained by pooling the C, D and *Lines* sources confounded with the same source.

3.2 The algebraic analysis of a single structure

We outline useful results obtained from the analysis of the relationship algebra generated by the set of terms derived from the factors in a Tjur structure (Tjur, 1984, section 4.1; Bailey, 1984), although results for the special case of a simple orthogonal structure (Nelder (1965a) will also be given. The results for simple orthogonal structures are contained in the papers by Nelder (1965a), Haberman (1975), Khuri (1982), Speed and Bailey (1982), Tjur (1984), Speed (1986) and Speed and Bailey (1987); the results for a Tjur structure are obtained from Tjur (1984) and Bailey (1984). In deriving results from Tjur (1984), in particular, one should bear in mind that Tjur's factors and nestedness of factors correspond to my terms and marginality of terms, respectively. Also, my minima of terms and intersection of model subspaces correspond to Tjur's minima of factors. Further, it is important to note that, whereas the presentations of some of these authors are intimately bound up with the models for the data, in this section we consider only properties that derive solely from the structure and layout as summarized in the summation/relationship matrices.

A feature of the class of structures presented in this thesis is that, while there has to be a maximal term derived from the structure to which all other terms derived from the structure are marginal, there does not have to be a unit term derived from the structure. But, to derive the results given in this section, if the number of observed levels combinations for the factors in the structure is not equal to the number of observational units, n, a dummy factor is introduced to provide a unit term. This factor is nested within all the other factors in the structure. However, it will become apparent that the theorems given in this section for Tjur structures will produce the correct results for the original factors in a structure even if the dummy factor is omitted.

Any structure summarizes the relationships between a set of factors, $F_i = \{t_{ih}, h = 1, \ldots, f_i\}$ with the order of factor t_{ih} being $n_{t_{ih}}$. Levels of these factors are observed for each observational unit and so can be indexed by the index set for the observational units, I which has n elements. The set of terms in a structure, $T_i = \{T_{iv}, \quad v = 1, \ldots, t_i\}$, is obtained by expanding the formula for the structure according to the rules

given by Wilkinson and Rogers (1973). Of course, a term $T_{iv} \in T_i$ either corresponds to one of the factors t_{ih} from the original set of factors F_i or can be thought of as defining a new factor whose levels correspond to the levels combinations of the original factors (Tjur, 1984). However, I reserve the name factor for those in the original set. Terms will be either one of these factors or be composed of several factors. A term usually represents a meaningful partition of the observational units into subsets formed by placing in a subset those observational units that have the same levels combination of the factors in the term. The subsets formed in this way have been referred to as the term's observational-unit subsets. A term T_{iv} is marginal to T_{iw} ($T_{iv} \leq T_{iw}$) if the model space of T_{iv} is a subspace of the model space of T_{iw}, this being the case because of the innate relationship between the levels combinations of the two terms and being independent of the replication of the levels combination of the two terms. This will occur if the factors comprising T_{iv} are a subset of those comprising T_{iw}, i.e. $T_{iv} \subseteq T_{iw}$.

For a simple orthogonal structure, the factors are simple and either crossed or nested and $n = r_i \prod_{h=1}^{f_i} n_{t_{ih}}$.

Further, associated with any structure will be the sets of incidence matrices, $W_i = \{\mathbf{W}_{T_{iv}}, v = 1, \ldots, t_i\}$, summation matrices, $S_i = \{\mathbf{S}_{T_{iv}}, v = 1, \ldots, t_i\}$, and mutually orthogonal idempotent operators, $E_i = \{\mathbf{E}_{T_{iv}}, i = v, \ldots, t_i\}$. The matrices making up these sets are of order n. The elements of these sets are, for Tjur structures, specified by definitions 3.2 and 3.3 and theorem 3.5; for simple orthogonal structures, they are specified by theorems 3.6–3.8.

Example 3.2: Consider a study with $rcsu$ observational units and a single tier consisting of three factors, *Rows* (R) with r levels, *Columns* (C) with c levels and *Subplots* (S) with s levels. Further suppose that the structure for the study is $(R * C)/S$. As the levels combinations of the factors in the structure do not uniquely index the observational units, a dummy factor *Units* (U) with u levels has to be included in the structure; it is nested within the other factors in the structure so that the modified structure is $(R * C)/S/U$.

For this modified structure,

$$\begin{aligned} n &= rcsu, \\ f_1 &= 4 \\ F_1 &= \{\textit{Rows}, \textit{Columns}, \textit{Subplots}, \textit{Units}\}, \end{aligned}$$

$$\begin{aligned} n_R &= r, \quad n_C = c, \quad n_S = s \quad \text{and} \quad n_U = u, \\ t_1 &= 6, \\ T_1 &= \{G, R, C, R.C, R.C.S, R.C.S.U\}, \\ W_1 &= \{\mathbf{W}_G, \mathbf{W}_R, \mathbf{W}_C, \mathbf{W}_{R.C}, \mathbf{W}_{R.C.S}, \mathbf{W}_{R.C.S.U}\}, \\ S_1 &= \{\mathbf{S}_G, \mathbf{S}_R, \mathbf{S}_C, \mathbf{S}_{R.C}, \mathbf{S}_{R.C.S}, \mathbf{S}_{R.C.S.U}\}, \text{and} \\ E_1 &= \{\mathbf{E}_G, \mathbf{E}_R, \mathbf{E}_C, \mathbf{E}_{R.C}, \mathbf{E}_{R.C.S}, \mathbf{E}_{R.C.S.U}\}. \end{aligned}$$

[To be continued.]

Before proceeding to establish the results of the analysis of the relationship algebra for a single structure, some mathematical definitions and results are provided; they have been taken from Grätzer (1971).

Definition 3.1 *A* **partially ordered set** *or* **poset** $\langle P; \leq \rangle$ *is a set* P *of elements* $a, b, c, \ldots$ *with a binary relation, denoted by '*$\leq$*', which satisfy the following properties:*

i)	$a \leq a$,	(Reflexive)
ii)	If $a \leq b$ and $b \leq c$, then $a \leq c$,	(Transitive)
iii)	If $a \leq b$ and $b \leq a$, then $a = b$	(Antisymmetric)

Clearly, a relation satisfying these properties establishes an ordering between the elements of P*. Note also that* $a \leq b$ *can be written* $b \geq a$ *and that we write* $a < b$ *(or* $b > a$*) if* $a \leq b$ *and* $a \neq b$*.*

If $\langle P; \leq \rangle$ *is a poset,* $a, b \in P$*, then* a *and* b *are* **comparable** *if* $a \leq b$ *or* $b \leq a$*. Otherwise,* a *and* b *are* **incomparable***, in notation* $a \| b$*.*

Let $H \subseteq P$*,* $a \in P$*. Then* a *is a* **lower bound** *of* H *if* $a \leq h$ *for all* $h \in H$*. A lower bound* a *of* H *is the unique* **greatest lower bound** *of* H *if, for any lower bound* b *of* H*,* $b \leq a$*. We shall write* $a = \bigwedge H$*. For two elements* $c, d \in P$*, we will denote their greatest lower bound by* $c \wedge d$ *where* $\wedge$ *is called the* **meet***. A* **meet-semilattice** *is a poset for which any two elements have a greatest lower bound.*

An **upper bound** *and a* **least upper bound** *are similarly defined. A least upper bound for two elements* $c, d \in P$ *will be denoted by* $c \vee d$ *where* $\vee$ *is called the* **join***. A* **join-semilattice** *is a poset for which any two elements have a least upper bound.*

A **lattice** *is a set* P *of elements* $a, b, c, \ldots$ *with two binary operations* $\vee$ *and* $\wedge$ *which satisfy the following properties:*

$$\begin{array}{lrcll}
\text{i)} & a \vee a & = & a \wedge a = a, & \text{(Idempotent)} \\
\text{ii)} & a \vee b & = & b \vee a, & \\
 & a \wedge b & = & b \wedge a, & \text{(Commutative)} \\
\text{iii)} & a \vee (b \vee c) & = & (a \vee b) \vee c, & \\
 & a \wedge (b \wedge c) & = & (a \wedge b) \wedge c, & \text{(Associative)} \\
\text{iv)} & a \vee (a \wedge b) & = & a \wedge (a \vee b) = a & \text{(Absorption)}
\end{array}$$

A poset P is a lattice if and only if it is a join-semilattice and a meet-semilattice. A **distributive lattice**, *in addition to satisfying the properties for a lattice, satisfies the following distributive property:*

$$(a \wedge b) \vee (a \wedge c) = a \vee (b \wedge c).$$

Suppose the poset P possesses unique minimal and maximal elements. The Zeta function of the poset signifies which elements of the poset satisfy its order relation; that is

$$\zeta(a, c) = \begin{cases} 1 & \text{if } a \leq c \\ 0 & \text{otherwise.} \end{cases}$$

The inverse of this function, in the incidence algebra, is known as the Möbius function of the poset which, for $a, c \in P$, is given by

$$\begin{aligned}
\mu(a, a) &= 1 \\
\mu(a, c) &= -\sum_{a \leq b < c} \mu(a, b) = -\sum_{a < b \leq c} \mu(b, c), \quad a < c
\end{aligned}$$

(for more detail see Aigner, 1979; Speed and Bailey, 1987).

Note that the Zeta function of a poset can be represented as a matrix whose elements are the Zeta function for a pair of elements of the poset. The Möbius function is then represented by the inverse of this matrix.

The use of the Zeta and Möbius functions of the poset in the present context has been advocated by Speed and Bailey (1982), Tjur (1984) and Speed and Bailey (1987). The interest in the Zeta function of a poset P arises from the fact that we will be concerned with sums of real-valued functions, $u(c)$ and $v(a)$ say, the sums being of the following forms:

$$u(c) = \sum_{a \in P} \zeta(a, c) v(a) \quad \text{or} \quad u(c) = \sum_{a \in P} \zeta(c, a) v(a).$$

To then obtain expressions for $v(c)$ in terms of $u(a)$ involves Möbius inversion as specified by the following theorem:

Theorem 3.1 (Möbius inversion) *Let P be a finite poset, and $u(a)$ and $v(a)$ be real-valued functions defined for $a \in P$. Then,*

(i) inversion from below is given by

$$u(c) = \sum_{a \leq c} v(a), = \sum_{a \in P} \zeta(a,c)v(a), c \in P \quad \Leftrightarrow \quad v(c) = \sum_{a \leq c} u(a)\mu(a,c), c \in P;$$

(ii) inversion from above is given by

$$u(c) = \sum_{a \geq c} v(a) = \sum_{a \in P} \zeta(c,a)v(a), c \in P \quad \Leftrightarrow \quad v(c) = \sum_{a \geq c} u(a)\mu(c,a), c \in P.$$

Proof: Theorem 4.18 from Aigner (1979, IV.2) specifies that the above formulae for inversion apply to locally finite posets with all principal ideals and filters finite; also, the maps must be to an integral domain containing the rationals.

Let the **principal ideal** L_c for $c \in P$ be the set $\{a \mid a \in P, \quad a \leq c\}$ and the **principal filter** G_c for $c \in P$ be the set $\{a \mid a \in P, \quad a \geq c\}$. All principal ideals and principal filters of a finite poset P are finite as they are subsets of a finite set.

Clearly, the theorem is a specialised version of theorem 4.18 from Aigner (1979, IV.2). □

The following theorem will be useful in calculating the Möbius function for the posets with which we will be dealing.

Theorem 3.2 *Let $\langle P; \leq \rangle$ be a meet-semilattice and define the set of immediate descendants of c to be the set*

$$\{b \mid b \in P, b \leq c, \text{ there exists no } d \text{ such that } b < d < c\}.$$

Let D_c be the set of all $a \in P$ that are the meets of immediate descendants of c.

If $a < c$ and $a \notin D_c$, then $\mu(a,c) = 0$.

If $\langle P; \leq \rangle$ is a finite distributive lattice, then

$$\mu(a,c) = \begin{cases} = (-1)^k & \text{if } a \in D_c, \\ 0 & \text{otherwise} \end{cases}$$

where

k is the number of distinct immediate descendants of c whose meet is a.

Proof: The result for a meet-semilattice is derived by application of the duality principle for posets (see Grätzer, 1971, p.3) to the theorem of P. Hall given by Berge (1971, p.88). The dual result for a finite distributive lattice is given by Rota (1964). □

The applicability of the above theorem is evident upon noting that the terms from a Tjur structure form a meet-semilattice where the relation is that of marginality between terms. This is because the minima ('meet') of two terms is their greatest lower bound and the terms from Tjur structures are closed under the formation of minima. Also note that a term is immediately marginal to another if it is an immediate descendant of the other. Further, the terms from a simple orthogonal structure form a finite distributive lattice (Bailey, 1981; Speed and Bailey, 1982; Speed and Bailey, 1987).

Next we establish the form of the three matrix types fundamental to our analysis.

Definition 3.2 $\mathbf{W}_{T_{iw}}$ *is the $n \times n$ symmetric incidence matrix with element*

$$w_{gh} = \begin{cases} 1 & \text{if observational units } g \text{ and } h,\ g,h \in I, \text{ have the same levels} \\ & \text{combination of the factors in } T_{iw} \text{ and there is no term } T_{iv} > \\ & T_{iw} \text{ such that observational units } g \text{ and } h \text{ have the same} \\ & \text{levels combination of the factors in } T_{iv}, \\ 0 & \text{otherwise.} \end{cases}$$

Corollary 3.3 *The* **maximum of terms** *is the term that is the union of the factors from the terms for which it is the maximum. If the terms in T_i are closed under the formation of maxima, then*

$$\sum_{T_{iw} \in T_i} \mathbf{W}_{T_{iw}} = \mathbf{J}.$$

Proof: As the grand mean term G is always included in the set of terms there must be, for every pair of observational units, some $\mathbf{W}_{T_{iw}}, T_{iw} \in T_i$ which has $w_{gh} = 1$, $g, h \in I$. Further there can be only one such matrix. Suppose there were two matrices, corresponding to terms T_{iw} and T_{iv}, for which $w_{gh} = 1$. However, the terms must be incomparable, otherwise, if one is marginal to the other, the element would be zero for the term to which the other is marginal. But the terms are closed under the formation of maxima. So there exists a term whose levels combinations will be equal only for units for which the levels combinations of both incomparable terms are equal. The two terms are marginal to this term, their maximum. Hence, the elements of the incidence matrices corresponding to the two incomparable terms must be zero. That is, there cannot be two terms for which $w_{gh} = 1$ and the condition given in the corollary follows. □

Definition 3.3 $\mathbf{S}_{T_{iw}}$ *is the* $n \times n$ *symmetric summation matrix with element*

$$s_{gh} = \begin{cases} 1 & \textit{if observational units } g \textit{ and } h,\ g, h \in I, \textit{ have the same levels} \\ & \textit{combination of the factors in } T_{iw}, \\ 0 & \textit{otherwise.} \end{cases}$$

Corollary 3.4

$$\mathbf{S}_{T_{iw}} = \sum_{T_{iv} \geq T_{iw}} \mathbf{W}_{T_{iv}}.$$

This corollary is obvious upon comparison of definition 3.2 with 3.3.

Theorem 3.5 *For each term* T_{iw} *from a Tjur structure, there exists an* $n \times n$ *symmetric idempotent matrix,* $\mathbf{E}_{T_{iw}}$*, that is given by*

$$\mathbf{E}_{T_{iw}} = \sum_{T_{iv} \in \{T_{iw}\} \cup D_{T_{iw}}} \mu(T_{iv}, T_{iw}) \mathbf{R}_{T_{iv}}^{-1} \mathbf{S}_{T_{iv}} \quad \textit{with} \sum_{T_{iw} \in T_i} \mathbf{E}_{T_{iw}} = \mathbf{I}$$

where

$D_{T_{iw}}$ *is the set of terms in the ith structure that are the minima of terms immediately marginal to the term* T_{iw}*, and*

$\mathbf{R}_{T_{iv}}$ *is the diagonal replications matrix of order n. A particular diagonal element is the replication of the levels combination of the factors in term* T_{iv} *for the observational unit corresponding to that element. For a regular term,* $\mathbf{R}_{T_{iv}} = r_{T_{iv}}\mathbf{I}$.

Proof: From theorem 1 of Tjur (1984), we have that the sample space can be written as the direct sum of a set of orthogonal subspaces, one subspace for each $T_{iw} \in T_i$. Then, denoting by $\mathbf{E}_{T_{iw}}$ the orthogonal idempotent that projects on the model space for T_{iw}, we have

$$\sum_{T_{iw} \in T_i} \mathbf{E}_{T_{iw}} = \mathbf{I}.$$

Further, from theorem 1 of Tjur (1984), we have that

$$\begin{aligned} \mathbf{R}_{T_{iw}}^{-1}\mathbf{S}_{T_{iw}} &= \sum_{T_{iv} \leq T_{iw}} \mathbf{E}_{T_{iv}} \\ &= \sum_{T_{iv} \in T_i} \zeta(T_{iv}, T_{iw})\mathbf{E}_{T_{iv}}. \end{aligned}$$

Next, this last expression is to be inverted. Consider a pair of corresponding elements from the matrices $\mathbf{R}_{T_{iw}}^{-1}\mathbf{S}_{T_{iw}}$ and $\mathbf{E}_{T_{iv}}$. We have two real-valued functions, a particular function mapping an element of T_i to an element of its matrix. Also the set T_i is finite. Hence, by Möbius inversion (theorem 3.1),

$$\mathbf{E}_{T_{iw}} = \sum_{T_{iv} \in T_i} \mu(T_{iv}, T_{iw})\mathbf{R}_{T_{iv}}^{-1}\mathbf{S}_{T_{iv}}.$$

But from theorem 3.2, $\mu(T_{iv}, T_{iw}) \neq 0$ only for T_{iw} and for $T_{iv} \in D_{T_{iw}}$ and so

$$\mathbf{E}_{T_{iw}} = \sum_{T_{iv} \in \{T_{iw}\} \cup D_{T_{iw}}} \mu(T_{iv}, T_{iw})\mathbf{R}_{T_{iv}}^{-1}\mathbf{S}_{T_{iv}}.$$

□

Theorems 3.6–3.8 specify the form of the incidence matrices, summation matrices and idempotent operators for a simple orthogonal structure. These theorems are given

without proof as the results are available in, for example, Nelder (1965a). The forms are given in terms of $\mathbf{I}$ or unit matrices, $\mathbf{J}$ or matrices of ones, $\mathbf{K}$ $(= \mathbf{J} - \mathbf{I})$ matrices and $\mathbf{G}$ $(= m^{-1}\mathbf{J}$ where m is the order of $\mathbf{J})$ matrices. The forms given apply only if the observational units are arranged in lexicographical order according to the factors in the structure. While this can be easily arranged for the first structure, it cannot be arranged concomitantly for the other structure(s). However, the form for structures other than the first can be obtained by premultiplying the matrices derived according to theorems 3.6–3.8 with a permutation matrix and postmultiplying by its transpose. The permutation matrix for a structure, $\mathbf{U}_i$, specifies the association between the observed levels combinations of the factors in the structure and the observational units. As noted above, if the number of observed levels combinations of the factors in the structure is not equal to the number of observational units, a dummy factor is included so that the factors in the structure uniquely index the observational units. Note that, except for theorems 3.6–3.8, the remainder of the theorems given in this section are independent of the ordering of the levels combinations of the factors in a structure.

A particular incidence matrix, $\mathbf{W}_{T_{iw}} \in W_i$, for each term from a simple orthogonal structure can be expressed as the direct product of $\mathbf{I}$, $\mathbf{J}$ and $\mathbf{K}$ matrices, premultiplied by $\mathbf{U}_i$ and postmultiplied by $\mathbf{U}_i'$. The direct product is given by the following theorem:

Theorem 3.6 *The direct product for an incidence matrix will contain an* $\mathbf{I}$*,* $\mathbf{J}$ *or* $\mathbf{K}$ *matrix of order* $n_{t_{ih}}$ *for each factor in the structure. In determining the incidence matrix for a particular term,* T_{iw}*, use: an* $\mathbf{I}$ *matrix for a factor* t_{ih} *if* $t_{ih} \in T_{iw}$*; a* $\mathbf{J}$ *matrix for a factor* t_{ih} *if there exists a factor that nests* t_{ih}*,* $t_{ih} \notin T_{iw}$ *and* $(t_{ih} \cup T_{iw}) \in T_i$*; and a* $\mathbf{K}$ *matrix otherwise.*

A particular summation matrix, $\mathbf{S}_{T_{iw}} \in S_i$, can be expressed as the direct product of $\mathbf{J}$ and $\mathbf{I}$ matrices, premultiplied by $\mathbf{U}_i$ and postmultiplied by $\mathbf{U}_i'$. The direct product is given by the following theorem:

Theorem 3.7 *The direct product for a summation matrix will contain an* $\mathbf{I}$ *or* $\mathbf{J}$ *matrix of order* $n_{t_{ih}}$ *for each factor in the structure. In determining the summation*

matrix for a particular term, use an $\mathbf{I}$ *matrix if the factor is in the term* ($t_{ih} \in T_{iw}$) *and a* $\mathbf{J}$ *otherwise.*

A particular idempotent matrix, $\mathbf{E}_{T_{iw}} \in E_i$, can be expressed as the direct product of $\mathbf{I}$, $\mathbf{G}$ and $\mathbf{I}-\mathbf{G}$ matrices, premultiplied by $\mathbf{U}_i$ and postmultiplied by $\mathbf{U}_i'$. The direct product is given by the following theorem:

Theorem 3.8 *The direct product for an idempotent matrix will contain an* $\mathbf{I}$, $\mathbf{G}$ *or* $\mathbf{I}-\mathbf{G}$ *matrix of order* $n_{t_{ih}}$ *for each factor in the structure. Let* $N_{T_{iw}}$ *be the set of factors in* T_{iw} *that nest other factors in* T_{iw}*. In determining the idempotent for a particular term,* $\mathbf{I}-\mathbf{G}$ *is included in the direct product for each of the factors in the term provided that they do not nest factors in the current term* ($t_{ih} \in (T_{iw} \cap \overline{N}_{T_{iw}})$)*, in which case an* $\mathbf{I}$ *matrix is included* ($t_{ih} \in N_{T_{iw}}$)*.* $\mathbf{G}$ *is included for factors not in the current term* ($t_{ih} \notin T_{iw}$)*.*

> **Example 3.2 (cont'd):** Application of theorems 3.6–3.8 to the example yields the expressions for the incidence, summation and idempotent matrices given in table 3.2. In this case $\mathbf{U}_1 = \mathbf{I}$ and so is not included in the table. [To be continued.]

Definitions 3.2 and 3.3 and theorem 3.5 establish the form of the three fundamental matrix types for Tjur structures; theorems 3.6 to 3.8 do the same for simple orthogonal structures. In general, we will be concerned with linear combinations of these matrices and changing from a linear combination based on one type of matrix to an equivalent linear combination based on another type. That is, suppose we have a matrix $\mathbf{Z}$, then we are interested in the following linear forms in the three matrix types:

$$\begin{aligned} \mathbf{Z} &= \boldsymbol{c}_i'\boldsymbol{w}_i \\ &= \boldsymbol{f}_i'\boldsymbol{s}_i \\ &= \boldsymbol{l}_i'\boldsymbol{e}_i \quad \text{with } \mathbf{1}'\boldsymbol{e}_i = \mathbf{I}. \end{aligned}$$

In order to be able to convert the basis of a linear form from one of the three matrix types to another, we establish below the form of the following set of six transformation matrices: $\mathbf{T}_{\boldsymbol{w}_i\boldsymbol{s}_i}$, $\mathbf{T}_{\boldsymbol{s}_i\boldsymbol{w}_i}$, $\mathbf{T}_{\boldsymbol{s}_i\boldsymbol{e}_i}$, $\mathbf{T}_{\boldsymbol{e}_i\boldsymbol{s}_i}$, $\mathbf{T}_{\boldsymbol{w}_i\boldsymbol{e}_i}$ and $\mathbf{T}_{\boldsymbol{e}_i\boldsymbol{w}_i}$. The matrix $\mathbf{T}_{\boldsymbol{a}_i\boldsymbol{b}_i}$ is the

Table 3.2: Direct product expressions for the incidence, summation and idempotent matrices for $(\boldsymbol{R} * \boldsymbol{C})/\boldsymbol{S}/\boldsymbol{U}$[†]

	Incidence				Summation			
Factor	R	C	S	U	R	C	S	U
Term								
G	$\mathbf{K}$	$\mathbf{K}$	$\mathbf{J}$	$\mathbf{J}$	$\mathbf{J}$	$\mathbf{J}$	$\mathbf{J}$	$\mathbf{J}$
R	$\mathbf{I}$	$\mathbf{K}$	$\mathbf{J}$	$\mathbf{J}$	$\mathbf{I}$	$\mathbf{J}$	$\mathbf{J}$	$\mathbf{J}$
C	$\mathbf{K}$	$\mathbf{I}$	$\mathbf{J}$	$\mathbf{J}$	$\mathbf{J}$	$\mathbf{I}$	$\mathbf{J}$	$\mathbf{J}$
$R.C$	$\mathbf{I}$	$\mathbf{I}$	$\mathbf{K}$	$\mathbf{J}$	$\mathbf{I}$	$\mathbf{I}$	$\mathbf{J}$	$\mathbf{J}$
$R.C.S$	$\mathbf{I}$	$\mathbf{I}$	$\mathbf{I}$	$\mathbf{K}$	$\mathbf{I}$	$\mathbf{I}$	$\mathbf{I}$	$\mathbf{J}$
$R.C.S.U$	$\mathbf{I}$	$\mathbf{I}$	$\mathbf{I}$	$\mathbf{I}$	$\mathbf{I}$	$\mathbf{I}$	$\mathbf{I}$	$\mathbf{I}$

	Idempotent			
Factor	R	C	S	U
Term				
G	$\mathbf{G}$	$\mathbf{G}$	$\mathbf{G}$	$\mathbf{G}$
R	$(\mathbf{I}-\mathbf{G})$	$\mathbf{G}$	$\mathbf{G}$	$\mathbf{G}$
C	$\mathbf{G}$	$(\mathbf{I}-\mathbf{G})$	$\mathbf{G}$	$\mathbf{G}$
$R.C$	$(\mathbf{I}-\mathbf{G})$	$(\mathbf{I}-\mathbf{G})$	$\mathbf{G}$	$\mathbf{G}$
$R.C.S$	$\mathbf{I}$	$\mathbf{I}$	$(\mathbf{I}-\mathbf{G})$	$\mathbf{G}$
$R.C.S.U$	$\mathbf{I}$	$\mathbf{I}$	$\mathbf{I}$	$(\mathbf{I}-\mathbf{G})$

[†]The matrices in each direct product are of order r, c, s and u, respectively.

matrix that transforms the set of matrices in the symbolic t_i-vector $\boldsymbol{b}_i$ to the set of matrices in the symbolic t_i-vector $\boldsymbol{a}_i$; that is, $\boldsymbol{a}_i = \mathbf{T}_{\boldsymbol{a}_i \boldsymbol{b}_i} \boldsymbol{b}_i$.

For incidence matrices, we will be interested in linear combinations of the form:

$$\mathbf{Z} = \boldsymbol{c}_i' \boldsymbol{w}_i$$

where

$\boldsymbol{w}_i$ is the t_i-vector of incidence matrices for the ith structure.

Example 3.2 (cont'd): The elements of $\boldsymbol{c}_1'$ and $\boldsymbol{w}_1'$ are:

$$\begin{aligned} \boldsymbol{c}_1' &= \left[\begin{array}{cccccc} c_G & c_R & c_C & c_{R.C} & c_{R.C.S} & c_{R.C.S.U} \end{array} \right]; \text{ and} \\ \boldsymbol{w}_1' &= \left[\begin{array}{cccccc} \mathbf{W}_G & \mathbf{W}_R & \mathbf{W}_C & \mathbf{W}_{R.C} & \mathbf{W}_{R.C.S} & \mathbf{W}_{R.C.S.U} \end{array} \right]. \end{aligned}$$

Whence,

$$\begin{aligned} \mathbf{Z} = {} & c_G \mathbf{W}_G + c_R \mathbf{W}_R + c_C \mathbf{W}_C + c_{R.C} \mathbf{W}_{R.C} + c_{R.C.S} \mathbf{W}_{R.C.S} \\ & + c_{R.C.S.U} \mathbf{W}_{R.C.S.U}. \end{aligned}$$

[To be continued.]

We can re-express this linear combination $\mathbf{Z}$ in terms of the elements of the set, S_i, of summation matrices using the following relationship:

$$\boldsymbol{w}_i = \mathbf{T}_{\boldsymbol{w}_i \boldsymbol{s}_i} \boldsymbol{s}_i$$

where

$\boldsymbol{s}_i$ is the t_i-vector of summation matrices for the ith structure.

Clearly,

$$\begin{aligned} \mathbf{Z} &= \boldsymbol{c}_i' \mathbf{T}_{\boldsymbol{w}_i \boldsymbol{s}_i} \boldsymbol{s}_i \\ &= \boldsymbol{f}_i' \boldsymbol{s}_i \end{aligned}$$

so that

$$\boldsymbol{f}_i = \mathbf{T}'_{\boldsymbol{w}_i \boldsymbol{s}_i} \boldsymbol{c}_i$$

Similarly,

$$\boldsymbol{s}_i = \mathbf{T}_{\boldsymbol{s}_i \boldsymbol{w}_i} \boldsymbol{w}_i$$

so that

$$\boldsymbol{c}_i = \mathbf{T}'_{\boldsymbol{s}_i \boldsymbol{w}_i} \boldsymbol{f}_i$$

The elements of $\mathbf{T}'_{\boldsymbol{s}_i \boldsymbol{w}_i}$, which provide expressions for the elements of $\boldsymbol{c}_i$ in terms of the elements of $\boldsymbol{f}_i$ for Tjur structures, is given by the following theorem (Speed and Bailey, 1982; Tjur, 1984; Speed, 1986):

Theorem 3.9 *The element $c_{T_{iw}}$ of $\boldsymbol{c}_i$ is the sum of elements $f_{T_{iv}}$ of $\boldsymbol{f}_i$, a particular element being in the sum if $T_{iv} \leq T_{iw}$.*

Proof: From corollary 3.4, element (w, v) of $\mathbf{T}_{\boldsymbol{s}_i \boldsymbol{w}_i}$ is 1 if $T_{iv} \geq T_{iw}$, 0 otherwise. Hence, element (w, v) of $\mathbf{T}'_{\boldsymbol{s}_i \boldsymbol{w}_i}$ is 1 if $T_{iv} \leq T_{iw}$, 0 otherwise. □

The elements of $\mathbf{T}'_{\boldsymbol{w}_i \boldsymbol{s}_i}$, which provide expressions for the elements of $\boldsymbol{f}_i$ in terms of the elements of $\boldsymbol{c}_i$ for simple orthogonal and Tjur structures, is given by the following theorem:

Theorem 3.10 *The element $f_{T_{iw}}$ of $\mathbf{f}_i$ is a linear function of $c_{T_{iw}}$ and the elements $c_{T_{iv}}$ of $\boldsymbol{c}_i$ for which T_{iv} is:*

1. *marginal to T_{iw}; and*
2. *the minimum of a set of terms immediately marginal to T_{iw}.*

That is, $T_{iv} \in \{T_{iw}\} \cup D_{T_{iw}}$. The coefficient of $c_{T_{iv}}$ in the linear function is $\mu(T_{iv}, T_{iw})$. For a simple orthogonal structure, the coefficient of $c_{T_{iv}}$ is $(-1)^k$ where k is the number of terms immediately marginal to T_{iw} whose intersection is required to obtain T_{iv}.

Alternatively, use the Hasse diagram of term marginalities to obtain the expressions. To the left of each term in the Hasse diagram is the $c_{T_{iv}}$ for that term. To the right of a term is the expression for the $f_{T_{iw}}$ as a function of the $c_{T_{iv}}$ which, for a term, is computed by taking the difference between the $c_{T_{iv}}$ for that term and the sum of the $f_{T_{iw}}$s of all terms marginal to that term.

Proof: To obtain the linear function of the elements of $\boldsymbol{c}_i$ requires inversion of the expressions in theorem 3.9. That is, we have

$$\mathbf{S}_{T_{iw}} = \sum_{T_{iv} \geq T_{iw}} \mathbf{W}_{T_{iv}}$$

Hence, by Möbius inversion from above (theorem 3.1),

$$\mathbf{W}_{T_{iw}} = \sum_{T_{iv} \geq T_{iw}} \mu(T_{iv}, T_{iw}) \mathbf{S}_{T_{iv}}.$$

That is, element (w, v) of $\mathbf{T}_{\boldsymbol{w}_i \boldsymbol{s}_i}$ is $\mu(T_{iv}, T_{iw})$ if $T_{iv} \geq T_{iw}$, 0 otherwise. Hence, element (w, v) of $\mathbf{T}'_{\boldsymbol{w}_i \boldsymbol{s}_i}$ is $\mu(T_{iv}, T_{iw})$ if $T_{iv} \leq T_{iw}$, 0 otherwise.

The terms $T_{iv} \leq T_{iw}$ for which the Möbius function has to be calculated are specified in theorem 3.2; clearly, $T_{iv} \in \{T_{iw}\} \cup D_{T_{iw}}$. The expression for simple orthogonal structures is also given by theorem 3.2 since, as previously noted, the terms from a simple orthogonal block structure form a finite distributive lattice.

That the Hasse diagram of term marginalities can be used to obtain the expressions derives from the fact that it provides a diagrammatic representation of equations involving the Zeta function. The algorithm described amounts to a procedure for recursively inverting these equations. In this instance, it is clear from theorem 3.9 that the equations we need to invert are:

$$c_{T_{iw}} = \sum_{T_{iv} \in T_i} \zeta(T_{iv}, T_{iw}) f_{T_{iv}}, \text{ for all } T_{iw} \in T_i$$

□

Example 3.2 (cont'd): The elements of $\boldsymbol{f}'_1$ and $\boldsymbol{s}'_1$ are:

$$\begin{aligned} \boldsymbol{f}'_1 &= \left[\begin{array}{cccccc} f_G & f_R & f_C & f_{R.C} & f_{R.C.S} & f_{R.C.S.U} \end{array} \right]; \text{ and} \\ \boldsymbol{s}'_1 &= \left[\begin{array}{cccccc} \mathbf{S}_G & \mathbf{S}_R & \mathbf{S}_C & \mathbf{S}_{R.C} & \mathbf{S}_{R.C.S} & \mathbf{S}_{R.C.S.U} \end{array} \right]. \end{aligned}$$

Whence,

$$\mathbf{Z} = f_G \mathbf{S}_G + f_R \mathbf{S}_R + f_C \mathbf{S}_C + f_{R.C} \mathbf{S}_{R.C} + f_{R.C.S} \mathbf{S}_{R.C.S} + f_{R.C.S.U} \mathbf{S}_{R.C.S.U}.$$

Also,

$$\left[\begin{array}{c} c_G \\ c_R \\ c_C \\ c_{R.C} \\ c_{R.C.S} \\ c_{R.C.S.U} \end{array} \right] = \left[\begin{array}{cccccccccccc} f_G & & & & & & & & & & & \\ f_G & + & f_R & & & & & & & & & \\ f_G & & & + & f_C & & & & & & & \\ f_G & + & f_R & + & f_C & + & f_{R.C} & & & & & \\ f_G & + & f_R & + & f_C & + & f_{R.C} & + & f_{R.C.S} & & & \\ f_G & + & f_R & + & f_C & + & f_{R.C} & + & f_{R.C.S} & + & f_{R.C.S.U} \end{array} \right]$$

so that

$$\mathbf{T}_{\boldsymbol{s}_1\boldsymbol{w}_1} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

and its inverse is

$$\mathbf{T}_{\boldsymbol{w}_1\boldsymbol{s}_1} = \begin{bmatrix} 1 & -1 & -1 & 1 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

The second matrix, obtained by matrix inversion, gives us the expressions of the $f_{T_{iw}}$s in terms of the $c_{T_{iw}}$s. However, as outlined in theorem 3.10, these can also be obtained using the Hasse diagram of term marginalities as illustrated in figure 3.4. In addition, they can be derived by evaluating the Möbius function. To do this we require the sets of all possible minima of terms immediately marginal to the terms in the structure:

$$\begin{array}{rclrclrcl} D_G & = & \{G\}; & D_R & = & \{G\}; & D_C & = & \{G\}; \\ D_{R.C} & = & \{G, R, C\}; & D_{R.C.S} & = & \{R.C\}; & D_{R.C.S.U} & = & \{R.C.S\}. \end{array}$$

As this structure is a simple orthogonal structure, the coefficients in the linear combination can be calculated using the expression based on $(-1)^k$ given in theorem 3.10. [To be continued.]

Further, the matrix $\mathbf{Z}$ can be written as a linear combination of the elements of the set, E_i, of mutually orthogonal idempotents of the relationship algebra. We can use either of the relationships:

$$\boldsymbol{w}_i = \mathbf{T}'_{\boldsymbol{w}_i\boldsymbol{e}_i}\boldsymbol{e}_i \quad \text{or} \quad \boldsymbol{s}_i = \mathbf{T}'_{\boldsymbol{s}_i\boldsymbol{e}_i}\boldsymbol{e}_i.$$

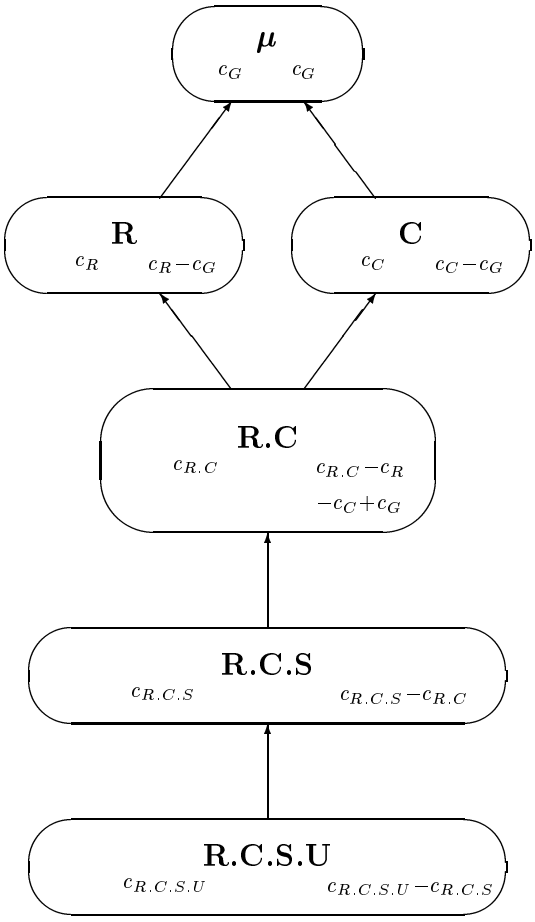
where

$\boldsymbol{e}_i$ is the t_i-vector of mutually orthogonal idempotent matrices for the ith structure.

Thus,

$$\mathbf{Z} = \boldsymbol{l}'_i\boldsymbol{e}_i \quad \text{with } \mathbf{1}'\boldsymbol{e}_i = \mathbf{I}.$$

Figure 3.4: Hasse diagram of term marginalities, including $f_{T_{iw}}$s, for the $(\boldsymbol{R} * \boldsymbol{C})/\boldsymbol{S}/\boldsymbol{U}$ example



The elements of $\mathbf{T}'_{\boldsymbol{s}_i \boldsymbol{e}_i}$, which provide expressions for the elements of $\boldsymbol{l}_i$ in terms of those of $\boldsymbol{f}_i$ for simple orthogonal and Tjur structures, are given by the following theorem (Tjur, 1984; Bailey, 1984):

Theorem 3.11 *The element $l_{T_{iw}}$ is a linear combination of the elements $f_{T_{iv}}$ of $\boldsymbol{f}_i$, a particular element having a nonzero coefficient if $T_{iw} \leq T_{iv}$. For a simple orthogonal structure, any nonzero coefficient is the product of the order of the factors not in the term T_{iv}, i.e. $\prod_{t_{ih} \notin T_{iv}} n_{t_{ih}}$. For a regular Tjur structure, any nonzero coefficient is the replication of the term T_{iv}, $r_{T_{iv}}$.*

Proof: In the proof of theorem 3.5 it was noted, that from theorem 1 of Tjur (1984), we have

$$\begin{aligned} \mathbf{R}_{T_{iw}}^{-1} \mathbf{S}_{T_{iw}} &= \sum_{T_{iv} \leq T_{iw}} \mathbf{E}_{T_{iv}} \\ &= \sum_{T_{iv} \in T_i} \zeta(T_{iv}, T_{iw}) \mathbf{E}_{T_{iv}} \end{aligned}$$

Hence, for a regular structure,

$$\mathbf{S}_{T_{iw}} = \sum_{T_{iv} \leq T_{iw}} r_{T_{iw}} \mathbf{E}_{T_{iv}}$$

The element (w, v) of the transformation matrix $\mathbf{T}_{\boldsymbol{s}_i \boldsymbol{e}_i}$ is thus $r_{T_{iw}}$ if $T_{iv} \leq T_{iw}$, 0 otherwise.

But it is the transpose of this transformation matrix that converts $f_{T_{iv}}$s to $l_{T_{iw}}$s. That is, element (w, v) of the transpose is $r_{T_{iv}}$ if $T_{iv} \geq T_{iw}$, 0 otherwise.

For simple orthogonal structures $n_i = \prod_{t_{ih} \in T_i} n_{t_{ih}}$ so that

$$\begin{aligned} r_{T_{iv}} &= \frac{n_i}{\prod_{t_{ih} \in T_{iv}} n_{t_{ih}}} \\ &= \prod_{t_{ih} \notin T_{iv}} n_{t_{ih}} \end{aligned}$$

□

The final transformation matrices can be obtained from those already given in that

$$\mathbf{T}_{\boldsymbol{w}_i \boldsymbol{e}_i} = \mathbf{T}_{\boldsymbol{w}_i \boldsymbol{s}_i} \mathbf{T}_{\boldsymbol{s}_i \boldsymbol{e}_i} \quad \text{and} \quad \mathbf{T}_{\boldsymbol{e}_i \boldsymbol{w}_i} = \mathbf{T}_{\boldsymbol{e}_i \boldsymbol{s}_i} \mathbf{T}_{\boldsymbol{s}_i \boldsymbol{w}_i}.$$

Example 3.2 (cont'd): The expressions for the elements of $\boldsymbol{l}_i$ in terms of $\boldsymbol{f}_i$ are as follows:

$$\begin{bmatrix} l_G \\ l_R \\ l_C \\ l_{R.C} \\ l_{R.C.S} \\ l_{R.C.S.U} \end{bmatrix} = \begin{bmatrix} rcsuf_G + csuf_R + rsuf_C + suf_{RC} + uf_{RCS} + f_{RCSU} \\ csuf_R + suf_{RC} + uf_{RCS} + f_{RCSU} \\ rsuf_C + suf_{RC} + uf_{RCS} + f_{RCSU} \\ suf_{RC} + uf_{RCS} + f_{RCSU} \\ uf_{RCS} + f_{RCSU} \\ f_{RCSU} \end{bmatrix}$$

so that

$$\mathbf{T}_{\boldsymbol{s}_1\boldsymbol{e}_1} = \begin{bmatrix} rcsu & 0 & 0 & 0 & 0 & 0 \\ csu & csu & 0 & 0 & 0 & 0 \\ rsu & 0 & rsu & 0 & 0 & 0 \\ su & su & su & su & 0 & 0 \\ u & u & u & u & u & 0 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix}$$

and its inverse is

$$\mathbf{T}_{\boldsymbol{e}_1\boldsymbol{s}_1} = \begin{bmatrix} \frac{1}{rcsu} & 0 & 0 & 0 & 0 & 0 \\ \frac{-1}{rcsu} & \frac{1}{csu} & 0 & 0 & 0 & 0 \\ \frac{-1}{rcsu} & 0 & \frac{1}{rsu} & 0 & 0 & 0 \\ \frac{1}{rcsu} & \frac{-1}{csu} & \frac{-1}{rsu} & \frac{1}{su} & 0 & 0 \\ 0 & 0 & 0 & \frac{-1}{su} & \frac{1}{u} & 0 \\ 0 & 0 & 0 & 0 & \frac{-1}{u} & 1 \end{bmatrix}$$

Thus

$$\mathbf{T}_{\boldsymbol{w}_1\boldsymbol{e}_1} = \begin{bmatrix} su(rc-c-r+1) & -su(c-1) & -su(r-1) & -su & 0 & 0 \\ su(c-1) & su(c-1) & -su & -su & 0 & 0 \\ su(r-1) & -su & su(r-1) & -su & 0 & 0 \\ u(s-1) & u(s-1) & u(s-1) & u(s-1) & -u & 0 \\ u-1 & u-1 & u-1 & u-1 & u-1 & -1 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{bmatrix}$$

and its inverse is

$$\mathbf{T}_{\boldsymbol{e}_1\boldsymbol{w}_1} = \begin{bmatrix} \frac{1}{rcsu} & \frac{1}{rcsu} & \frac{1}{rcsu} & \frac{1}{rcsu} & \frac{1}{rcsu} & \frac{1}{rcsu} \\ \frac{-1}{rcsu} & \frac{r-1}{rcsu} & \frac{-1}{rcsu} & \frac{r-1}{rcsu} & \frac{r-1}{rcsu} & \frac{r-1}{rcsu} \\ \frac{-1}{rcsu} & \frac{-1}{rcsu} & \frac{c-1}{rcsu} & \frac{c-1}{rcsu} & \frac{c-1}{rcsu} & \frac{c-1}{rcsu} \\ \frac{1}{rcsu} & \frac{-(r-1)}{rcsu} & \frac{-(c-1)}{rcsu} & \frac{-(rc-r-c+1)}{rcsu} & \frac{-(rc-r-c+1)}{rcsu} & \frac{-(rc-r-c+1)}{rcsu} \\ 0 & 0 & 0 & \frac{-1}{su} & \frac{s-1}{su} & \frac{s-1}{su} \\ 0 & 0 & 0 & 0 & \frac{-1}{u} & \frac{u-1}{u} \end{bmatrix}$$

[To be continued.]

In summary, theorem 3.9 specifies $\mathbf{T}_{\boldsymbol{s}_i\boldsymbol{w}_i}$, theorem 3.10 specifies $\mathbf{T}_{\boldsymbol{w}_i\boldsymbol{s}_i}$, theorem 3.11 specifies $\mathbf{T}_{\boldsymbol{s}_i\boldsymbol{e}_i}$, $\mathbf{T}_{\boldsymbol{e}_i\boldsymbol{s}_i}$ is obtained by inversion of $\mathbf{T}_{\boldsymbol{s}_i\boldsymbol{e}_i}$, and $\mathbf{T}_{\boldsymbol{w}_i\boldsymbol{e}_i}$ and $\mathbf{T}_{\boldsymbol{e}_i\boldsymbol{w}_i}$ are obtained as the product of two of the first four matrices. These results will be utilised in section 3.3.1

Next expressions for the degrees of freedom of terms from a single structure are provided.

Theorem 3.12 *The degrees of freedom of a term from a simple orthogonal structure is given by:*

$$\nu_{T_{iw}} = \prod_{t_{ih} \in N_{T_{iw}}} n_{t_{ih}} \prod_{t_{ih} \in (T_{iw} \cap \overline{N}_{T_{iw}})} (n_{t_{ih}} - 1).$$

More generally, for a Tjur structure, use the Hasse diagram of term marginalities to obtain the degrees of freedom for the terms derived from the structure. Each term in the Hasse diagram has to its left the number of levels combinations of the factors comprising that term for which there are observations. To the right of the term is the degrees of freedom which is computed by taking the difference between the number to the left of that term and the sum of the degrees of freedom to the right of all terms marginal to that term.

Proof: To derive the expression for simple orthogonal structures note that, for $\mathbf{I}$ and $\mathbf{G}$ of order $n_{t_{ih}}$,

$$\mathrm{tr}(\mathbf{I}) = n_{t_{ih}}, \quad \mathrm{tr}(\mathbf{G}) = 1, \quad \mathrm{tr}(\mathbf{I} - \mathbf{G}) = n_{t_{ih}} - 1,$$

and

$$\mathrm{tr}(\mathbf{B} \otimes \mathbf{C}) = \mathrm{tr}(\mathbf{B})\,\mathrm{tr}(\mathbf{C}).$$

Now

$$\nu_{T_{iw}} = \mathrm{tr}(\mathbf{E}_{T_{iw}}).$$

But from theorem 3.8, $\mathbf{E}_{T_{iw}}$ is the direct product of matrices, premultiplied by $\mathbf{U}_i$ and postmultiplied by $\mathbf{U}_i'$; there is one matrix in the direct product for each factor in the structure. As $\mathbf{U}_i$ is orthogonal, $\mathbf{U}_i' = \mathbf{U}_i^{-1}$, $\mathrm{tr}(\mathbf{U}_i\mathbf{D}\mathbf{U}_i') = \mathrm{tr}(\mathbf{D}\mathbf{U}_i\mathbf{U}_i') = \mathrm{tr}(\mathbf{D})$. Hence, the permutation matrix can be ignored in obtaining $\mathrm{tr}(\mathbf{E}_{T_{iw}})$. Now, an $\mathbf{I} - \mathbf{G}$

matrix is included in the direct product for factors $t_{ih} \in (T_{iw} \cap \overline{N}_{T_{iw}})$, an $\mathbf{I}$ matrix for $t_{ih} \in N_{T_{iw}}$, and a $\mathbf{G}$ matrix for $t_{ih} \notin T_{iw}$.

Clearly, the degrees of freedom for a simple orthogonal structure are as stated in the theorem.

Tjur (1984, section 5) outlines the use of the Hasse diagram, based on the marginality relationships between the terms to obtain the degrees of freedom for a Tjur structure. To derive this procedure, note that from theorem 3.5 we have that

$$\mathrm{tr}(\mathbf{E}_{T_{iw}}) = \sum_{T_{iv} \in \{T_{iw}\} \cup D_{T_{iw}}} \mu(T_{iv}, T_{iw}) \mathrm{tr}\left(\mathbf{R}_{T_{iv}}^{-1} \mathbf{S}_{T_{iv}}\right)$$

with

$$\mathrm{tr}\left(\mathbf{R}_{T_{iv}}^{-1} \mathbf{S}_{T_{iv}}\right) = n_{T_{iv}}.$$

A similar argument to that given in the proof of theorem 3.10, about the use of the Hasse diagram, yields the procedure outlined by Tjur for using the Hasse diagram to compute the degrees of freedom. □

> **Example 3.2 (cont'd):** Using the expression for simple orthogonal structures, we have that the degrees of freedom of $R.C$ is $(r-1)(c-1)$ and of $R.C.S$ is $rc(s-1)$. [To be continued.]

Expressions for the sums of squares of the terms from simple orthogonal and Tjur structures are given in the following theorem:

Theorem 3.13 *For a simple orthogonal structure, write down the algebraic expression for the degrees of freedom in terms of the components given in theorem 3.12; use symbols for the order of the factors, not the observed orders. Expand this expression and replace each product of orders of the factors in this expression by the means vector for the same set of factors. The effects vector for the term is this linear form in the means vectors. The sum of squares for the term is then the sum of squares of the elements of the effects vector.*

That is, the sum of squares is given by:

$$\boldsymbol{y}' \mathbf{E}_{T_{iw}} \boldsymbol{y} = \boldsymbol{d}'_{T_{iw}} \boldsymbol{d}_{T_{iw}}$$

where

$\boldsymbol{y}$ is *the observation n-vector which we assume is arranged in lexicographical order with respect to the factors indexing the first tier,*

$\boldsymbol{d}_{T_{iw}} = \sum_{T_{iv} \in \{T_{iw}\} \cup D_{T_{iw}}} (-1)^k \overline{\boldsymbol{y}}_{T_{iv}}$ *is the effects n-vector for term* T_{iw}*, and*

$\overline{\boldsymbol{y}}_{T_{iv}}$ *is the means n-vector containing, for each observational unit, the mean of the elements of* $\boldsymbol{y}$ *corresponding to that unit's levels combination of the factors in term* T_{iv}*.*

More generally, for a Tjur structure, use the Hasse diagram of term marginalities to obtain the expression for the effects vector in terms of the mean vectors. For each term in the Hasse diagram there is to the left the mean vector for the set of factors in the term. To the right of the term is the effects vector which is computed by taking the difference between the mean vector to the left of that term and the sum of the effects vectors to the right of all terms marginal to that term. Again the sum of squares for a term is then the sum of squares of the elements in the effects vector.

Proof: For simple orthogonal structures Nelder (1965a) gives the algorithm outlined above. To show that

$$\boldsymbol{d}_{T_{iw}} = \sum_{T_{iv} \in \{T_{iw}\} \cup D_{T_{iw}}} (-1)^k \overline{\boldsymbol{y}}_{T_{iv}}$$

note that, from theorem 3.5,

$$\begin{aligned} \boldsymbol{y}' \mathbf{E}_{T_{iw}} \boldsymbol{y} &= \sum_{T_{iv} \in \{T_{iw}\} \cup D_{T_{iw}}} \mu(T_{iv}, T_{iw}) \boldsymbol{y}' \mathbf{R}_{T_{iv}}^{-1} \mathbf{S}_{T_{iv}} \boldsymbol{y} \\ &= \sum_{T_{iv} \in \{T_{iw}\} \cup D_{T_{iw}}} \mu(T_{iv}, T_{iw}) \overline{\boldsymbol{y}}'_{T_{iv}} \overline{\boldsymbol{y}}_{T_{iv}} . \end{aligned}$$

The expression for $\mu(T_{iv}, T_{iw})$, in the case of simple orthogonal structures, follows from the fact that terms from such structures form a distributive lattice and theorem 3.2.

For Tjur structures, Tjur (1984) gives the method. □

Example 3.2 (cont'd): As the example is a simple orthogonal structure, the expanded expression for the degrees of freedom can be used to obtain the effects vector. For example, for the term $R.C$, the expanded expression for the degrees of freedom is $rc - r - c + 1$ so that the effects vector from which the sum of squares for $R.C$ is calculated is the following linear form in the means vectors:

$$\overline{\boldsymbol{y}}_{R.C} - \overline{\boldsymbol{y}}_R - \overline{\boldsymbol{y}}_C + \overline{\boldsymbol{y}}_G.$$

The expanded expression for the degrees of freedom for $R.C.S$ is $rcs - rc$ and the effects vector for $R.C.S$ is:

$$\overline{\boldsymbol{y}}_{R.C.S} - \overline{\boldsymbol{y}}_{R.C}.$$

As indicated at the outset, a dummy factor may have to be included in a structure to ensure that there is a unit term derived from the structure and that the results of previous authors are applicable. However, it is evident that the modifications to be made, to theorems 3.9–3.13 so that they can be applied to the original structure, can be determined by setting the coefficients of the unit term to zero. It is clear that all the theorems except theorem 3.11 can be applied as stated to the original structure. In the case of this theorem, only the part specific to a simple orthogonal structure does not apply to the original structure.

3.3 Derivation of rules for analysis of variance quantities

In this section we derive expressions for the mean squares that constitute the analysis of variance for the study, consider the form of the linear models that can be used to describe the study and obtain expressions for the expected mean squares on which testing and estimation for the study will be based.

3.3.1 Analysis of variance for the study

The analysis of variance for a study provides a partition of the sample variance into a set of mean squares, each of which is based on effects that are homogeneous in that they are influenced by differences between the levels combinations of the same term(s). We require expressions for this set of mean squares, which must take into account the s structures in the structure set for the study. We will obtain the required expressions by separately finding expressions for the sums of squares and degrees of freedom of the mean squares.

In order to find expressions for the sums of squares, we first consider the set of mutually orthogonal idempotents derived from the first structure for the study; these

will be the elements $\mathbf{P}_{1k}$ of the set, P_1, of projection operators for the first structure. As the factors in the first tier will uniquely index the observational units, these idempotents will sum to $\mathbf{I}$ and a partition of the *Total* variance will be obtained. This partition is given by

$$\boldsymbol{y}'\boldsymbol{y} = \sum_k \boldsymbol{y}'\mathbf{P}_{1k}\boldsymbol{y}.$$

After this we successively partition the *Total* variation by obtaining the set, P_i, of projection operators that specify the decomposition of the sample space into a set of orthogonal subspaces corresponding to the terms from the first i structures. This is done by determining the relationship of each matrix $\mathbf{E}_{T_{iw}}$ to the projection matrices of the previous structure; that is, to the matrices in the set P_{i-1} (see theorem 3.14).

The elements, $\mathbf{P}_{ik}$ $(k = 1, \ldots, p_i)$, of the set P_i have the property that

$$\sum_k \mathbf{P}_{ik} = \mathbf{I}.$$

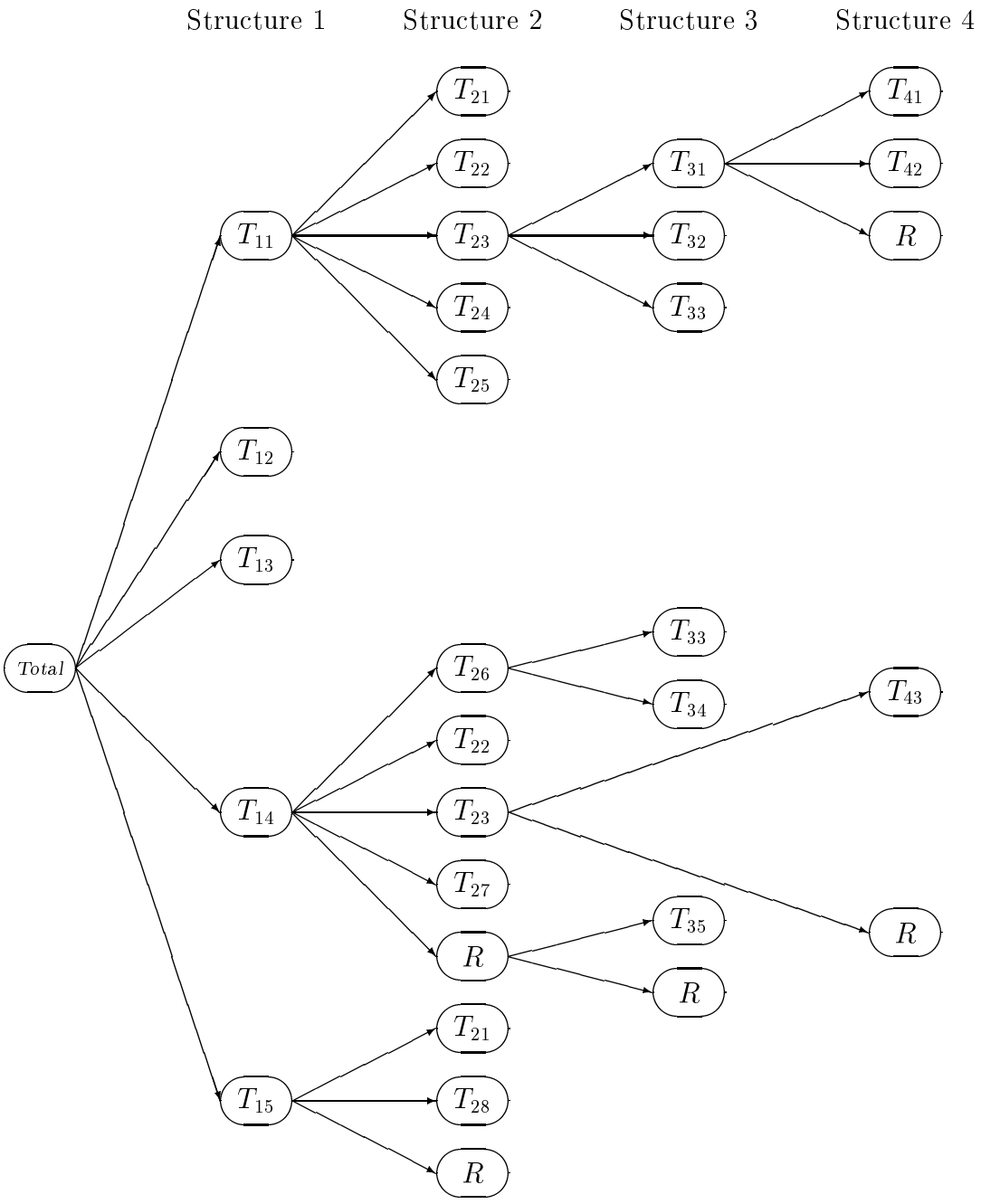
That this holds for the first structure follows directly from the results presented in section 3.2. For subsequent structures it follows from the hierarchical decomposition of projection operators from the previous structure given in theorem 3.14.

The corresponding partition of the *Total* sum of squares is given by

$$\boldsymbol{y}'\boldsymbol{y} = \sum_k \boldsymbol{y}'\mathbf{P}_{ik}\boldsymbol{y}.$$

The set of sums of squares, and hence mean squares, derived from the set, P_s, of projection operators for structure s constitutes the full analysis of variance for the study in that it results in a decomposition of the sample variance that takes into account all terms included in the model for the study. This decomposition of the sample space can be represented in a decomposition tree with each node corresponding to the subspace of a projector $\mathbf{P}_{ik}$ such that the descendants of any node are orthogonal subspaces of that node.

Figure 3.5: Decomposition tree for a four-tiered experiment with 5,8,5, and 3 terms arising from each of structures 1–4, respectively†



†The term T_{iw} is the wth term from the ith structure and R is the *Residual* corresponding to a source from a lower structure.

Example 3.3: The decomposition tree given in figure 3.5 is for a hypothetical example illustrating a wide range of potential situations that can arise in such a tree. Ultimately, the sample space is divided into 22 orthogonal subspaces so that there will be 22 **P**s corresponding to structure 4. There would be 22 sources, derived from various structures, to be considered in the analysis of variance table.

Further examples of decomposition trees are given in figures 3.3 and 3.6.

In this thesis we consider only structure-balanced experiments. That is we restrict our attention to those experiments for which the relationship between mutually orthogonal idempotent matrices, $\mathbf{E}_{T_{iw}}$, and a projection matrix from a previous structure, $\mathbf{P}_{(i-1)c}$, is as specified in the following definition:

Definition 3.4 *An experiment is said to exhibit* **structure balance** *if, with* $r = i-1$, *there exist scalars* $e^c_{T_{iw}}$ *such that*

$$\mathbf{E}_{T_{iw}}\mathbf{P}_{rc}\mathbf{E}_{T_{iv}} = \begin{cases} e^c_{T_{iw}}\mathbf{E}_{T_{iw}}, & \text{for all } w = v, T_{iw} \in T_i, i = 2, \ldots, s, c = 1, \ldots, p_r \\ 0 & \text{otherwise} \end{cases}$$

where

$e^c_{T_{iw}}$ *is the efficiency factor for term* T_{iw} *when it is estimated from the range of the* c*th projection operator for the* $(i-1)$*th structure; for orthogonal terms* $e^c_{T_{iw}} = 1$*; and*

$\mathbf{P}_{rc}$ *is the* c*th projection operator of order* n *from the* r*th structure.*

That is, as discussed in section 1.2.2.2, the terms generated from a single structure are orthogonal and terms from different structures display first-order balance. This definition is just Nelder's (1965b, 1968) definition of general balance applied to all structures. Experiments satisfying this condition are generally balanced under the Houtman and Speed (1983) definition. As Houtman and Speed point out,

$$0 \leq e^c_{T_{iw}} \leq 1 \quad \text{and} \quad \sum_c e^c_{T_{iw}} = 1.$$

This condition does not apply to first-order balanced experiments as the projection-operator product is not required to be zero for $w \neq v$. Consequently, the $e^c_{T_{iw}}$s do not necessarily sum to one.

Theorem 3.14 *Denote by q_{ik} the sum of squares $\boldsymbol{y}'\mathbf{P}_{ik}\boldsymbol{y}$ for the kth projection operator from the ith structure and by $T_{jw}, j \leq i$, the defining term for the source corresponding to $\mathbf{P}_{ik}$. Then, the form of $\mathbf{P}_{ik}$ is:*

$$\mathbf{P}_{ik} = \begin{cases} \mathbf{E}_{T_{1w}}, & i = j = 1 \\ \mathbf{P}_{jq}, & j < i, \text{ for a source from the } j\text{th structure having no terms from structure } (j+1) \text{ through to the } i\text{th structure confounded with it,} \\ \mathbf{P}_{rc}\mathbf{E}^c_{T_{iw}}\mathbf{P}_{rc}, & j = i > 1, \quad r = i-1, \text{ for sources whose defining term arises in the } i\text{th structure } (= \mathbf{E}_{T_{iw}} \text{ for an orthogonal term}), \\ \mathbf{P}_{jq} - \sum_{j<g\leq i}\sum_{u\in U^{gi}_{jq}} \mathbf{P}_{gu}, & j < i, \text{ for residual sources,} \end{cases}$$

where

$\mathbf{E}^c_{T_{iw}}$ = $(e^c_{T_{iw}})^{-1}\mathbf{E}_{T_{iw}}$ *is the adjusted idempotent matrix for term T_{iw} when term T_{iw} is estimated from the cth source in the $(i-1)$th structure; for an orthogonal term $\mathbf{E}^c_{T_{iw}} = \mathbf{E}_{T_{iw}}$;*

$e^c_{T_{iw}}$ *is the efficiency factor corresponding to term T_{iw} when it is estimated from the cth source of the $(i-1)$th structure; for an orthogonal term $e^c_{T_{iw}} = 1$;*

$\mathbf{P}_{rc}$ *is the cth projection operator from the rth structure; and*

U^{gi}_{jq} *is the set of indices specifying the projection operators that correspond to the sources in the gth structure which:*

- *are confounded with the source corresponding to the qth projection operator from the jth structure; and*
- *have no terms from structure $(j+1)$ through to the ith structure confounded with them.*

That is, the projection operators such that, for $u \in U^{gi}_{jq}$,

$$\mathbf{P}_{jq}\mathbf{P}_{gu} = \mathbf{P}_{gu}, \text{ and}$$

$$\mathbf{E}_{T_{hz}}\mathbf{P}_{gu} = 0, \quad \text{for all } T_{hz} \in T_h, \quad g < h \leq i.$$

Proof: For the purposes of this proof, the four forms of projection operator given in the theorem will be referred to as:

(i) pivotal projection operator from first structure;

(ii) previous-structure projection operator;

(iii) pivotal projection operator; and

(iv) residual projection operator, respectively.

Note that, except for those of type (ii), any projection operator is said to correspond to a source in that it is the projection operator for the source associated with the structure from which the source arises.

(i) Pivotal projection operator from first structure. The form of $\mathbf{P}_{ik}$ for $i = 1$, that is of a pivotal projection operator from the first structure, follows immediately from the results presented in section 3.2.

(ii) Previous-structure projection operator. There is nothing to prove when sources from a previous structure have no terms from the ith structure confounded with them.

(iii) Pivotal projection operator. For sources corresponding to terms from the ith structure, consider the idempotent operator $\mathbf{E}_{T_{iw}}$ for defining term T_{iw}. Let $\mathbf{P}_{rc}$ be a projection operator such that $\mathbf{E}_{T_{iw}}\mathbf{P}_{rc} \neq 0$ for $r = i - 1$. Then, by lemma 1 of theorem 1 and the associated discussion of James and Wilkinson (1971),

$$\mathcal{R}(\mathbf{P}_{rc}) = \mathcal{R}(\mathbf{P}_{rc}\mathbf{E}_{T_{iw}}\mathbf{P}_{rc}) \oplus \mathcal{R}(\mathbf{P}_{rc}) \cap \mathcal{R}(\mathbf{P}_{rc}\mathbf{E}_{T_{iw}}\mathbf{P}_{rc})^{\perp}$$

where

$\mathcal{R}(\mathbf{B})$ denotes the range of $\mathbf{B}$.

That is, in effecting the decomposition corresponding to the ith structure, a subspace from a previous structure will be partitioned into two orthogonal subspaces. The projection operator whose range is $\mathcal{R}(\mathbf{P}_{rc}\mathbf{E}_{T_{iw}}\mathbf{P}_{rc})$ is a pivotal projection operator and has been denoted as $\mathbf{P}_{ik}$. We next derive the expressions given in theorem 3.14 for this projection operator; the projection operator for the other subspace, a residual projection operator, will be considered below.

Note that for a structure-balanced experiment there is only one nonzero eigenvalue, $e^c_{T_{iw}}$ when T_{iw} is estimated from the range of the cth projection operator for structure $(i-1)$. Thus, $\mathcal{R}(\mathbf{P}_{rc}\mathbf{E}_{T_{iw}}\mathbf{P}_{rc})$ will be the eigenspace of $\mathbf{P}_{rc}\mathbf{E}_{T_{iw}}\mathbf{P}_{rc}$ corresponding to the nonzero eigenvalue and $\mathbf{P}_{ik}$ the projection operator onto this eigenspace.

Also, let $\mathbf{E}^{\star}_{T_{iw}}$ be the projection operator on the single eigenspace of $\mathbf{E}_{T_{iw}}\mathbf{P}_{rc}\mathbf{E}_{T_{iw}}$ with a nonzero eigenvalue.

Also, from definition 3.4, we have that $\mathbf{E}_{T_{iw}}\mathbf{P}_{rc}\mathbf{E}_{T_{iw}} = e^c_{T_{iw}}\mathbf{E}_{T_{iw}}$ so that $\mathbf{E}_{T_{iw}}$ is the projection operator on the single eigenspace of $\mathbf{E}_{T_{iw}}\mathbf{P}_{rc}\mathbf{E}_{T_{iw}}$ with nonzero eigenvalue.

Now, by corollary 2 of theorem 1 of James and Wilkinson (1971),

$$\mathbf{P}_{rc}\mathbf{E}_{T_{iw}}\mathbf{P}_{rc} = e^c_{T_{iw}}\mathbf{P}_{ik}.$$

Hence,

$$\begin{aligned}\mathbf{P}_{ik} &= (e^c_{T_{iw}})^{-1}\mathbf{P}_{rc}\mathbf{E}_{T_{iw}}\mathbf{P}_{rc} \\ &= \mathbf{P}_{rc}\mathbf{E}^c_{T_{iw}}\mathbf{P}_{rc} \qquad \text{as } \mathbf{E}^c_{T_{iw}} = (e^c_{T_{iw}})^{-1}\mathbf{E}_{T_{iw}}\end{aligned}$$

For orthogonal experiments, $\mathbf{E}_{T_{iw}}\mathbf{P}_{rc}\mathbf{E}_{T_{iw}} = \mathbf{E}_{T_{iw}}$ and $\mathbf{E}_{T_{iw}}$ and $\mathbf{P}_{rc}$ commute. Thus, $\mathbf{P}_{rc}\mathbf{E}^c_{T_{iw}}\mathbf{P}_{rc} = \mathbf{E}_{T_{iw}}$.

(iv) Residual projection operator. The residual projection operator after a single term has been eliminated from a source is the projection on $\mathcal{R}(\mathbf{P}_{rc}) \cap \mathcal{R}(\mathbf{P}_{rc}\mathbf{E}_{T_{iw}}\mathbf{P}_{rc})^{\perp}$ and, by corollary 2 of theorem 1 of James and Wilkinson (1971), this is given by

$$\begin{aligned}\mathbf{P}_{rc} - \mathbf{P}_{ik} &= \mathbf{P}_{rc} - \mathbf{P}_{rc}\mathbf{E}^c_{T_{iw}}\mathbf{P}_{rc} \\ &= \mathbf{P}_{rc}(\mathbf{I} - \mathbf{E}^c_{T_{iw}})\mathbf{P}_{rc} \\ &= \mathbf{P}_{rc} - \mathbf{E}_{T_{iw}} \qquad \text{for orthogonal experiments.}\end{aligned}$$

More generally, the residual source derived from $\mathbf{P}_{rc}$ will be obtained after all the terms confounded with the source corresponding to $\mathbf{P}_{rc}$ have been eliminated. That is the projection operator for this residual source is given by

$$\mathbf{P}_{rc} - \sum_{u \in U^{ii}_{rc}} \mathbf{P}_{iu}$$

where

U_{rc}^{ii} is the set of indices specifying the projection operators that correspond to the sources in the ith structure confounded with the cth source from the rth structure.

That this is the case derives from the fact that $\mathbf{P}_{rc}\mathbf{P}_{iu} = \mathbf{P}_{iu}$ and that, for $u, v \in U_{rc}^{ii}$, $\mathbf{P}_{iu}\mathbf{P}_{iv} = 0$. The latter fact is a consequence of definition 3.4. That is, the range of the cth projection operator for the rth structure is partitioned into the direct sum of the orthogonal subspaces corresponding to the set of terms from the ith structure estimated from it, and the subspace orthogonal to these.

However, in general, the defining term for a residual source may not arise in the immediately preceding, that is rth, structure (see figure 3.5 in which a *Residual* source for T_{14} is associated with the third structure). Thus, the expression for a residual source given above may not involve the defining term for the source. To derive a general expression for a residual source that involves its defining term, one must start with the projection operator from the jth structure corresponding to the defining term for this source; to obtain the projection operator for the residual source one has to subtract the projection operators for all sources confounded with it, but which do not have sources confounded with them. Hence, the general expression for a residual source is

$$\mathbf{P}_{ik} = \mathbf{P}_{jq} - \sum_{j<g\leq i} \sum_{u \in U_{jq}^{gi}} \mathbf{P}_{gu}, \quad j < i.$$

□

Wood, Williams and Speed (1988) have independently derived similar expressions for the projection operators, but for a more restricted class of experiments. The steps given in table 2.3 for the sums of squares can be deduced from the results given in this theorem.

To complement the expressions for the sums of squares, we also require expressions for the degrees of freedom. They are given by the following theorem.

Theorem 3.15 *Denote by ν_{ik} the degrees of freedom for q_{ik} the sum of squares for the kth projection operator from the ith structure; that is, ν_{ik} is* $\mathrm{rank}(\mathbf{P}_{ik})$. *Let $T_{jw}, j \leq i$, be the defining term for the source corresponding to the kth projection operator from the ith structure. Then,*

$$\nu_{ik} = \begin{cases} \mathrm{tr}\left(\mathbf{E}_{T_{jw}}\right), & j \leq i, \textit{if sources with defining term } T_{jw} \textit{ have no terms confounded with them} \\ \mathrm{tr}\left(\mathbf{P}_{jq}\right) - \sum_{j<g\leq i} \sum_{u \in U_{jq}^{gi}} \mathrm{tr}\left(\mathbf{P}_{gu}\right), & j < i, \textit{for residual sources} \end{cases}$$

where

$$\begin{aligned} \mathrm{tr}\left(\mathbf{E}_{T_{jw}}\right) &= \textit{for simple orthogonal structures,} \\ \mathrm{tr}(\mathbf{P}_{jq}) &= \mathrm{tr}\left(\mathbf{E}_{T_{jw}}\right), j < i, \textit{ and} \\ \mathrm{tr}(\mathbf{P}_{gu}) &\textit{ is a linear form in } \mathrm{tr}(\mathbf{E}s). \end{aligned}$$

PROOF: From theorem 3.14, we have that $\mathbf{P}_{ik}$ is idempotent, so that

$$\nu_{ik} = \mathrm{rank}(\mathbf{P}_{ik}) = \mathrm{tr}\left(\mathbf{P}_{ik}\right).$$

Trivially, for a pivotal projection operator from the first structure,

$$\mathrm{tr}\left(\mathbf{P}_{1k}\right) = \mathrm{tr}\left(\mathbf{E}_{T_{1u}}\right)$$

A projection operator from the previous structure will be either a pivotal or a residual projection operator and so its degrees of freedom can be computed using the expression for whichever of these is appropriate; however, one has to take into account that the defining term is from a structure below the ith structure.

For a pivotal projection operator from other than the first structure,

$$\begin{aligned} \mathrm{tr}(\mathbf{P}_{ik}) &= \mathrm{tr}\left(\mathbf{P}_{rc}\mathbf{E}_{T_{jw}}^{c}\mathbf{P}_{rc}\right), \quad j \leq i, r = j-1 \\ &= \mathrm{tr}\left(\mathbf{E}_{T_{jw}}^{c}\mathbf{P}_{rc}\right) \end{aligned}$$

$$
\begin{aligned}
&= (e^c_{T_{jw}})^{-1}\mathrm{tr}\left(\mathbf{E}_{T_{jw}}\mathbf{P}_{rc}\right)\\
&= (e^c_{T_{jw}})^{-1}\mathrm{tr}\left(\mathbf{E}_{T_{jw}}\mathbf{P}_{rc}\mathbf{E}_{T_{jw}}\right)\\
&= e^c_{T_{jw}}\,\mathrm{tr}\left(\mathbf{E}^c_{T_{jw}}\mathbf{P}_{rc}\mathbf{E}^c_{T_{jw}}\right)\\
&= e^c_{T_{jw}}\,\mathrm{tr}\left(\mathbf{E}^c_{T_{jw}}\right)\\
&= \mathrm{tr}\left(\mathbf{E}_{T_{jw}}\right)
\end{aligned}
$$

The expression for ν_{ik} for a residual projection operator, follows immediately from the expression for it given in theorem 3.14.

The expression for $\mathrm{tr}\left(\mathbf{E}_{T_{jw}}\right)$ is given by theorem 3.12. That for $\mathrm{tr}(\mathbf{P}_{jq})$ follows from the fact that it is a pivotal projection operator corresponding to the source with defining term T_{jw}. The comments on the $\mathrm{tr}(\mathbf{P}_{gu})$ follow from the fact that it may be either a pivotal or a residual projection operator. □

The steps given in table 2.2 for the degrees of freedom can be deduced from the results given in this theorem.

Example 2.1: Consider again the split-plot experiment presented in section 2.2; the structure set for the study has been given in section 2.2.4 and the analysis of variance table in table 2.4. The Hasse diagrams of term marginalities for this kind of experiment, giving the terms derived from the structure set for the study and their degrees of freedom, are shown in figure 2.2; the decomposition tree is given in figure 3.6. The analysis table, incorporating expressions for the projection operators, is given in table 3.3. [To be continued.]

Figure 3.6: Decomposition tree for a split-plot experiment

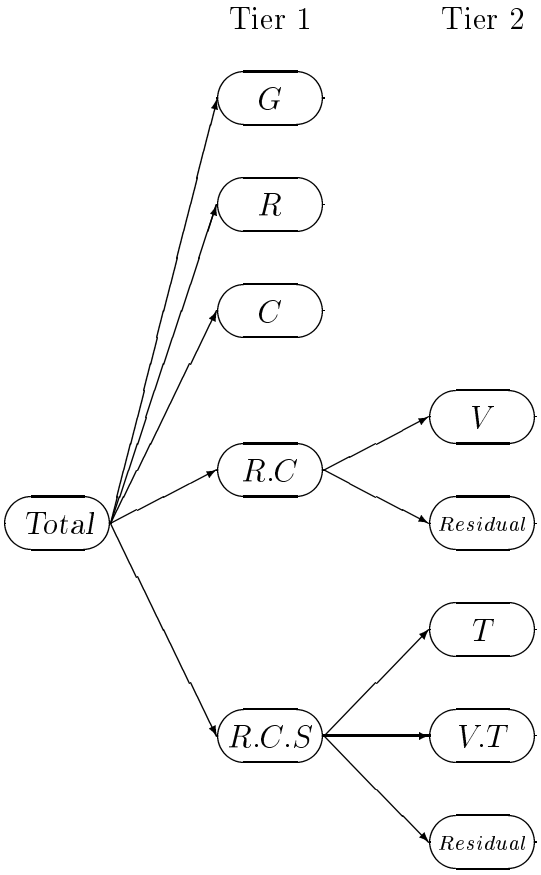


Table 3.3: Analysis of variance table, including projection operators, for a split-plot experiment

SOURCE	DF	PROJECTION OPERATORS
Rows	$v-1$	$\mathbf{P}_{11} = \mathbf{P}_{21} = \mathbf{E}_R$
Columns	$v-1$	$\mathbf{P}_{12} = \mathbf{P}_{22} = \mathbf{E}_C$
Rows.Columns	$(v-1)^2$	$\mathbf{P}_{13} = \mathbf{E}_{RC}$
Varieties	$v-1$	$\mathbf{P}_{23} = \mathbf{E}_V$
Residual	$(v-1)(v-2)$	$\mathbf{P}_{24} = \mathbf{P}_{13} - \mathbf{P}_{23}$
Rows.Columns.Subplots	$(t-1)v^2$	$\mathbf{P}_{14} = \mathbf{E}_{RCS}$
Treatments	$t-1$	$\mathbf{P}_{25} = \mathbf{E}_T$
Varieties.Treatments	$(v-1)(t-1)$	$\mathbf{P}_{26} = \mathbf{E}_{VT}$
Residual	$(v-1)(t-1)v$	$\mathbf{P}_{27} = \mathbf{P}_{14} - \mathbf{P}_{25} - \mathbf{P}_{26}$

Example 3.1 (cont'd): The Hasse diagrams of term marginalities for the simple lattice experiment, giving the terms derived from the structure set for the study and their degrees of freedom, are shown in figure 3.2; the decomposition tree is given in figure 3.3 and the analysis table and projection operators for this experiment are given in table 3.4. [To be continued.]

Table 3.4: Analysis of variance table, including projection operators, for a simple lattice experiment

SOURCE	DF	PROJECTION OPERATORS
Reps	1	$\mathbf{P}_{11} = \mathbf{P}_{21} = \mathbf{E}_R$
Reps.Blocks	$2(b-1)$	$\mathbf{P}_{12} = \mathbf{E}_{RB}$
C	$b-1$	$\mathbf{P}_{22} = (e_C^2)^{-1}\mathbf{E}_C$
D	$b-1$	$\mathbf{P}_{23} = (e_D^2)^{-1}\mathbf{E}_D$
Reps.Blocks.Plots	$2b(b-1)$	$\mathbf{P}_{13} = \mathbf{E}_{RBP}$
C	$b-1$	$\mathbf{P}_{24} = (e_C^3)^{-1}\mathbf{E}_C$
D	$b-1$	$\mathbf{P}_{25} = (e_D^3)^{-1}\mathbf{E}_D$
Lines	$(b-1)^2$	$\mathbf{P}_{26} = \mathbf{E}_L$
Residual	$(b-1)^2$	$\mathbf{P}_{27} = \mathbf{P}_{13} - \mathbf{P}_{24} - \mathbf{P}_{25} - \mathbf{P}_{26}$

3.3.1.1 Recursive algorithm for the analysis of variance

The computation of the analysis of variance can be achieved using a generalization of Wilkinson's algorithm (Wilkinson, 1970; Payne and Wilkinson, 1977). This algorithm is the natural method of implementing what Yates (1975) has described as Fisher's 'major extension of Gaussian least square theory' to incorporate the analysis of multiple errors. The essence of what is required in this situation is estimation of a term from those sources with which it is confounded; for example, in analysing a split-plot experiment, the treatment contrasts confounded with main plots are to be estimated from the main-plot source.

Wilkinson's algorithm applies to two-tiered experiments and involves performing a two-stage series of sweeps. For each **sweep**, the means for a prescribed factor combination are calculated from the input vector, initially the data vector. The resulting (effective) means, divided by an efficiency factor if appropriate, are then subtracted from the input vector to form a residual vector. Either the residual vector, for a residual sweep, or the (effective) means, for a pivotal sweep, produced from one sweep will become the input for subsequent sweeps. Subsequent sweeps may involve **backsweeps** for previously fitted terms nonorthogonal to the current source. Of course, a two-stage decomposition could also be achieved using matrix inversion techniques to perform the sweeps.

To cover multitiered studies, the algorithm must be generalized to effect a multistage decomposition of the sample space such as that depicted in figure 3.5 for a four-tiered experiment. The stages correspond to the structures in the structure set for the study. In the first stage, the components of the data vector are obtained for the subspaces corresponding to the terms derived from the first structure; this can be achieved by applying recursively the appropriate sequence of residual sweeps. In subsequent stages, each of the subspaces formed in the previous stage is decomposed to obtain the components of the data vector in the subspaces corresponding to terms arising from the current structure. To achieve this requires the application of pivotal sweeps, together with appropriate backsweeps, for each subspace of the previous stage that contains a subspace of a term arising from the current structure. To the vectors

produced by the pivotal sweeps, one recursively applies a sequence of (adjusted) residual idempotent operators corresponding to the sources arising in the current structure. The sweep sequences for examples involving nonorthogonal three-tiered experiments are presented in sections 5.2.2, 5.2.3 and 5.2.4.

That the additive decomposition $\boldsymbol{y} = \sum_{k=1}^{p_i} \mathbf{P}_{ik}\boldsymbol{y}$ can be achieved by recursive application of adjusted idempotent operators, $\mathbf{E}^c_{T_{iw}}$, and adjusted residual idempotent operators, $(\mathbf{I} - \mathbf{E}^c_{T_{iw}})$, derives from the general form of projection operators as given in theorem 3.14 using an inductive argument.

The decomposition corresponding to the first structure is given by

$$\boldsymbol{y} = \sum_{T_{1z} \in T_1} \mathbf{E}_{T_{1z}}\boldsymbol{y}$$

where

$$T_{1z} \text{ is the defining term for the source corresponding to } \mathbf{P}_{1k}.$$

Suppose that, in general, the projection operators, $\mathbf{P}_{ik}, k = 1, \ldots, p_i$, are ordered so that marginal terms occur before terms to which they are marginal and that fitting is being done in the same order as the projection operators. Then it is easy to show that

$$\begin{aligned} \mathbf{P}_{1m}\boldsymbol{y} &= \mathbf{E}_{T_{1w}}\boldsymbol{y} \\ &= \mathbf{E}_{T_{1w}} \prod_{k=1}^{m-1} (\mathbf{I} - \mathbf{P}_{1k})\boldsymbol{y} \end{aligned}$$

where

$$T_{1w} \text{ is the defining term for the source corresponding to } \mathbf{P}_{1m}.$$

That is, take the residuals after fitting the first $(m-1)$ sources and apply the idempotent operator for the mth source to them. The result of this operation will then be subtracted from the input residuals to form the residuals after fitting the first m sources.

Now we assume that the effects $\mathbf{P}_{rk}\boldsymbol{y}$ are obtained by recursive application of idempotent and residual idempotent operators. So that we need to demonstrate that effects $\mathbf{P}_{im}\boldsymbol{y}, i = r+1$, can be obtained from $\mathbf{P}_{rk}\boldsymbol{y}$ by the same type of recursive procedure.

For the ith structure and with $r = i - 1$, projection operators, $\mathbf{P}_{im}$s can be of the following forms (theorem 3.14):

(i) previous-structure projection operator, $\mathbf{P}_{rk}$;

(ii) pivotal projection operator, $\mathbf{P}_{rk}\mathbf{E}^{c}_{T_{iw}}\mathbf{P}_{rk}$; and

(iii) residual projection operator,

$$\mathbf{P}_{rk} - \sum_{u \in U^{ii}_{rk}} \mathbf{P}_{iu} = \mathbf{P}_{rk} - \sum_{u \in U^{ii}_{rk}} \mathbf{P}_{rk}\mathbf{E}^{c}_{T_{iz}}\mathbf{P}_{rk}$$

where

T_{iz} is the defining term for the source corresponding to $\mathbf{P}_{iu}$; and

U^{ii}_{rk} is the set of indices specifying the projection operators corresponding to the sources in the ith structure which are estimated from the range of the kth projection operator from the rth structure.

So, if a projection operator from the ith structure is a previous-structure projection operator, there is no term from the ith structure confounded with it; we have assumed that its fitting has been achieved, using a recursive procedure, in the decomposition for the previous structures. For pivotal projection operators, the fitting can be achieved by

1. taking the effects $\mathbf{P}_{rk}\boldsymbol{y}$ and applying the adjusted idempotent operator to them to form $\mathbf{E}^{c}_{T_{iw}}\mathbf{P}_{rk}\boldsymbol{y}$;
2. subtracting the result of the previous step from its input to yield $(\mathbf{I}-\mathbf{E}^{c}_{T_{iw}})\mathbf{P}_{rk}\boldsymbol{y}$; and
3. applying, to the results of the two previous steps, the assumed recursive sequence corresponding to $\mathbf{P}_{rk}$; this is called backsweeping and results in the formation of $\mathbf{P}_{im}\boldsymbol{y}$ and associated residuals.

For residual projection operators from the ith structure, it can be shown that

$$\mathbf{P}_{im}\boldsymbol{y} \;=\; (\mathbf{P}_{rk} - \sum_{u \in U^{ii}_{rk}} \mathbf{P}_{rk}\mathbf{E}^{c}_{T_{iz}}\mathbf{P}_{rk})\boldsymbol{y}$$

$$= \prod_{u \in U^{ii}_{rk}} \mathbf{P}_{rk}(\mathbf{I} - \mathbf{E}^c_{T_{iz}})\mathbf{P}_{rk}\boldsymbol{y}$$

To derive the last result note that

$$\begin{aligned} \mathbf{P}_{iu}\mathbf{P}_{iu'} &= 0, \quad u \neq u' \text{ and} \\ \mathbf{P}_{rk}(\mathbf{I} - \mathbf{E}^c_{T_{iz}})\mathbf{P}_{rk}(\mathbf{I} - \mathbf{E}^c_{T_{iz'}})\mathbf{P}_{rk} &= \mathbf{P}_{rk} - \mathbf{P}_{rk}\mathbf{E}^c_{T_{iz}}\mathbf{P}_{rk} - \mathbf{P}_{rk}\mathbf{E}^c_{T_{iz'}}\mathbf{P}_{rk} \end{aligned}$$

where

T_{iz} is the defining term for the source corresponding to $\mathbf{P}_{iu}$, and
$T_{iz'}$ is the defining term for the source corresponding to $\mathbf{P}_{iu'}$.

Clearly, the fitting of terms from the ith structure to yield the projection operators for the ith structure can be achieved by recursive application of adjusted idempotent and adjusted residual idempotent operators to the effects corresponding to the projection operator from which it is estimated; that is, to $\mathbf{P}_{rk}\boldsymbol{y}$.

Hence, by induction, the fitting can be achieved by recursive application of the appropriate sequence of adjusted idempotent and adjusted residual idempotent operators.

Further, **averaging operators** $\mathbf{A}_{T_{iw}}$ can be substituted for the idempotent operators $\mathbf{E}_{T_{iw}}$ in this procedure so that adjusted idempotent operators $\mathbf{E}^c_{T_{iw}}$ can be replaced by the operators $(e^c_{T_{iw}})^{-1}\mathbf{A}_{T_{iw}}$. That this is the case rests on the fact that an idempotent for a particular term is a linear combination of the summation matrices for terms marginal to the idempotent's term; this result follows from theorem 3.11. Thus, if $\mathbf{P}\boldsymbol{y}$ is the residual vector after sweeping out sources for which $T_{iv} < T_{iw}$, then

$$\mathbf{E}^c_{T_{iw}}\mathbf{P}\boldsymbol{y} = (e^c_{T_{iw}})^{-1}\mathbf{A}_{T_{iw}}\mathbf{P}\boldsymbol{y}$$

where

$$\mathbf{A}_{T_{iw}} = \mathbf{R}^{-1}_{T_{iw}}\mathbf{S}_{T_{iw}}.$$

The pivotal operator is a substantial innovation of the Wilkinson algorithm. However, whereas Wilkinson (1970) regards a pivotal operator as having been defined by a sequence of residual operators, the pivotal operator used herein will, in general, be

defined by a sequence of residual and pivotal operators. While Wilkinson's form is sufficient for two-tiered experiments, the more general form is required for experiments consisting of more than two tiers.

3.3.2 Linear models for the study

So far in section 3.3 we have not mentioned linear models; the analysis of variance has been derived solely from the structure set for the study and factor incidences (Brien, 1983; Tjur, 1984). The analysis of variance provides us with invaluable information for the next step in the analysis process: the formulation and/or selection of linear models. It can be used to assist in determining the models to be considered, with estimation and hypothesis testing being most straightforward for those models whose subspaces correspond to the decomposition of the sample space on which the analysis of variance is based.

As outlined in section 2.2.6, the linear models for a study consist of sets of alternative models for the expectation and variation. In determining these models, one has first to classify the factors as either expectation or variation factors as described in section 2.2.3. Then the terms derived from a structure can be similarly classified; the expectation terms contain only expectation factors and variation terms contain at least one variation factor. Thus, the maximum of two expectation terms, if it exists, will be an expectation term; for a structure closed under the formation of maxima, such as a simple orthogonal structure, the highest order expectation term will be comprised of all the expectation factors in that structure. Further, any term to which a variation term is marginal must also be a variation term. Thus, if there is a variation term in a structure, the maximal term for that structure will be a variation term.

Definition 3.5 *The general form of the maximal expectation model is as follows:*

$$\begin{aligned} \mathrm{E}[\boldsymbol{y}] = \boldsymbol{\mu} &= \sum \boldsymbol{\mu}_i \\ &= \sum_i \sum_{T_{iw} \in T_{\boldsymbol{\mu}_i}} \boldsymbol{\mu}_{T_{iw}} \end{aligned}$$

where

$\boldsymbol{\mu}_i$ *is the n-vector of parameters corresponding to the terms from the ith structure that have been included in the maximal expectation model expectation model for the ith structure. The parameters are arranged in the vector in a manner consistent with the ordering of the summation matrices for the structure. The vector contains only zeros if there is no expectation factor in the structure, or if a structure contains the same set of expectation factors as a previous structure;*

$T_{\boldsymbol{\mu}_i}$ *is the set of terms from the ith structure that have been included in the maximal expectation model; and*

$\boldsymbol{\mu}_{T_{iw}}$ *is the n-vector of expectation parameters for an expectation term T_{iw}. A particular element of the vector corresponds to a particular observational unit and will be the parameter for the levels combination of the term T_{iw} observed for that observational unit; there will be $n_{T_{iw}}$ unique elements in the vector.*

The maximal expectation model can be written symbolically as

$$\mathrm{E}[Y] = \sum_i \sum_{T_{iw} \in T_{\boldsymbol{\mu}_i}} T_{iw}$$

Definition 3.6 *The general form of the maximal variation model is as follows:*

$$\mathrm{Var}[\boldsymbol{y}] = \mathbf{V} = \sum_i \mathbf{V}_i = \sum_i \boldsymbol{\phi}_i' \mathbf{s}_i = \sum_i \boldsymbol{\gamma}_i' \mathbf{w}_i = \sum_i \boldsymbol{\lambda}_i' \mathbf{e}_i$$

where

$\boldsymbol{\phi}_i$, $\boldsymbol{\gamma}_i$ *and* $\boldsymbol{\lambda}_i$ *are the* t_i*-vectors of canonical covariance, covariance and spectral parameters, respectively; that is, there is an element in the vector for each term in the* i*th structure; elements of* $\boldsymbol{\phi}_i$ *will be set to zero if they correspond to:*

- *expectation terms, or*
- *terms that also arise from lower structures;*

the elements of $\boldsymbol{\gamma}_i$ *and* $\boldsymbol{\lambda}_i$ *will be modified to reflect this;*

$$\begin{aligned}\boldsymbol{\gamma}_i &= \mathbf{T}'_{\boldsymbol{s}_i \boldsymbol{w}_i}\boldsymbol{\phi}_i; \text{ and}\\ \boldsymbol{\lambda}_i &= \mathbf{T}'_{\boldsymbol{s}_i \boldsymbol{e}_i}\boldsymbol{\phi}_i.\end{aligned}$$

Symbolically, the variation model can be written

$$\mathrm{Var}[Y] = \sum_i \sum_{T_{iw} \in T_{\mathbf{V}_i}} T_{iw}$$

where

$T_{\mathbf{V}_i}$ is the set of terms from the ith structure that have been included in the maximal variation model; that is, terms corresponding to the nonzero elements of $\boldsymbol{\phi}_i$.

In as much as there can be variation terms in more than one structure and that the terms from the different structures need only exhibit structure balance, these variation models represent a class exhibiting **nonorthogonal variation structure**.

The handling of pseudoterms (Alvey *et al.*, 1977) merits special note. When pseudoterms are included they result in a decomposition of the subspace corresponding to the term to which they are linked; thus they affect the set E_i for the structure in which they arise, and hence the sets $P_i, \ldots, P_s$ of projection operators. However, for the purpose of determining the expected mean squares, pseudoterms should be excluded from both the expectation and variation models.

While we have provided expressions for the variance matrices in terms of canonical covariance, covariance and spectral components for each structure, the relationship between these components needs clarification. We begin by specifying the component of the variance matrix corresponding to the ith structure in terms of the canonical

covariance components ($\phi_{T_{iw}}$s), which may well be a subset of the coefficients of the summation matrices ($f_{T_{iw}}$s). However, expressions for the covariance components ($\gamma_{T_{iw}}$s) in terms of the canonical covariance components are still given by theorem 3.9 with all covariance components being nonzero if the canonical component for G is always included. The γs will be actual covariances when variation terms arise from the first structure only and the set of variation terms is closed under the formation of both minima and maxima of terms. The expressions for the $\phi_{T_{iw}}$s in terms of the $\gamma_{T_{iw}}$s can be obtained using the Möbius function as described by Tjur (1984) on the subset of the Hasse diagram of term marginalities that involves only the terms for which there is a nonzero $\phi_{T_{iw}}$; however, the values of the Möbius function may no longer be given by theorem 3.10. The expressions for the $\phi_{T_{iw}}$s can also be obtained by using theorem 3.10 to obtain the $f_{T_{iw}}$s in terms of the $c_{T_{iw}}$s and setting to zero the $f_{T_{iw}}$s for which $\phi_{T_{iw}}$ is zero; the implication of this is that particular linear functions of $c_{T_{iw}}s$ are zero and expressions for the nonzero $f_{T_{iw}}$s, in terms of the $c_{T_{iw}}$s, will have to be adjusted to reflect this. It is also clear that expressions for the spectral components ($\lambda_{T_{iw}}$s) in terms of the canonical covariance components ($\phi_{T_{iw}}$s) are still given by theorem 3.11, provided that the structure involved is regular. Note that it is not necessary to require, as does Tjur (1984), that the terms from a structure contributing to the variation model be closed under the formation of minima. It is only necessary that, as specified in section 2.2.4, the full set of terms in the structure is closed under the formation of minima.

Example 2.1 (cont'd): If the factors in the first tier of a split-plot experiment of the kind presented in section 2.2 are classified as being variation factors and those in the second tier as expectation factors, then the maximal expectation and variation models, previously given in section 2.2.6.1, are:

$$\begin{aligned} \boldsymbol{\mu} &= \boldsymbol{\mu}_{VT} \qquad \text{with } \mathrm{E}[y_{klm}] = (\zeta\tau)_{ij}, \text{ and} \\ \mathbf{V} &= \phi_G\mathbf{S}_G + \phi_R\mathbf{S}_R + \phi_C\mathbf{S}_C + \phi_{RC}\mathbf{S}_{RC} + \phi_{RCS}\mathbf{S}_{RCS}. \end{aligned}$$

The symbolic expressions for these models, also previously given in section 2.2.6.1, are:

$$\mathrm{E}[Y] = V.T \qquad \text{and} \qquad \mathrm{Var}[Y] = G + R + C + R.C + R.C.S.$$

[To be continued.]

Example 3.1 (cont'd): If the factors in both tiers of a simple lattice experiment are classified as being variation factors, then the maximal expectation model is:

$$\boldsymbol{\mu} = \boldsymbol{\mu}_G \qquad \text{with } \mathrm{E}[y_{klm}] = \mu$$

where

y_{klm} is an observation with klm indicating the levels of the factors *Reps*, *Blocks*, and *Plots*, respectively, for that observation.

The maximal variation model is:

$$\mathbf{V} = \mathbf{V}_1 + \mathbf{V}_2$$

where

$$\begin{aligned}
\mathbf{V}_1 &= \phi_G \mathbf{S}_G + \phi_R \mathbf{S}_R + \phi_{RB} \mathbf{S}_{RB} + \phi_{RBP} \mathbf{S}_{RBP} \\
&= \phi_G \mathbf{J} \otimes \mathbf{J} \otimes \mathbf{J} + \phi_R \mathbf{I} \otimes \mathbf{J} \otimes \mathbf{J} + \phi_{RB} \mathbf{I} \otimes \mathbf{I} \otimes \mathbf{J} \\
&\quad + \phi_{RBP} \mathbf{I} \otimes \mathbf{I} \otimes \mathbf{I}; \\
\mathbf{V}_2 &= \phi_L \mathbf{S}_L \\
&= \phi_L \mathbf{U}_2 (\mathbf{I} \otimes \mathbf{J}) \mathbf{U}_2',
\end{aligned}$$

ϕ_j is the canonical covariance component arising from the factor combination of the factor set j;

the three matrices in the direct products for $\mathbf{V}_1$ correspond to *Reps*, *Blocks* and *Plots*, respectively, and so are of orders 2, b and b, respectively;

the two matrices in the direct product for $\mathbf{V}_2$ correspond to *Lines* and a dummy factor *Units*, respectively, and so are of orders b^2 and 2, respectively; and

$\mathbf{U}_2$ is the permutation matrix of order n giving the assignment of the levels combinations of *Lines* and *Units*, from the second tier to the observational units; it is assumed that the observational units are ordered lexicographically according to the factors in the first tier.

The symbolic expressions for these models, previously given in section 3.1, are:

$$\mathrm{E}[Y] = G \qquad \text{and} \qquad \mathrm{Var}[Y] = G + R + R.B + R.B.P + L.$$

[To be continued.]

3.3.3 Expectation and distribution of mean squares for the study

We are interested in finding the expectation and distribution of mean squares of the form

$$\boldsymbol{y}'\mathbf{P}_{sk}\boldsymbol{y}/\nu_{sk}.$$

Firstly, in determining the expectation of the mean squares we have, using Searle (1971b, section 2.5a, theorem 1),

$$\mathrm{E}[\boldsymbol{y}'\mathbf{P}_{sk}\boldsymbol{y}] = \boldsymbol{\mu}'\mathbf{P}_{sk}\boldsymbol{\mu} + \mathrm{tr}(\mathbf{P}_{sk}\mathbf{V}).$$

Thus we can consider the contribution of expectation and variation terms separately. Theorems 3.16 and 3.18, given below, provide expressions for each of these contributions.

Theorem 3.16 *The contribution to the expected mean squares from the expectation factors is given by*

$$\sum_i \sum_j \boldsymbol{\mu}_i'\mathbf{P}_{sk}\boldsymbol{\mu}_j/\nu_{sk}.$$

For a study in which expectation factors are either unrandomized or randomized only to variation factors, the contribution to the kth source from structure s reduces to

$$\boldsymbol{\mu}_i'\mathbf{P}_{sk}\boldsymbol{\mu}_i/\nu_{sk}$$

where

> *i is the structure in which the defining term for the kth source from the sth structure arises.*

Proof: The result is obtained straightforwardly by substituting the general form of the expectation model, given in definition 3.5, into $\boldsymbol{\mu}'\mathbf{P}_{sk}\boldsymbol{\mu}$. □

That is, in general, the contribution to the expected mean squares by the expectation factors will be quadratic and bilinear forms in the expectation parameters,

these forms parallelling those for the sums of squares. For studies in which expectation factors are either unrandomized or randomized only to variation factors, the usual situation, this reduces to quadratic forms in the expectation vector. The matrix of one of these quadratic forms is the same as that for the corresponding sum of squares and hence the step given in table 2.8 for determining the contribution of the expectation terms to an expected mean square.

In order to obtain the contribution of the variation terms to the expected mean squares, we first derive, using the following lemmas, an expression for $\mathbf{V}$ in terms of the $\mathbf{P}_{sk}$s.

Lemma 3.1 $\mathbf{P}_{im}\mathbf{E}_{T_{iw}} = 0$ *unless* $\mathbf{P}_{im}$ *is a pivotal projection operator with defining term* T_{iw}.

Proof: As outlined in theorem 3.14, $\mathbf{P}_{im}$ may be one of four possible general forms. We derive the results for each of these four forms.
(i) Pivotal projection operator from first structure. In this case, $i = 1$. Suppose that T_{iv} is the defining term for $\mathbf{P}_{im}$. Then, $\mathbf{P}_{1m} = \mathbf{E}_{T_{1v}}$ and it follows immediately from the results presented in section 3.2 that

$$\mathbf{P}_{1m}\mathbf{E}_{T_{1w}} = \mathbf{E}_{T_{1v}}\mathbf{E}_{T_{1w}} = \delta_{wv}\mathbf{E}_{T_{1w}}.$$

(ii) Previous-structure projection operator. That is, $\mathbf{P}_{im} = \mathbf{P}_{rc}$, $r = i - 1$. Being a previous-structure operator, it must be that no term from the ith structure is confounded with it and so $\mathbf{P}_{im}\mathbf{E}_{T_{iw}} = \mathbf{P}_{rc}\mathbf{E}_{T_{iw}} = 0$.
(iii) Pivotal projection operator. Suppose that the defining term for $\mathbf{P}_{im}$ is T_{iv} and that $\mathbf{P}_{rc}$, $r = i - 1$, is the projection operator such that

$$\mathbf{P}_{im} = (e^c_{T_{iv}})^{-1}\mathbf{P}_{rc}\mathbf{E}_{T_{iv}}\mathbf{P}_{rc}.$$

Now,

$$\begin{aligned}\mathbf{P}_{im}\mathbf{E}_{T_{iw}} &= (e^c_{T_{iv}})^{-1}\mathbf{P}_{rc}\mathbf{E}_{T_{iv}}\mathbf{P}_{rc}\mathbf{E}_{T_{iw}} \\ &= \delta_{wv}\mathbf{P}_{rc}\mathbf{E}_{T_{iw}}, \quad \text{by definition 3.4.}\end{aligned}$$

(iv) Residual projection operator. In this case, there exists $\mathbf{P}_{rc}$, $r = i - 1$ such that

$$\mathbf{P}_{im} = \mathbf{P}_{rc} - \sum_{u \in U_{rc}^{ii}} \mathbf{P}_{iu}, \quad r = i - 1.$$

where

U_{rc}^{ii} is the set of indices specifying the projection operators that correspond to the sources in the ith structure confounded with the cth source from the rth structure.

First, suppose that $\mathbf{P}_{rc}\mathbf{E}_{T_{iw}} \neq 0$. Let $\mathbf{E}_{T_{iv}}$ be the defining term for $\mathbf{P}_{iu}$ so that

$$\mathbf{P}_{iu} = (e_{T_{iv}}^{c})^{-1}\mathbf{P}_{rc}\mathbf{E}_{T_{iv}}\mathbf{P}_{rc}.$$

Now,

$$\begin{aligned}
\mathbf{P}_{im}\mathbf{E}_{T_{iw}} &= \mathbf{P}_{rc}\mathbf{E}_{T_{iw}} - \sum_{u \in U_{rc}^{ii}} \mathbf{P}_{iu}\mathbf{E}_{T_{iw}} \\
&= \mathbf{P}_{rc}\mathbf{E}_{T_{iw}} - \sum_{u \in U_{rc}^{ii}} (e_{T_{iv}}^{c})^{-1}\mathbf{P}_{rc}\mathbf{E}_{T_{iv}}\mathbf{P}_{rc}\mathbf{E}_{T_{iw}} \\
&= \mathbf{P}_{rc}\mathbf{E}_{T_{iw}} - \mathbf{P}_{rc}\mathbf{E}_{T_{iw}}, \quad \text{by definition 3.4} \\
&= 0.
\end{aligned}$$

Second, if $\mathbf{P}_{rc}\mathbf{E}_{T_{iw}} = 0$,

$$\mathbf{P}_{iu}\mathbf{P}_{rc}\mathbf{E}_{T_{iw}} = \mathbf{P}_{iu}\mathbf{E}_{T_{iw}} = 0$$

and so

$$\mathbf{P}_{im}\mathbf{E}_{T_{iw}} = 0.$$

Examination of the results for the four forms reveals that the lemma is true. □

Lemma 3.2 *Denote by* $\mathbf{P}_{sk}$ *the* k*th projection operator from the* s*th structure. Let* P_{sk} *be the set of pivotal projection operators for which*

$$\mathbf{P}_{sk}\mathbf{P}_{im} = \mathbf{P}_{im}\mathbf{P}_{sk} = \mathbf{P}_{sk}, \quad \mathbf{P}_{im} \in P_{sk} \text{ and } i = 1, \ldots, s.$$

Let T_{iw} *be the defining term for* $\mathbf{P}_{im}$ *and* $\mathbf{P}_{rc}$ *be the projection operator from the* r*th structure, where* $r = i - 1$*, corresponding to the source from which the source corresponding to* $\mathbf{P}_{im}$ *is estimated.*

Then,

$$\mathbf{P}_{sk}\mathbf{E}_{T_{iw}}\mathbf{P}_{sk'} = \begin{cases} e^c_{T_{iw}}\mathbf{P}_{sk} & \text{when } k = k' \text{ and } T_{iw} \text{ is the defining term for a } \mathbf{P}_{im} \in P_{sk} \\ 0 & \text{otherwise} \end{cases}$$

where

$e^c_{T_{iw}}$ *is the efficiency factor for* T_{iw} *when it is estimated from the range of the* c*th projection operator from the* $(i-1)$*th structure.*

Proof: Firstly note that there will be one projection operator for each i such that $\mathbf{P}_{im}\mathbf{P}_{sk} = \mathbf{P}_{sk}\mathbf{P}_{im} = \mathbf{P}_{sk}$, $i = 1 \ldots s$. The operator may not be a pivotal projection operator.

$$\begin{aligned} \mathbf{P}_{sk}\mathbf{E}_{T_{iw}} &= \mathbf{P}_{sk}\mathbf{P}_{im}\mathbf{E}_{T_{iw}}, \quad \text{for the } \mathbf{P}_{im} \text{ such that } \mathbf{P}_{sk}\mathbf{P}_{im} = \mathbf{P}_{sk} \\ &= 0 \quad \text{unless } T_{iw} \text{ is the defining term for } \mathbf{P}_{im} \in P_{sk} \text{ (by lemma 3.1).} \end{aligned}$$

Secondly, on also noting that, for $\mathbf{P}_{im'}\mathbf{E}_{T_{iw}} = 0$, $(\mathbf{P}_{im'}\mathbf{E}_{T_{iw}})' = \mathbf{E}_{T_{iw}}\mathbf{P}_{im'} = 0$,

$$\begin{aligned} \mathbf{E}_{T_{iw}}\mathbf{P}_{sk'} &= \mathbf{E}_{T_{iw}}\mathbf{P}_{im'}\mathbf{P}_{sk'} \quad \text{for the } \mathbf{P}_{im'} \text{ such that} \mathbf{P}_{im'}\mathbf{P}_{sk'} = \mathbf{P}_{sk'} \\ &= 0 \quad \text{unless } T_{iw} \text{ is the defining term for } \mathbf{P}_{im'} \in P_{sk'} \text{ (by lemma 3.1).} \end{aligned}$$

Hence, $\mathbf{P}_{sk}\mathbf{E}_{T_{iw}}\mathbf{P}_{sk'} = 0$ unless T_{iw} is the defining term for $\mathbf{P}_{im} \in P_{sk} \cap P_{sk'}$.

If T_{iw} is the defining term for $\mathbf{P}_{im} \in P_{sk} \cap P_{sk'}$,

$$\mathbf{P}_{im} = (e^c_{T_{iw}})^{-1}\mathbf{P}_{rc}\mathbf{E}^c_{T_{iw}}\mathbf{P}_{rc}$$

so that

$$\mathbf{P}_{sk}\mathbf{P}_{im}\mathbf{P}_{sk'} = (e^c_{T_{iw}})^{-1}\mathbf{P}_{sk}\mathbf{P}_{rc}\mathbf{E}^c_{T_{iw}}\mathbf{P}_{rc}\mathbf{P}_{sk'}$$

and

$$\mathbf{P}_{sk}\mathbf{P}_{sk'} = (e^c_{T_{iw}})^{-1}\mathbf{P}_{sk}\mathbf{E}^c_{T_{iw}}\mathbf{P}_{sk'},$$

as $\mathcal{R}(\mathbf{P}_{sk}) \subseteq \mathcal{R}(\mathbf{P}_{im}) \subseteq \mathcal{R}(\mathbf{P}_{rc})$.

Now $\mathbf{P}_{sk}\mathbf{P}_{sk'} = 0$ for $k \neq k'$ and the lemma follows straightforwardly. □

Theorem 3.17 *The variance matrix can be written*

$$\mathbf{V} = \sum_k \sum_{\mathbf{P}_{im} \in P_{sk}} e^c_{T_{iw}} \lambda_{T_{iw}} \mathbf{P}_{sk}$$

where

$\lambda_{T_{iw}}$ *is the spectral component for term* T_{iw}.

Proof:

$$\begin{aligned}
\mathbf{V} &= \sum_{j=1}^{s} \sum_{T_{jz} \in T_j} \lambda_{T_{jz}} \mathbf{E}_{T_{jz}}, \quad \text{(from definition 3.6)} \\
&= \sum_{k=1}^{t_s} \mathbf{P}_{sk} \left(\sum_{j=1}^{s} \sum_{T_{jz} \in T_j} \lambda_{T_{jz}} \mathbf{E}_{T_{jz}} \right) \sum_{k'=1}^{t_s} \mathbf{P}_{sk'} \\
&= \sum_{k=1}^{t_s} \sum_{k'=1}^{t_s} \sum_{j=1}^{s} \sum_{T_{jz} \in T_j} \lambda_{T_{jz}} \mathbf{P}_{sk} \mathbf{E}_{T_{jz}} \mathbf{P}_{sk'} \\
&= \sum_k \sum_{\mathbf{P}_{im} \in P_{sk}} e^c_{T_{iw}} \lambda_{T_{iw}} \mathbf{P}_{sk}, \quad \text{(by lemma 3.2).}
\end{aligned}$$

□

Theorem 3.18 *Denote by* ξ_{sk} *the contribution of the variation to the expected mean square for the source corresponding to the* k*th projection operator from the* s*th structure,* $\mathbf{P}_{sk}$*. Then, provided that the structures giving rise to the defining terms,* T_{iw}*, of the elements of* P_{sk} *are regular Tjur structures,*

$$\xi_{sk} = \sum_{\mathbf{P}_{im} \in P_{sk}} e^c_{T_{iw}} \sum_{\substack{T_{iv} \geq T_{iw} \\ T_{iv} \in T_{\mathbf{V}_i}}} r_{T_{iv}} \phi_{T_{iv}}$$

where

$e^c_{T_{iw}}$ *is the efficiency factor for term* T_{iw} *when it is estimated from the range of the* c*th projection operator for the* $(i-1)$*th structure;*

$r_{T_{iv}}$ *is the replication of regular term* T_{iv} *which, for simple orthogonal structures, is given by* $n\prod_{t_{ih}\in T_{iv}} n^{-1}_{t_{ih}} = r_i \prod_{t_{ih}\notin T_{iv}} n_{t_{ih}}$*; and*

$\phi_{T_{iv}}$ *is the canonical covariance component for the term* T_{iv}*.*

Proof: Now,

$$\begin{aligned}
\xi_{sk} &= \operatorname{tr}(\mathbf{P}_{sk}\mathbf{V})/\nu_{sk} \\
&= \operatorname{tr}\left(\mathbf{P}_{sk}\sum_{k'}\sum_{\mathbf{P}_{im}\in P_{sk'}} e^c_{T_{iw}}\lambda_{T_{iw}}\mathbf{P}_{sk'}\right)/\nu_{sk}, \quad \text{(by theorem 3.17)} \\
&= \operatorname{tr}\left(\sum_{\mathbf{P}_{im}\in P_{sk}} e^c_{T_{iw}}\lambda_{T_{iw}}\mathbf{P}_{sk}\right)/\nu_{sk} \\
&= \sum_{\mathbf{P}_{im}\in P_{sk}} e^c_{T_{iw}}\lambda_{T_{iw}}\operatorname{tr}(\mathbf{P}_{sk})/\nu_{sk} \\
&= \sum_{\mathbf{P}_{im}\in P_{sk}} e^c_{T_{iw}}\lambda_{T_{iw}} \\
&= \sum_{\mathbf{P}_{im}\in P_{sk}} e^c_{T_{iw}} \sum_{\substack{T_{iv}\geq T_{iw}\\ T_{iv}\in T_i}} r_{T_{iv}}\phi_{T_{iv}}, \quad \text{(by theorem 3.11)} \\
&= \sum_{\mathbf{P}_{im}\in P_{sk}} e^c_{T_{iw}} \sum_{\substack{T_{iv}\geq T_{iw}\\ T_{iv}\in T_{\mathbf{V}_i}}} r_{T_{iv}}\phi_{T_{iv}}, \quad \text{as for } T_{iv}\notin T_{\mathbf{V}_i},\ \phi_{T_{iv}} = 0.
\end{aligned}$$

□

As mentioned previously, pseudoterms are not included in the models for the study. Hence, a variation pseudoterm will have the element of the vector $\boldsymbol{\phi}_i$ corresponding to it set to zero. In effect, this is no different to including a component for it initially and setting this to zero after the expected mean squares have been determined.

Of course for a valid analysis of variance we require that the ξ_{sk}s are strictly positive. In particular, note that $\mathbf{V} = \sum_k \xi_{sk}\mathbf{P}_{sk}$ so that, if the ξ_{sk}s are strictly positive, $\mathbf{V}$ will be nonsingular with $\mathbf{V}^{-1} = \sum_k \xi^{-1}_{sk}\mathbf{P}_{sk}$. The ξ_{sk}s will be strictly positive if

- the canonical covariance components for unit terms, which are also the spectral components for these terms, are strictly positive, and

- the spectral components for other than unit terms is nonnegative.

Of course, this allows canonical covariance components to be negative.

The results contained in theorem 3.18 justify the steps given in table 2.8 for obtaining the contribution of the variation terms to the expected mean squares.

Further, if the F distribution is to be used in performing hypothesis tests based on ratios of mean squares, we require that the mean squares are independently distributed as χ^2s. The following theorem provides the necessary results.

Theorem 3.19 *When* $\boldsymbol{y}$ *is normally distributed with mean* $\boldsymbol{\mu}$ *and variance* $\mathbf{V}$*, then* $(\xi_{sk}\nu_{sk})^{-1}\boldsymbol{y}'\mathbf{P}_{sk}\boldsymbol{y}$ *is distributed as a* χ^2 *with degrees of freedom* ν_{sk} *and noncentrality parameter* $(2\xi_{sk}\nu_{sk})^{-1}\boldsymbol{\mu}'\mathbf{P}_{sk}\boldsymbol{\mu}$*.*

Also, $(\xi_{sk'}\nu_{sk'})^{-1}\boldsymbol{y}'\mathbf{P}_{sk'}\boldsymbol{y}$ *is distributed independently of* $(\xi_{sk}\nu_{sk})^{-1}\boldsymbol{y}'\mathbf{P}_{sk}\boldsymbol{y}$ *for* $k \neq k'$*.*

Proof: From Searle (1971b, section 2.5a, theorem 2), $(\xi_{sk}\nu_{sk})^{-1}\boldsymbol{y}'\mathbf{P}_{sk}\boldsymbol{y}$ will be distributed as specified if $(\xi_{sk}\nu_{sk})^{-1}\mathbf{P}_{sk}\mathbf{V}$ is idempotent.

Further, from Searle (1971b, section 2.5a, theorem 4), $(\xi_{sk'}\nu_{sk'})^{-1}\boldsymbol{y}'\mathbf{P}_{sk'}\boldsymbol{y}$ is distributed independently of $(\xi_{sk}\nu_{sk})^{-1}\boldsymbol{y}'\mathbf{P}_{sk}\boldsymbol{y}$ for $k \neq k'$ if $(\xi_{sk}\nu_{sk}\xi_{sk'}\nu_{sk'})^{-1}\mathbf{P}_{sk}\mathbf{V}\mathbf{P}_{sk'} = 0$.

Now,

$$(\xi_{sk}\nu_{sk})^{-1}\mathbf{P}_{sk}\mathbf{V} = (\xi_{sk}\nu_{sk})^{-1}\mathbf{P}_{sk}.$$

As $\mathbf{P}_{sk}$ is idempotent, $(\xi_{sk}\nu_{sk})^{-1}\mathbf{P}_{sk}\mathbf{V}$ is idempotent.

Also, as $\mathbf{P}_{sk}\mathbf{P}_{sk'} = 0$ for $k \neq k'$, $(\xi_{sk}\nu_{sk}\xi_{sk'}\nu_{sk'})^{-1}\mathbf{P}_{sk}\mathbf{V}\mathbf{P}_{sk'} = 0$ for $k \neq k'$. □

Example 2.1 (cont'd): The analysis table, including projection operators, for split-plot experiments of the kind presented in section 2.2 is shown in table 3.5.

Example 3.1 (cont'd): The analysis table, including projection operators, for the simple lattice experiment is shown in table 3.6.

Table 3.5: Analysis of variance table, including projection operators, for a split-plot experiment

SOURCE	DF	PROJECTION OPERATORS	EXPECTED MEAN SQUARES Coefficients of ϕ_{RCS}	ϕ_{RC}	ϕ_R	ϕ_C	$\boldsymbol{\mu}_{VT}$
Rows	$v-1$	$\mathbf{P}_{11} = \mathbf{P}_{21} = \mathbf{E}_R$	1	t	vt		
Columns	$v-1$	$\mathbf{P}_{12} = \mathbf{P}_{22} = \mathbf{E}_C$	1	t		vt	
Rows.Columns	$(v-1)^2$	$\mathbf{P}_{13} = \mathbf{E}_{RC}$					
Varieties	$v-1$	$\mathbf{P}_{23} = \mathbf{E}_V$	1	t			$f_V(\boldsymbol{\mu}_{VT})^\dagger$
Residual	$(v-1)(v-2)$	$\mathbf{P}_{24} = \mathbf{P}_{13}-\mathbf{P}_{23}$	1	t			
Rows.Columns.Subplots	$(t-1)v^2$	$\mathbf{P}_{14} = \mathbf{E}_{RCS}$					
Treatments	$t-1$	$\mathbf{P}_{25} = \mathbf{E}_T$	1				$f_T(\boldsymbol{\mu}_{VT})^\dagger$
Varieties.Treatments	$(v-1)(t-1)$	$\mathbf{P}_{26} = \mathbf{E}_{VT}$	1				$f_{VT}(\boldsymbol{\mu}_{VT})^\dagger$
Residual	$(v-1)(t-1)v$	$\mathbf{P}_{27} = \mathbf{P}_{14}-\mathbf{P}_{25}-\mathbf{P}_{26}$	1				

†The functions for the expectation contribution are as follows:

$$
\begin{aligned}
f_V(\boldsymbol{\mu}_{VT}) &= vt\sum((\overline{\zeta\tau})_{i.} - (\overline{\zeta\tau})_{..})^2/(v-1),\\
f_T(\boldsymbol{\mu}_{VT}) &= v^2\sum((\overline{\zeta\tau})_{.j} - (\overline{\zeta\tau})_{..})^2/(t-1),\\
f_{VT}(\boldsymbol{\mu}_{VT}) &= v\sum((\zeta\tau)_{ij} - (\overline{\zeta\tau})_{i.} - (\overline{\zeta\tau})_{.j} + (\overline{\zeta\tau})_{..})^2/(v-1)(t-1),
\end{aligned}
$$

where the dot subscript denotes summation over that subscript.

3.4 Discussion

A summary of the conditions to be met by an study if it is to be covered by this approach is given in sections 2.2.5 and 6.1. It is also noted that, in some circumstances, the structure balance condition can be relaxed in part at least.

The basis for inference outlined here is the 'analysis of variance method'. That

Table 3.6: Analysis of variance table, including projection operators, for a simple lattice experiment

SOURCE	DF	PROJECTION OPERATORS	EXPECTED MEAN SQUARES Coefficients of ϕ_{RBP}	ϕ_{RB}	ϕ_R	ϕ_L
Reps	1	$\mathbf{P}_{11} = \mathbf{P}_{21} = \mathbf{E}_R$	1	b	b^2	
Reps.Blocks	$2(b-1)$	$\mathbf{P}_{12} = \mathbf{E}_{RB}$				
C	$b-1$	$\mathbf{P}_{22} = (e_C^2)^{-1}\mathbf{E}_C$	1	b		$e_C^2 2$
D	$b-1$	$\mathbf{P}_{23} = (e_D^2)^{-1}\mathbf{E}_D$	1	b		$e_D^2 2$
Reps.Blocks.Plots	$2b(b-1)$	$\mathbf{P}_{13} = \mathbf{E}_{RBP}$				
C	$b-1$	$\mathbf{P}_{24} = (e_C^3)^{-1}\mathbf{E}_C$	1			$e_C^3 2$
D	$b-1$	$\mathbf{P}_{25} = (e_D^3)^{-1}\mathbf{E}_D$	1			$e_D^3 2$
Lines	$(b-1)^2$	$\mathbf{P}_{26} = \mathbf{E}_L$	1			2
Residual	$(b-1)^2$	$\mathbf{P}_{27} = \mathbf{P}_{13} - \mathbf{P}_{24} - \mathbf{P}_{25} - \mathbf{P}_{26}$	1			

is, having established an analysis of variance and a model, we use them to produce expected mean squares. One method of obtaining estimates of canonical covariance components is to use a generalized linear model for the stratum mean squares; in fitting this model to the stratum mean squares, one would specify a gamma error distribution, a linear link and weights which are the degrees of freedom of the mean squares divided by two (McCullagh and Nelder, 1983, section 7.3.5). In situations where there are the same number of canonical components as there are strata and the stratum components are linearly independent, as is often the case, estimation of the canonical components is merely a matter of solving the moment equations.

Estimates of the expectation effects confounded with a particular source are obtained straightforwardly. Further, when an expectation term is confounded with more than one source, the combination of information about that term can be accomplished provided suitable estimates of the canonical covariance components are

available. However, it remains to establish the properties of the resulting estimators. For example, are they generalized least squares estimators? To establish whether or not this is the case would involve the simplification of the normal equations providing the BLUEs of $\boldsymbol{\mu}$. These are

$$\mathbf{M}\mathbf{V}^{-1}\mathbf{M}\boldsymbol{\mu} = \mathbf{M}\mathbf{V}^{-1}\boldsymbol{y}$$

where

$\mathbf{M} = \sum_i \sum_{T_{iw} \in T_{\boldsymbol{\mu}_i}} \mathcal{R}(\mathbf{A}_{T_{iw}})$
is the projection operator onto the subspace of the sample space corresponding to the expectation model.

As discussed in section 1.2.2.2, Houtman and Speed (1983) provide expressions for the case in which the study exhibits orthogonal variation structure. Wood, Williams and Speed (1988) give expressions for a class exhibiting nonorthogonal variation structure; in particular, they cover three-tiered experiments in which:

1. the factors in tiers 1 and 2 are classified as variation factors and those in tier 3 as expectation factors;
2. the terms derived from structure 1 are orthogonal to those from structure 2; and
3. the sources derived from structure 2 are generally balanced with respect to those derived from structure 3.

However, their results are not generally applicable to the class of studies discussed here as we place no restriction on the number of structures that can occur and we do not impose the first two of their conditions.

In this chapter, two relatively straightforward examples have been presented. Further examples will be treated in chapter 4.

Chapter 4

Analysis of two-tiered experiments

4.1 Introduction

In this chapter a number of examples are presented which either demonstrate the application of the approach or in which the use of the approach clarifies aspects of the analysis. Attention here is restricted to two-tiered experiments; the factors from the first tier will be referred to as unrandomized factors and those from the second tier as randomized factors. The structure sets for the orthogonal examples will accordingly correspond to those obtained using Nelder's (1965a,b) method. However, a detailed examination of the structure set for the range of experiments considered here is currently not available in the literature.

For all experiments, it will be assumed that the analyses discussed will only be applied to data that conform to the assumptions necessary for them to be valid. In particular, homogeneity of variance and correlation assumptions have to be made. This requires a particular form for the expected variance matrix of the observations (see, for example, Huynh and Feldt, 1970; Rouanet and Lépine, 1970).

4.2 Application of the approach to two-tiered experiments

4.2.1 A two-tiered sensory experiment

In this section we outline the analysis of a two-tiered sensory experiment whose analysis has been presented previously by Brien (1989). An experiment was conducted in which wine was made from 3 randomly selected batches of fruit from each of 4 areas specifically of interest to the investigator. The 12 wines were then presented for sensory evaluation to 2 evaluators selected from a group of experienced evaluators. For each evaluator, 12 glasses were positioned in a row on a bench and each wine poured into a glass selected at random. Each evaluator scored the wine from the 12 glasses starting with the first position and continuing to the twelfth. The whole process was repeated on a second occasion with the same evaluators. The scores from the experiment are given in appendix A.1.

The observational unit for this experiment is a glass in a particular position to be evaluated by an evaluator on an occasion. The structure set for the experiment, derived using the method described in sections 2.2.1–2.2.4, is as follows:

Tier	Structure
1	*(2 Occasion∗2 Evaluator)/12 Position* [or $(O * E)/P$]
2	*(4 Area/3 Batch)∗Occasion∗Evaluator* [or $(A/B) * O * E$]

That is, the factors *Occasion*, *Evaluator* and *Position* are unrandomized factors; *Area* and *Batch* are randomized factors. *Evaluator* is included in the Tier 2 structure since it is likely that interactions between it and the randomized factors *Area* and *Batch* will arise. The Hasse diagram of term marginalities, used to compute the degrees of freedom as described in table 2.2, is given in figure 4.1.

The analysis of variance table derived from the structure set for a study, as prescribed in table 2.1, is given in table 4.1.

Figure 4.1: Hasse diagram of term marginalities for a two-tiered sensory experiment

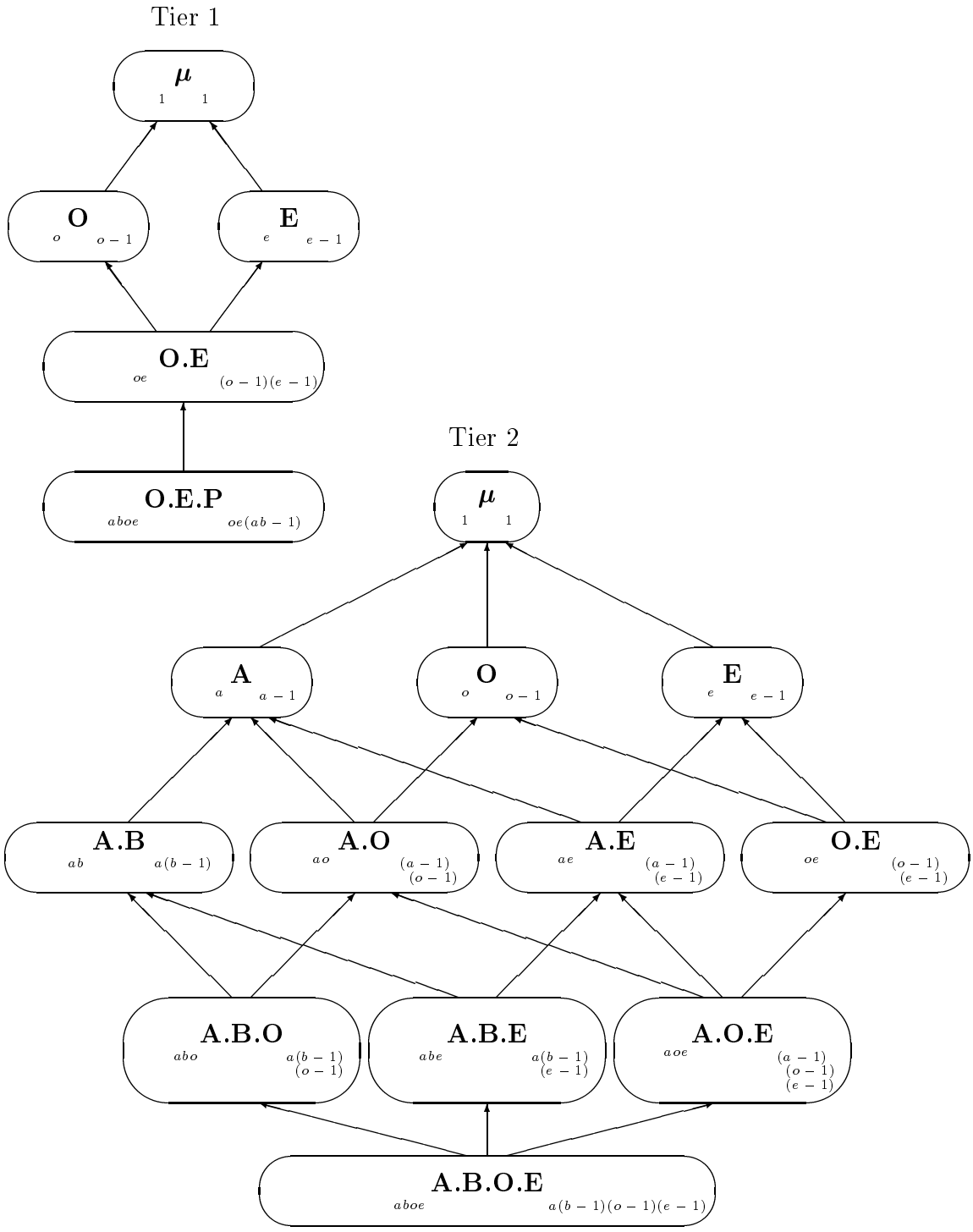


Table 4.1: Analysis of variance table for a two-tiered sensory experiment.

(O = *Occasion*; E = *Evaluator*; P = *Position*; A = *Area*; B = *Batch*)

SOURCE	DF	EXPECTED MEAN SQUARES Coefficients of ϕ_{OEP}	ϕ_{OE}	ϕ_O	ϕ_{ABOE}	ϕ_{AOE}	ϕ_{ABE}	ϕ_{ABO}	ϕ_{AO}	ϕ_{AB}	$\boldsymbol{\mu}$	MSq	F†
O	1	1	12	24	1	3		2	6			.19	$.28^{ns}$
E	1	1	12		1	3	2				$f_E(\boldsymbol{\mu})$‡	33.33	9.01^{ns}
OE	1	1	12		1	3						1.69	4.12^{ns}
$O.E.P$	44												
A	3	1			1	3	2	2	6	4	$f_A(\boldsymbol{\mu})$‡	14.83	$.98^{ns}$
$A.B$	8	1			1		2	2		4		15.78	3.20^{ns}
$A.O$	3	1			1	3		2	6			.41	$.52^{ns}$
$A.E$	3	1			1	3	2				$f_{AE}(\boldsymbol{\mu})$‡	2.06	$.54^{ns}$
$A.B.O$	8	1			1			2				1.01	3.13^{ns}
$A.B.E$	8	1			1		2					4.03	12.48^{***}
$A.O.E$	3	1			1	3						.41	1.27^{ns}
$A.B.O.E$	8	1			1							.32	
Total	47												

†The F values that are the ratios of combinations of mean squares are specified below, together with approximate degrees of freedom calculated according to Satterthwaite's (1946) approximation.

Source	Numerator	Denominator	ν_1	ν_2
O	$O + A.O.E$	$O.E + A.O$	3.91	1.51
E	$E + A.O.E$	$O.E + A.E$	1.02	3.29
A	$A + A.B.O$	$A.B + A.O$	3.42	8.41
$A.B$	$A.B + A.B.O.E$	$A.B.O + A.B.E$	8.33	11.77
$A.O$	$A.O + A.B.O.E$	$A.B.O + A.O.E$	7.78	10.99
$A.E$	$A.E + A.B.O.E$	$A.B.E + A.O.E$	3.98	9.45

‡The functions f_A, f_E and f_{AE} of $\boldsymbol{\mu}$ are similar in form to those given in table 2.10.

In order to determine the models for the experiment, the factors *Occasion*, *Position* and *Batch* are categorized as variation factors because particular occasions, positions or batches are of no special interest and will be assumed to have homogeneous variation. *Evaluator*, on the other hand, is categorized as an expectation factor because it is thought that performance of the evaluators is likely to be more heterogeneous than is appropriate for a variation factor (Jill's assessments of the wines are likely to be quite different from Jane's). *Area* is categorized as an expectation factor because there is interest in comparing the performance of different areas.

The maximal expectation model for the example, derived using the steps contained in table 2.5, is $A.E$ which can be expressed formally as

$$\mathrm{E}[y_{jkl}] = (\alpha\epsilon)_{il}$$

where

y_{jkl} is an observation with jkl indicating the levels of the factors *Occasion*, *Position*, and *Evaluator*, respectively, for that observation, and

$(\alpha\epsilon)_{il}$ is the expected response when the response depends on the combination of *Area* and *Evaluator* with il being the levels combination of the respective factors which is associated with observation jkl.

The maximal variation model, also derived as prescribed in table 2.5, is

$$G + O + O.E + O.E.P + A.B + A.O + A.B.O + A.B.E + A.O.E + A.B.O.E,$$

which corresponds to the following variance matrix for the observations, assuming the data are lexicographically ordered on *Occasion*, *Evaluator* and *Position*,

$$\mathbf{V} = \mathbf{V}_1 + \mathbf{V}_2$$

where

$$\begin{aligned}
\mathbf{V}_1 &= \phi_G \mathbf{J}\otimes\mathbf{J}\otimes\mathbf{J} + \phi_O \mathbf{I}\otimes\mathbf{J}\otimes\mathbf{J} + \phi_{OE}\mathbf{I}\otimes\mathbf{I}\otimes\mathbf{J} + \phi_{OEP}\mathbf{I}\otimes\mathbf{I}\otimes\mathbf{I},\\
\mathbf{V}_2 &= \mathbf{U}_2(\phi_{AB}\mathbf{I}\otimes\mathbf{I}\otimes\mathbf{J}\otimes\mathbf{J} + \phi_{AO}\mathbf{I}\otimes\mathbf{J}\otimes\mathbf{I}\otimes\mathbf{J} + \phi_{ABO}\mathbf{I}\otimes\mathbf{I}\otimes\mathbf{I}\otimes\mathbf{J}\\
&\quad + \phi_{ABE}\mathbf{I}\otimes\mathbf{I}\otimes\mathbf{J}\otimes\mathbf{I} + \phi_{AOE}\mathbf{I}\otimes\mathbf{J}\otimes\mathbf{I}\otimes\mathbf{I}\\
&\quad + \phi_{ABOE}\mathbf{I}\otimes\mathbf{I}\otimes\mathbf{I}\otimes\mathbf{I})\mathbf{U}_2', \text{ and}
\end{aligned}$$

$\mathbf{U_2}$ is the permutation matrix of order 48 specifying the assigning of the levels combinations of *Area* and *Batch* to position of presentation for each evaluator on each occasion.

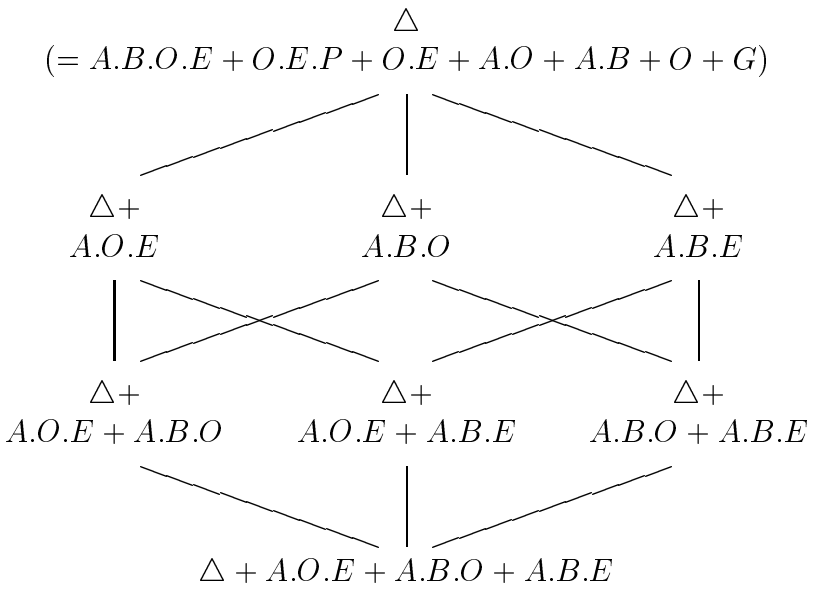
The expected mean squares for the maximal expectation and variation models, presented in table 4.1, are obtained using the steps outlined in table 2.8. The canonical covariance components are arranged in columns in table 4.1 so that for all sources the components in the first three columns of the expected mean squares arise from unrandomized factors, while those in columns four to nine arise from randomized factors. The contribution of the expectation terms is shown in the last column of the expected mean squares in table 4.1.

As outlined in section 2.2.8, subsequent model selection utilizes the expectation and variation lattices of models which are derived as described in table 2.6. The expectation lattice for this example is essentially the same as that given in figure 2.4. The full variation lattice for this experiment is rather large; however, it is possible to consider sublattices in which the differences between models involve terms all of the same order. The variation sublattices showing models that differ in either third or second order terms are shown in figure 4.2, the unit terms $A.B.O.E$ and $O.E.P$ and the term G being included in every model; the corresponding sublattice for first order terms is not included as it is trivial since there is only the one term, O, to be considered.

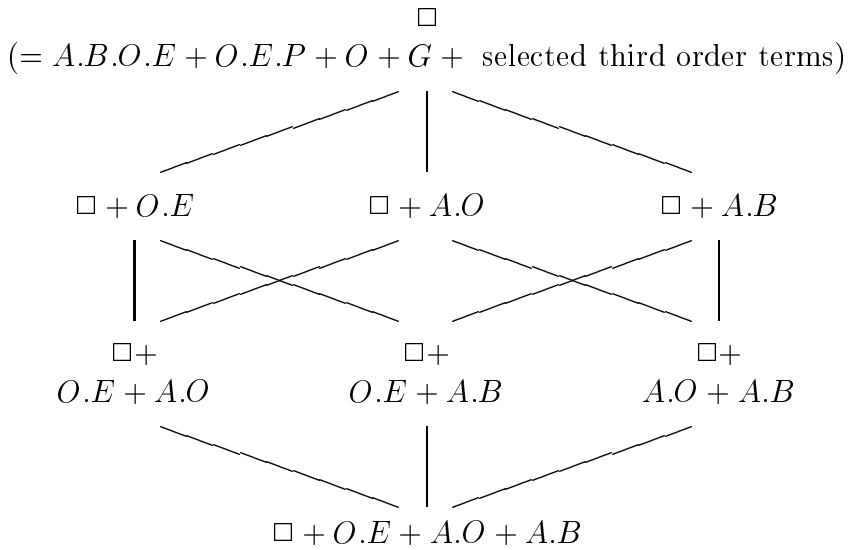
The results of the tests associated with model selection, without pooling, are also given in table 4.1. The selected model for expectation is G and that for variation $O.E.P + A.B.O.E + A.B.E + G$. The tests performed in selecting these models, in most instances, involved the use of Satterthwaite's (1946) approximation to the distribution of a linear combination of mean squares. For example, the F statistic for

Figure 4.2: Sublattices of variation models for second and third order model selection in a sensory experiment

A. Third Order Model Selection



B. Second Order Model Selection



Area is calculated as

$$\frac{14.8333 + 1.0104}{15.7812 + 0.4097} = 0.9786$$

and the degrees of freedom are given by

$$\nu_1 = \frac{(14.8333 + 1.0104)^2}{14.8333^2/3 + 1.0104^2/8} = 4.42, \qquad \nu_2 = \frac{(15.7812 + 0.4097)^2}{15.7812^2/8 + 0.4097^2/3} = 8.41$$

This is not the only F statistic for *Area*; an alternative F statistic is

$$\frac{14.8333}{15.7812 + 0.4097 - 1.0104} = 0.9771$$

However, Snedecor and Cochran (1980, section 16.14) point out that the latter statistic, while it has more power, has the disadvantage that Satterthwaite's approximation to the degrees of freedom of its denominator is not so good.

The significance of the $A.B.E$ source indicates that evaluators contribute to the variability in the evaluation of the batch of wine made from an area in that evaluations of that wine performed by the same evaluator differ in their covariance (and hence correlation) than those that are not. The canonical covariance component for $A.B.E$ is clearly positive so that evaluations by the same evaluator exhibit greater, rather than less, covariance than those that are not. If the source had not been significant it would indicate that scores for a wine from the same evaluator exhibited the same covariance as scores from different evaluators; in this case, it would be concluded that evaluators do not contribute to the variability in the evaluation of the individual wines. Of course, the reason for the significant interaction needs to be investigated and may suggest reanalysis such as a separate analysis of each evaluator's scores.

4.2.1.1 Split-plot analysis of a two-tiered sensory experiment

Kempthorne (1952, section 28.3), among others, suggests that sensory experiments be analysed using a split-plot analysis. The experimental structure underlying the split-plot analysis of the two-tiered sensory experiment presently being discussed is as follows:

Tier	Structure
1	*4 Area.3 Batch/2 Occasion.2 Evaluator*
2	*Area∗Occasion∗Evaluator*

The analysis derived from this structure is presented in table 4.2. The essential differences in determining this analysis, as compared to the analysis in table 4.1, are that:

1. *Evaluator* and *Occasion* are regarded as being nested within *Area.Batch* in the structure in which they occur together; and
2. following Kempthorne (1952, section 28.3), *Evaluator* is designated a variation factor.

As a result, the estimate of individual score variability from the analysis in table 4.2, *Error(b)*, is greater than that from table 4.1, $A.B.O.E$, because $A.B.O$, $A.B.E$ and $A.B.O.E$ from table 4.1 have been pooled into *Error(b)* from table 4.2. Consequently, the two analyses lead to different conclusions. The analysis in table 4.2 leads one to conclude that $A.B$ is (highly) significant, whereas the analysis in table 4.1 suggests it is not significant. Thus, one of the scientifically important conclusions is reversed according to the form of the analysis used. The analysis presented in table 4.1 was derived according to the method proposed in this thesis and is the more appropriate analysis as it separates out terms incorrectly pooled in that presented in table 4.2. This example demonstrates the advantage of the proposed method which is based on the careful consideration of the appropriate structure set for a study and the derivation of the analysis of variance table from that structure set.

4.2.2 Nonorthogonal two-factor experiment

To illustrate the process of selecting an expectation model for nonorthogonal experiments, consider a two-factor completely randomized design with unequal replication of the combinations of the levels of the two factors and with all combinations being replicated at least once. This example does not satisfy the conditions set out in section 2.2.5 as the terms arising from the randomized factors are not orthogonal; however, much of the approach remains applicable if the randomized factors are designated as expectation factors.

The structure set for a study, determined as described in section 2.2.4, is given in

Table 4.2: Split-plot analysis of variance table for a two-tiered sensory experiment

(O = *Occasion*; E = *Evaluator*; P = *Position*; A = *Area*; B = *Batch*)

SOURCE	DF	EXPECTED MEAN SQUARES Coefficients of ϕ	ϕ_{AOE}	ϕ_{AE}	ϕ_{AO}	ϕ_{OE}	ϕ_O	ϕ_E	ϕ_{AB}	$\boldsymbol{\mu}$	MSq	F†
A.B												
A	3	1	3	6	6				4	$f_A(\boldsymbol{\mu})$‡	14.83	0.93^{ns}
Error(a)	8	1							4		15.78	8.82^{***}
A.B.O.E												
O	1	1	3		6	12	24				0.19	0.29^{ns}
E	1	1	3	6		12		24			33.33	9.01^{*}
O.E	1	1	3			12					1.69	4.12^{ns}
A.O	3	1	3		6						0.41	1.00^{ns}
A.E	3	1	3	6							2.06	5.02^{ns}
A.O.E	3	1	3								0.41	0.23^{ns}
Error(b)	24	1									1.79	
Total	47											

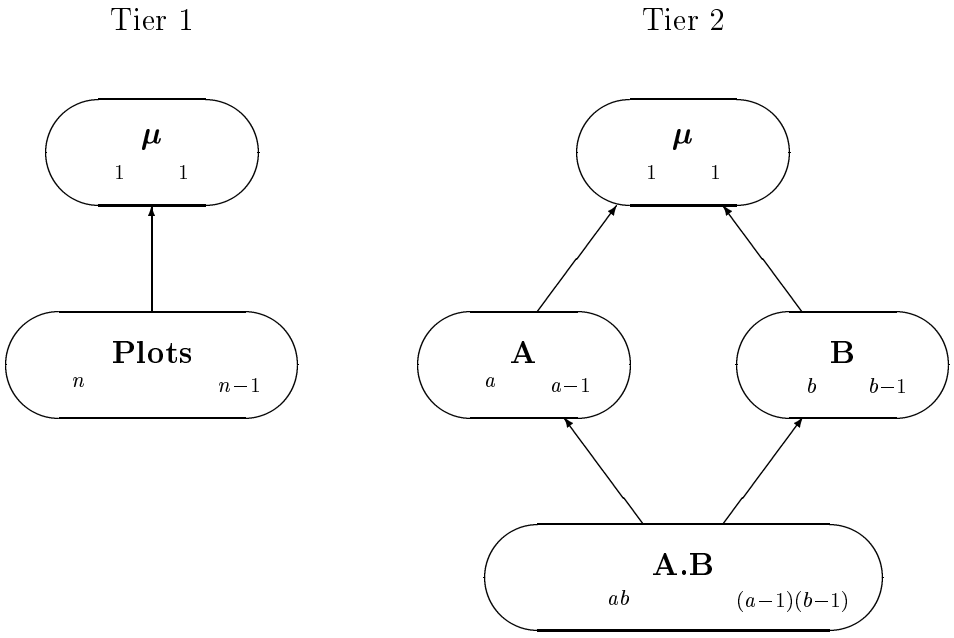
†F ratios for A, O and E are ratios of combinations of mean squares which, together with degrees of freedom calculated according to Satterthwaite's (1946) approximation, are shown below.

Source	Numerator	Denominator	ν_1	ν_2
A	$A + A.O.E + Error(b)$	$Error(a) + A.O + A.E$	3.94	10.21
O	$O + A.O.E$	$A.O + O.E$	3.91	1.51
E	$E + A.O.E$	$A.E + O.E$	1.02	3.29

‡$f_A(\boldsymbol{\mu}) = 12\Sigma(\mu_i - \overline{\mu}_.)^2/3$ where μ_i is the expectation for the ith *Area*, and $\overline{\mu}_.$ is the mean of the μ_is.

table 4.3. The Hasse diagrams of term marginalities, used in determining the degrees of freedom as described in table 2.2, are given in figure 4.3. The analysis of variance table, derived from the structure set for a study as prescribed in table 2.1, is given in table 4.3. The lattices of models, for unrandomized factors regarded as variation factors and randomized factors as expectation factors, are shown in figure 4.4; these are obtained using the steps given in table 2.6.

Figure 4.3: Hasse Diagram of term marginalities for a nonorthogonal two-factor completely randomized design



In this example, the variation lattice is trivial and interest is centred on the expectation lattice. The expectation lattice is the same as that given in figure 2.4 and so the form of the expectation models is the same as for the example discussed in section 2.2.6.2. In this case, the steps given in table 2.8 cannot be used to derive the expected mean squares; they are computed using the expression given by Searle (1971b, section 2.5a) which is presented in section 3.3.3.

Table 4.3: The structure set and analysis of variance for a nonorthogonal two-factor completely randomized design

STRUCTURE SET

Tier	Structure
1	n *Plots*
2	$a\,A * b\,B$

ANALYSIS OF VARIANCE TABLE

SOURCE	DF	SSq
Plots	$n-1$	$\sum\sum\sum(y_{ijk}-\overline{y}_{...})^2$
A	$a-1$	$\sum r_{i.}(\overline{y}_{i..}-\overline{y}_{...})^2$
B	$b-1$	$\boldsymbol{r}'\mathbf{C}^{-1}\boldsymbol{r}^{\dagger}$
A.B	$(a-1)(b-1)$	$\sum\sum r_{ij}\overline{y}_{ij.}-\boldsymbol{r}'\mathbf{C}^{-1}\boldsymbol{r}-\sum r_{i.}\overline{y}_{i..}$
Residual	$n-ab$	$\sum\sum\sum(y_{ijk}-\overline{y}_{ij.})^2$
Total	$n-1$	

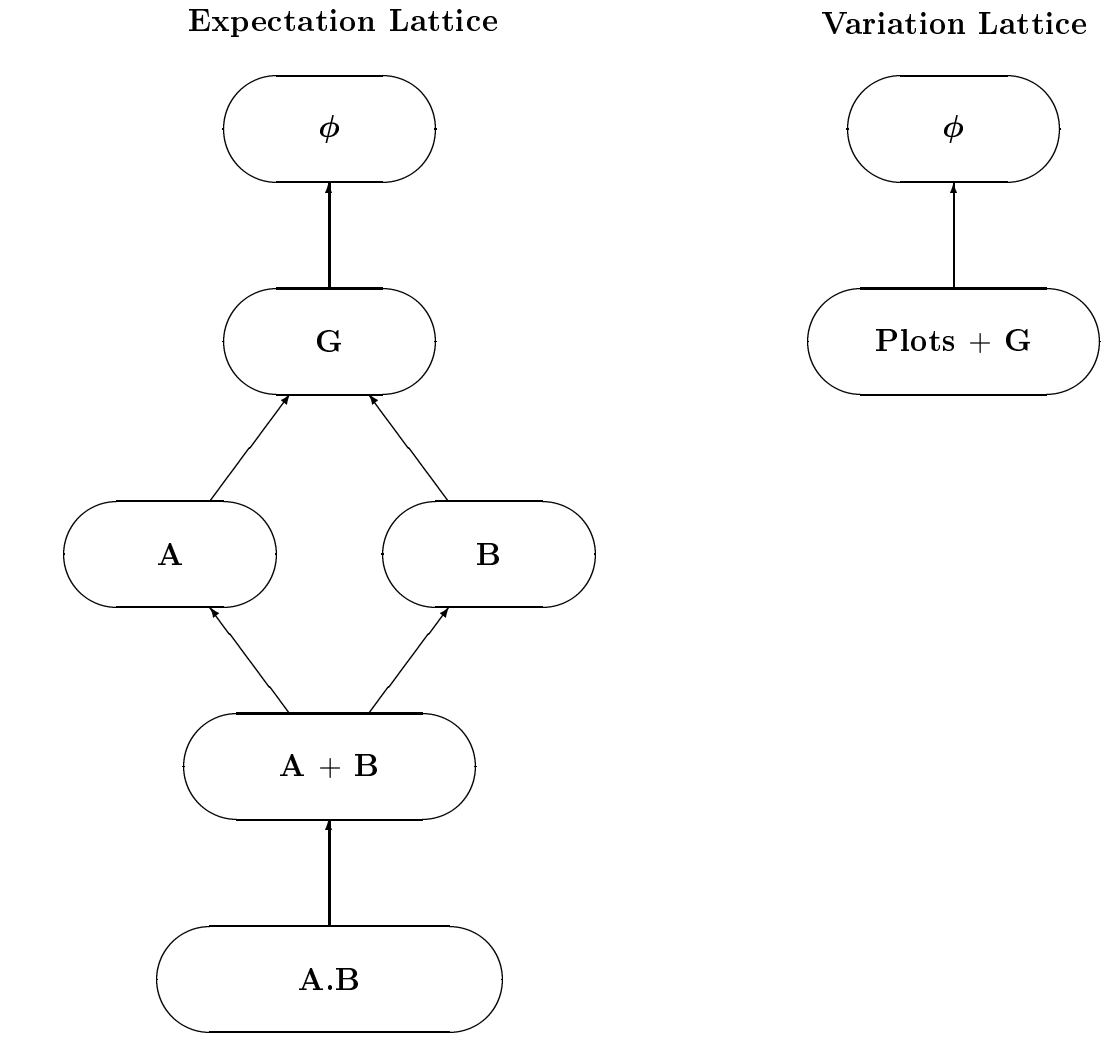
†Searle (1971b, section 7.2d) gives the general expression for this source. For the 2×2 case it reduces to:

$$\frac{\{\frac{r_{11}r_{12}}{r_{1.}}(\overline{y}_{11.}-\overline{y}_{12.})+\frac{r_{21}r_{22}}{r_{2.}}(\overline{y}_{21.}-\overline{y}_{22.})\}^2}{\frac{r_{11}r_{12}}{r_{1.}}+\frac{r_{21}r_{22}}{r_{2.}}}$$

where

r_{ij} is the number of observations for the jth level of B and the ith level of A, and the dot subscript denotes summation over that subscript.

Figure 4.4: Lattices of models for the two-factor completely randomized design



Choosing between mutually exclusive models will involve, in this nonorthogonal situation, two hierarchical fitting sequences corresponding to the two orders in which the terms A and B can be added to the set of fitted terms (Aitkin, 1978). This involves a set of model comparisons equivalent to that outlined by Appelbaum and Cramer (1974); the strategy is outlined in figure 4.5. The necessity for this procedure is evident upon examination of table 4.4 which contains, for each model, the expected mean squares for the hierarchical sequence in which A is fitted before B. To choose between the models $A.B$ and $A+B$, the $A.B$ mean square is appropriate since it is the only mean square whose expectation does not involve models marginal to $A.B$. If $A.B$ is selected as the appropriate model then, contrary to the suggestion of Hocking, Speed and Coleman (1980), there is no need to go further at this stage. In these circumstances, to examine main effects is seen to be irrelevant; to do so would be to attempt to fit two different models to the same data (as noted in section 2.2.8.2).

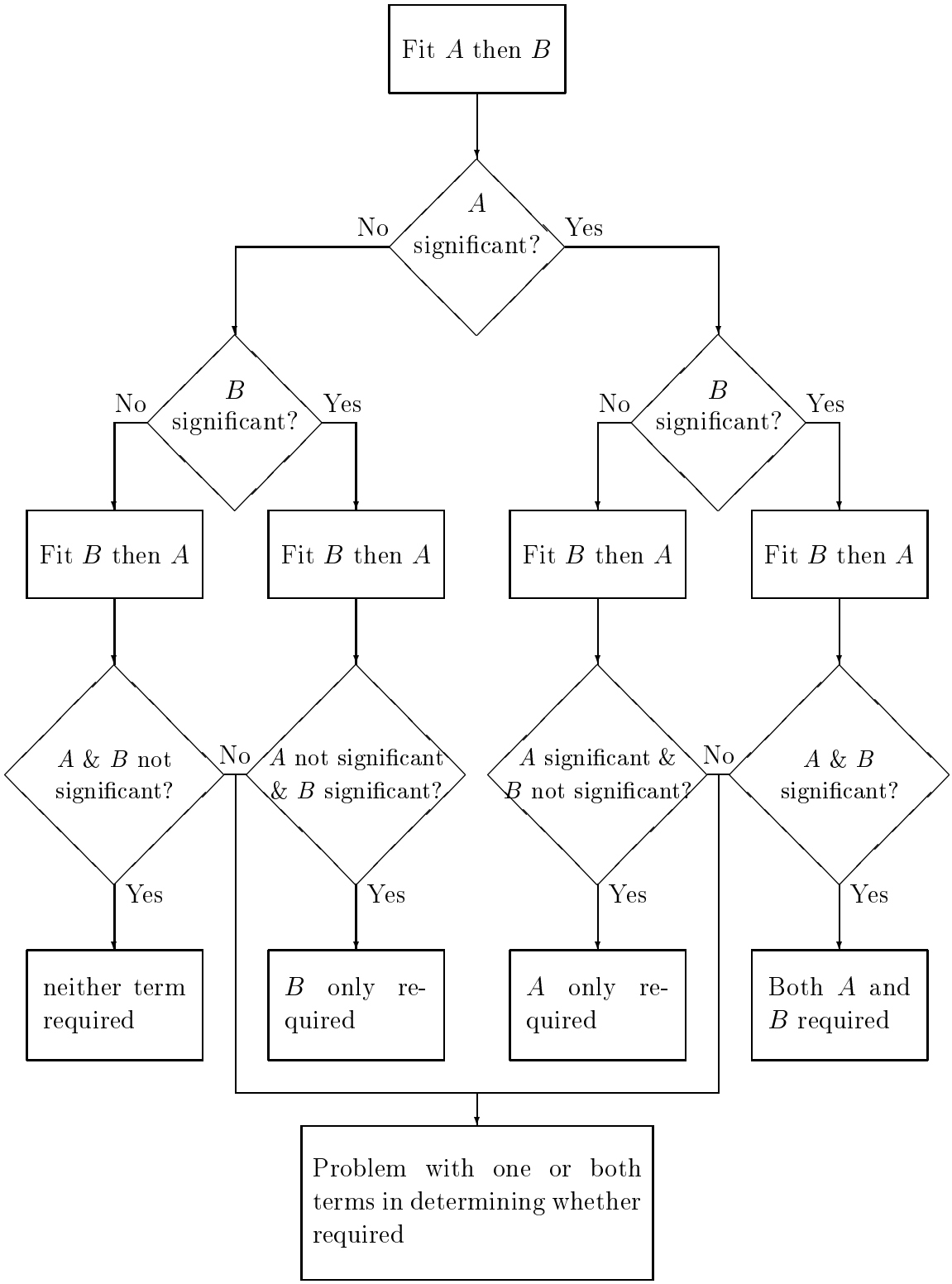
Table 4.4: Contribution to the expected mean squares from the expectation factors for the two-factor experiment under alternative models†

SOURCE	MODEL A	B	$A+B$	$A.B$
A	$f_A(\boldsymbol{\mu}_A)$	$f_A(\boldsymbol{\mu}_B)$	$f_A(\boldsymbol{\mu}_{A+B})$	$f_A(\boldsymbol{\mu}_{A.B})$
B	–	$f_B(\boldsymbol{\mu}_B)$	$f_B(\boldsymbol{\mu}_B)$	$f_B(\boldsymbol{\mu}_{A.B})$
$A.B$	–	–	–	$f_{A.B}(\boldsymbol{\mu}_{A.B})$
Residual	–	–	–	–

†In all cases the contribution arising from the variation factors is ϕ_P, the variance of the plots. The functions $f_A()$, $f_B()$ and $f_{A.B}()$ are functions of the parameters contained in the expectation vector $\boldsymbol{\mu}$; expressions for the functions are obtained by replacing the observations by their expectation in the expressions for the sums of squares given in table 4.3.

If $A.B$ is rejected, then to choose between A and $A+B$, the B (adjusted for A) mean square is appropriate. In the event that B is to be retained in the model, there is no source in the sequence underlying table 4.4 for testing between B and $A+B$,

Figure 4.5: Strategy for expectation model selection for a nonorthogonal two-factor completely randomized design



as there is no source that involves $A + B$ but not the marginal model B. The A mean square in the sequence where B is fitted first will provide this test. However, as Aitkin (1978) and Nelder (1982) warn, if A (or B) is to be excluded from the model $A + B$, the need for the model B (or A) should be tested using the analysis in which the term B (or A) is fitted first in the sequence.

4.2.3 Nested treatments

Usually, if the treatments involve more than one factor, they involve a set of crossed factors. However, as outlined by Baxter and Wilkinson (1970), Bailey (1985) and Payne and 13 other authors (1987), the treatment differences in some experiments can best be examined by employing nested relationships between some factors. Examples are given in this section and it is demonstrated that employing the proposed approach clarifies model selection for these experiments.

4.2.3.1 Treated-versus-control

Cochran and Cox (1957, section 3.2) present the results of an experiment examining the effects of soil fumigants on the number of eelworms. There were four different fumigants each applied in both single and double dose rates as well as a control treatment in which no fumigant was applied. The experiment was laid out as a randomized complete block design with 4 blocks each containing 12 plots; in each block, the 8 treatment combinations were each applied once and the control treatment four times and the 12 treatments randomly allocated to plots. The number of eelworm cysts in 400g samples of soil from each plot was determined.

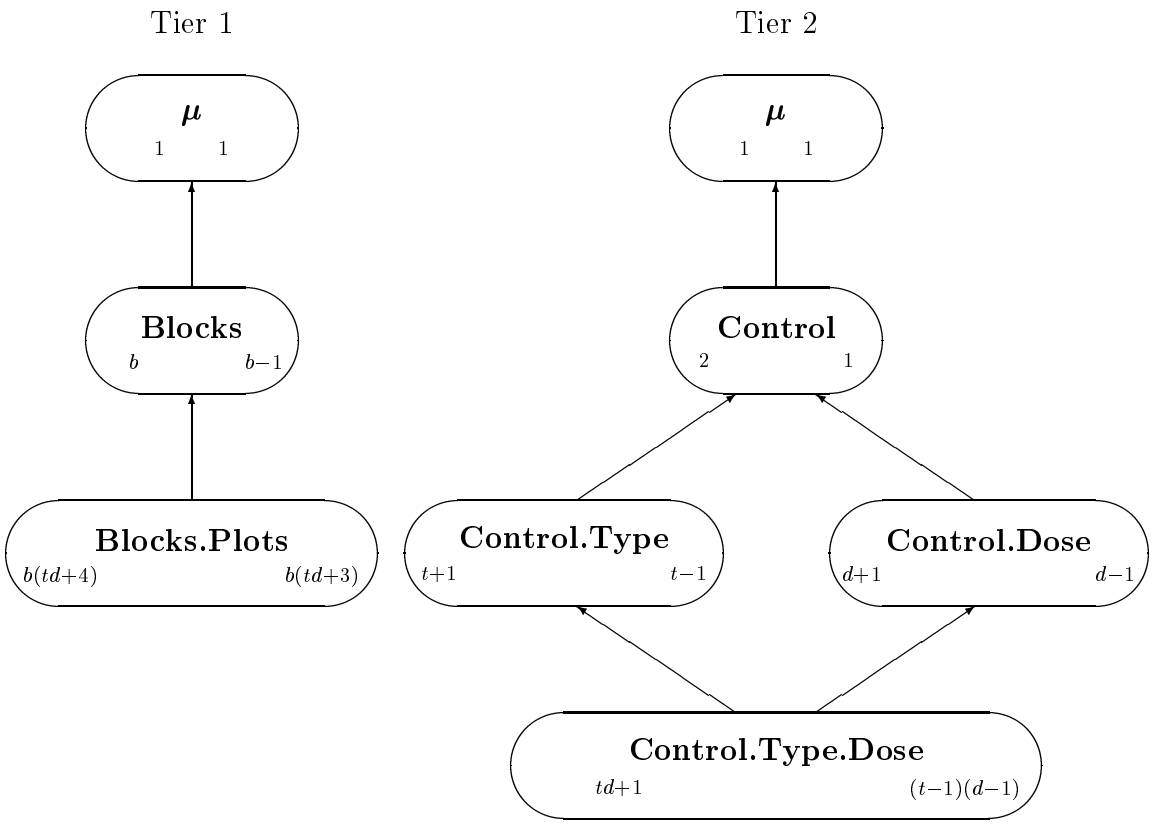
The experimental structure for this experiment is as follows:

Tier	Structure
1	*4 Blocks/12 Plots*
2	*2 Control/(4 Type∗2 Dose)*

The Hasse diagrams of term marginalities, used in determining the degrees of freedom of terms derived from the structure set for the study as described in table 2.2, are

given in figure 4.6. The manner in which the three factors index the nine treatment combinations is evident from the table of treatment means presented in table 4.6. The entries to the left of the Tier 2 terms in figure 4.6 are the number of nonempty cells for that factor combination.

Figure 4.6: Hasse diagram of term marginalities for the treated-versus-control experiment



The analysis of variance table, which can be obtained from the structure set for the study using the rules given in table 2.1, has been derived from Payne *et al.* (1987); it is given in table 4.5.

Table 4.5: Analysis of variance table for the treated-versus-control experiment

SOURCE	DF	EXPECTED MEAN SQUARES Coefficients of ϕ_{BP}	ϕ_B	$\boldsymbol{\mu}$	MSq	F
Blocks	3	1	12		1.34	
Blocks.Plots	43(1)†					
Control	1	1		$f_C(\boldsymbol{\mu})$‡	0.69	3.73
Control.Type	3	1		$f_{CT}(\boldsymbol{\mu})$‡	0.06	0.35
Control.Dose	1	1		$f_{CD}(\boldsymbol{\mu})$‡	0.22	1.20
Control.Type.Dose	3	1		$f_{CTD}(\boldsymbol{\mu})$‡	0.04	0.22
Residual	35(1)†	1			0.19	
Total	46					

†The bracketed one indicates that these sources have had their degrees of freedom reduced by one to adjust for a single missing value.
‡The functions for the expectation contribution under the maximal model are as follows:

$$
\begin{aligned}
f_C(\boldsymbol{\mu}) &= 16((\overline{\alpha\zeta\tau})_{1..} - (\overline{\alpha\zeta\tau})_{...})^2 + 32((\overline{\alpha\zeta\tau})_{2..} - (\overline{\alpha\zeta\tau})_{...})^2 \\
f_{CT}(\boldsymbol{\mu}) &= 8\sum((\overline{\alpha\zeta\tau})_{2j.} - (\overline{\alpha\zeta\tau})_{2..})^2/3 \\
f_{CD}(\boldsymbol{\mu}) &= 16\sum((\overline{\alpha\zeta\tau})_{2.k} - (\overline{\alpha\zeta\tau})_{2..})^2 \\
f_{CTD}(\boldsymbol{\mu}) &= 4\sum\sum((\alpha\tau\zeta)_{2jk} - (\overline{\alpha\zeta\tau})_{2j.} - (\overline{\alpha\zeta\tau})_{2.k} + (\overline{\alpha\zeta\tau})_{2..})^2/3
\end{aligned}
$$

where

$\mathrm{E}[y_{lm}]$ = $(\alpha\tau\zeta)_{ijk}$ is the maximal expectation model;
y_{lm} is the observation from the mth plot in the lth block;
$(\alpha\tau\zeta)_{ijk}$ is the expected response when the response depends on the combination of *Control*, *Type* and *Dose* with ijk being the levels combination of the respective factors which is associated with observation lm; and
the dot subscript denotes summation over that subscript.

Table 4.6: Table of means for the treated-versus-control experiment

Dose	*Control Type*	Not Fumigated	Fumigated			
		Not Fumigated	CN	CS	CM	CK
Not Fumigated		5.79				
Single			5.48	5.28	5.82	5.37
Double			5.58	5.46	5.71	5.57

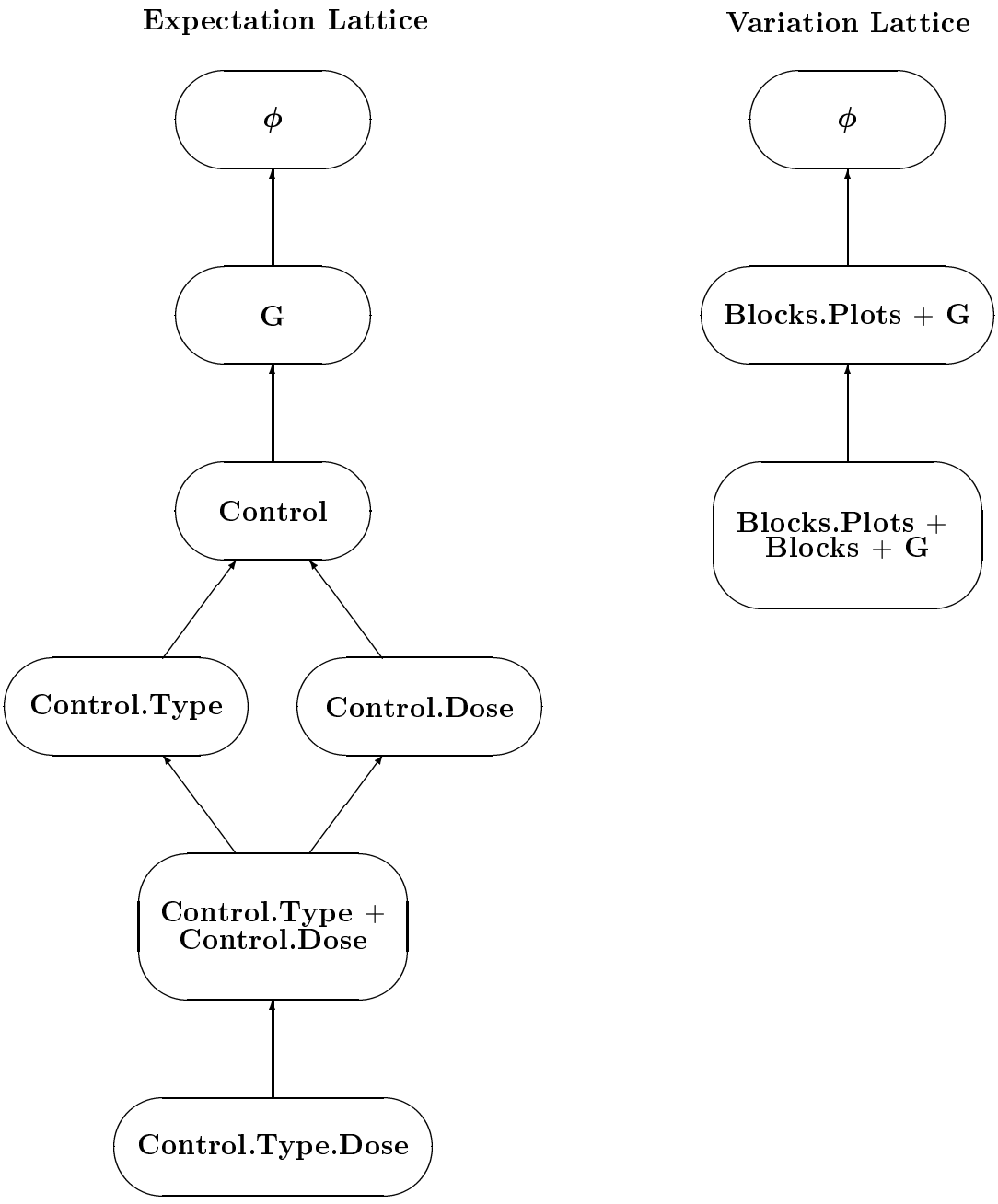
The maximal expectation and variation models, generated using the steps given in table 2.5, are:

$$\begin{aligned} \mathrm{E}[Y] &= \mathit{Control.Type.Dose}, \text{ and} \\ \mathrm{Var}[Y] &= G + \mathit{Blocks} + \mathit{Blocks.Plots}. \end{aligned}$$

Since the set of variation factors comprises all the factors in the first tier and the structure from this tier is regular, the steps given in table 2.8 can be used to obtain the expected mean squares; they are given in table 4.5.

As outlined in section 2.2.5, the alternative models to be considered for the experiment can be conveniently summarized in the Hasse diagrams of the lattices of models. The lattices of models for this experiment, derived using the steps given in table 2.6, are given in figure 4.7. Of particular interest in this example is the expectation lattice of models because the investigation of expectation models is independent of which variation model is selected. As discussed in section 2.2.8, testing begins with deciding whether or not the maximal model can be reduced. In this case, can the model in which the response depends on the combination of *Type* and *Dose* be reduced to one in which *Type* and *Dose* are additively independent. If it cannot be reduced then testing ceases and the maximal model is retained. In particular, in these circumstances it makes no sense to test the one-degree-of-freedom contrast involving the comparison of the mean of the nonfumigated or control treatment plots versus the mean of

Figure 4.7: Lattices of models for the treated-versus-control experiment



all fumigated plots — eminent commonsense. Indeed, only if all models involving differences between the type and dose of fumigant are rejected, is a model involving the comparison of the nonfumigated plots to the overall mean of the fumigated plots permissible.

As it turns out, the analysis presented in table 4.5 indicates that the model can be reduced to $\mathrm{E}[\boldsymbol{y}] = \mathit{Control}$. Hence one concludes that there is no difference between fumigated plots, but that nonfumigated plots (mean of 5.79) are different from fumigated plots (mean of 5.33).

4.2.3.2 Sprayer experiment

A further example of nested treatments is provided by an experiment to investigate the effects of tractor speed and spray pressure on the quality of dried sultanas (Clingeleffer, Trayford, May and Brien, 1977). The aspect of quality on which we shall concentrate is the lightness of the dried sultanas which is measured using a Hunterlab D25 L colour difference meter. Lighter sultanas are considered to be of better quality and these will have a higher lightness measurement (L). There were four tractor speeds and three spray pressures resulting in 12 treatment combinations which were applied to 12 plots, each consisting of 12 vines, using a randomized complete block design. However, these 12 treatment combinations resulted in only 6 rates of spray application as indicated in table 4.7.

The structure set for this experiment is given as follows:

Tier	Structure
1	*3 Blocks/12 Plots*
2	*6 Rates/(2 Rate2+3 Rate3+3 Rate4+2 Rate5)*

Note that there is a factor, *Rates*, for differences between treatments having different rates and factors *Rate2*, *Rate3*, *Rate4* and *Rate5* for differences between treatments having the same rate but different speed-pressure combinations. Each of these latter factors has one level assigned to all observations except those at the rate whose differences it indexes; for this rate, the factor has different levels for each of the speed-pressure combinations that produce the rate (see table 4.7). The order of one of these

Table 4.7: Table of application rates and factor levels for the sprayer experiment

			FLOW RATES			
		Tractor Speed (km hour^{-1})	3.6	2.6	1.8	1.3
	140		**2090**	2930	**4120**	5770
Pressure	330		2930	**4120**	5770	**8100**
(kPa)	550		**4120**	5770	**8100**	11340

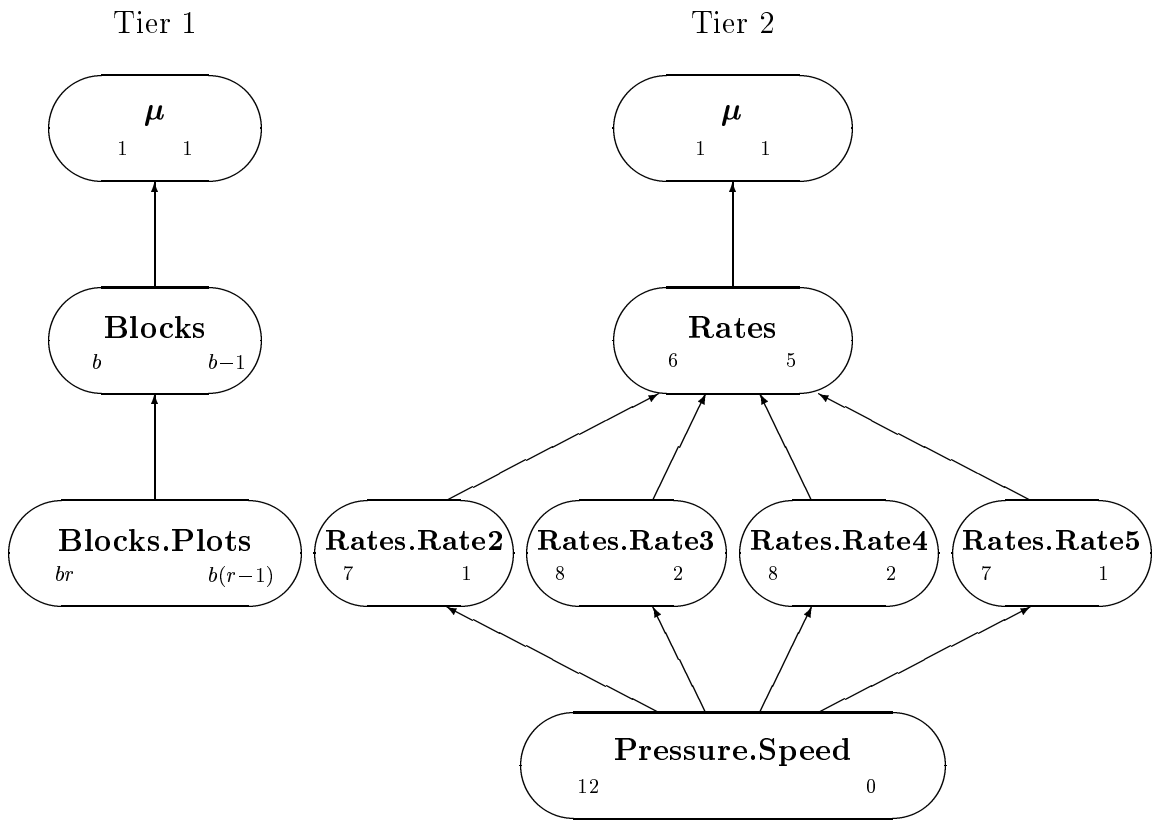
			LEVELS OF RATE2, RATE3, RATE4 AND RATE5															
			Rate factor															
			Rate2				*Rate3*				*Rate4*				*Rate5*			
		Tractor Speed (km hour^{-1})	3.6	2.6	1.8	1.3	3.6	2.6	1.8	1.3	3.6	2.6	1.8	1.3	3.6	2.6	1.8	1.3
	140		**1**	2	**1**	1	1	**1**	2	**1**	**1**	1	**1**	2	1	**1**	1	**1**
Pressure	330		3	**1**	1	**1**	**1**	3	**1**	1	1	**1**	3	**1**	**1**	1	**1**	2
(kPa)	550		**1**	1	**1**	1	4	**1**	1	**1**	**1**	4	**1**	1	1	**1**	3	**1**

latter factors is then the number of different speed-pressure combinations at their rate.

The Hasse diagrams of term marginalities, used in determining the degrees of freedom of terms derived from the structure set for the study as described in table 2.2, are given in figure 4.8. As for the treated-versus-control experiment presented in section 4.2.3.1, the entries to the left of the Tier 2 terms are the number of nonempty

cells for that factor combination. Further, a term (*Pressure.Speed*) whose model space corresponds to the union of the model spaces of all the factors in the experiment is included to satisfy the first condition for a Tjur structure (see section 2.2.4). This term is shown to be redundant in that it has no degrees of freedom.

Figure 4.8: Hasse diagram of term marginalities for the sprayer experiment



The analysis of variance table is generated using the rules given in table 2.1. The analysis, for a set of generated data (appendix A.2) with the same lightness (L) means as those presented in Clingeleffer *et al.* (1977), is given in table 4.8; the full table of means is given in table 4.9.

The maximal expectation and variation models, generated using the steps given in table 2.5, are:

$$\begin{aligned} \mathrm{Var}[Y] &= G + Blocks + Blocks.Plots, \text{ and} \\ \mathrm{E}[Y] &= Rates.Rate2 + Rates.Rate3 + Rates.Rate4 + Rates.Rate5. \end{aligned}$$

Table 4.8: Analysis of variance table for the sprayer experiment

SOURCE	DF	EXPECTED MEAN SQUARES Coefficients of ϕ_{BP}	ϕ_B	$\boldsymbol{\mu}$	MSq	F
Blocks	2	1	12		2.5011	
Blocks.Plots	33					
Rates	5	1		$f_R(\boldsymbol{\mu})^\dagger$	1.2447	7.78
Rates.Rate2	1	1		$f_{R2}(\boldsymbol{\mu})^\dagger$	1.9267	12.05
Rates.Rate3	2	1		$f_{R3}(\boldsymbol{\mu})^\dagger$	1.7144	10.72
Rates.Rate4	2	1		$f_{R4}(\boldsymbol{\mu})^\dagger$	0.2678	1.67
Rates.Rate5	1	1		$f_{R5}(\boldsymbol{\mu})^\dagger$	0.0817	0.51
Residual	22	1			0.1599	

†The functions f_R, f_{R2}, f_{R3}, f_{R4} and f_{R5} of $\boldsymbol{\mu}$ for the maximal model are similar, in form, to those given in table 4.5.

Again, since the variation factors are all those in the first tier and the structure derived from this tier is regular, the steps given in table 2.8 can be used to obtain the expected mean squares. They are given in table 4.8.

The alternative models to be considered are derived as described in table 2.6. The variation lattice will be the same as that presented in figure 4.7 and again the investigation of expectation models is independent of which variation model is selected. The expectation lattice consists of the models G, *Rates* and models consisting of all possible combinations of the terms *Rates.Rate2*, *Rates.Rate3*, *Rates.Rate4*, *Rates.Rate5*.

Table 4.9: Table of means for the sprayer experiment

FULL TABLE OF MEANS

(P = *Pressure*; L = Lightness)

	Tractor Speed								
	3.6		2.6		1.8		1.3		Mean
	P	L	P	L	P	L	P	L	
Rates									
2090	**140**	**18.7**							
2930	330	20.4	140	19.2					19.80
4120	**550**	**20.5**	**330**	**20.2**	**140**	**19.1**			**19.96**
5770			550	19.6	330	19.1	140	19.6	19.44
8100					**550**	**19.9**	**330**	**19.7**	**19.82**
11340							550	20.5	

FITTED TABLE OF MEANS

(P = *Pressure*; L = Lightness)

	Tractor Speed								
	3.6		2.6		1.8		1.3		Mean
	P	L	P	L	P	L	P	L	
Rates									
2090	**140**	**18.7**							
2930	330	20.4	140	19.2					
4120	**550**	**20.5**	**330**	**20.2**	**140**	**19.1**			
5770									19.44
8100									**19.82**
11340							550	20.5	

Thus, model selection firstly involves deciding which, if any, of the terms *Rate2*, *Rate3*, *Rate4* and *Rate5* need to be included in the model. If none are required because there are no differences within *Rates*, one next determines if the term *Rates* should be included. In the example, only *Rate2* and *Rate3* are significant so that the model for the expectation should be:

$$\mathrm{E}[Y] = \mathit{Rates}.\mathit{Rate2} + \mathit{Rates}.\mathit{Rate3}.$$

The fitted values for this model are given in table 4.9.

4.3 Clarifying the analysis of complex two-tiered experiments

The application of the method described in chapter 2 to more complicated two-tiered experiments will be described with some simple steps left implicit for brevity. Further, to obtain expected mean squares, unless otherwise stated, the unrandomized factors will be taken to be variation factors and the randomized factors to be expectation factors.

The experiments covered include split-plot experiments, series of experiments, repeated measurements experiments and change-over experiments. In all but one of these experiments, the expectation terms are confounded with different sources from the first structure and the stratum components used in estimation and testing differ between them. Consequently, most of them would normally be analysed within the framework of the split-plot analysis, this being the classic analysis in which expectation terms are confounded with different sources. It is therefore not uncommon to find experiments with procedures quite different from the split-plot experiment being treated as if they were split-plot experiments. The use of the structure set in specifying the analysis of variance table for such experiments will be found to be especially illuminating, differences in the experimental population and procedures being faithfully reproduced in the analysis table.

4.3.1 Split-plot designs

Most generally the split-plot principle can be defined as the randomizing of two or more factors so that the randomized factors differ in the experimental unit to which they are randomized. By modifying the restrictions on the randomization of treatments and different aggregations of observational units into experimental units, a wide range of designs can be obtained, all of which conform to the general definitions given above (see, for example, Cochran and Cox, 1957; Federer, 1975). A feature of these, and many textbook designs, is that they involve only a single class of replication factors. **Replication factors** are those whose primary function is to provide a range of conditions, resulting from uncontrolled variation, under which the treatments are observed. The classes of replication factors that commonly occur include factors indexing plots, animals, subjects and production runs.

The analysis for the 'standard' split-plot is presented here, while a more difficult, three-tiered example involving row-and-column designs is discussed in section 5.4.3.

The usual textbook example of a split-plot experiment (Federer, 1975, p.11) involves two treatment factors, C and D say, one of which (C) has been randomized to main plots according to a randomized complete block design. The main plots are further subdivided into subplots and the set of treatments corresponding to the factor D randomized to the subplots within each main plot. Clearly, the *Block*, *Plots* and *Subplots* are the unrandomized factors, while C and D are the randomized factors. *Plots* are nested within *Blocks* and *Subplots* are nested within *Plots*, primarily because of the randomization. The structure set and analysis of variance table appropriate in this situation are shown in table 4.10. The symbolic forms of the maximal models for this experiment, derived according to the rules given in table 2.5, are as follows:

$$\begin{aligned} \mathrm{E}[Y] &= C.D \\ \mathrm{Var}[Y] &= G + Blocks + Blocks.Plots + Blocks.Plots.Subplots \end{aligned}$$

The expected mean squares under these models are given in table 4.10.

The layout of the analysis table derived from the structure set parallels that usually presented in textbooks. It differs in that the error sources (residuals) are not viewed as interactions (or pooled interactions), but as residual information about nested terms

arising in the bottom tier. That is, the error sources are seen to be of a different type of variability (see section 6.6.2) from that usually implied.

Table 4.10: Structure set and analysis of variance table for the standard split-plot experiment

STRUCTURE SET

Tier	Structure
1	*b Blocks/c Plots/d Subplots*
2	*c C*d D*

ANALYSIS OF VARIANCE TABLE

SOURCE	DF	EXPECTED MEAN SQUARES Coefficients of ϕ_{BPS}	ϕ_{BP}	ϕ_B	$\boldsymbol{\mu}$
Blocks	$(b-1)$	1	d	cd	
Blocks.Plots	$b(c-1)$				
C	$(c-1)$	1	d		$f_C(\boldsymbol{\mu})$
Residual	$(b-1)(c-1)$	1	d		
Blocks.Plots.Subplots	$bc(d-1)$				
D	$(d-1)$	1			$f_D(\boldsymbol{\mu})$
C.D	$(c-1)(d-1)$	1			$f_{CD}(\boldsymbol{\mu})$
Residual	$c(d-1)(b-1)$	1			

The structure set and table for the situation in which it is thought to be appropriate to isolate the *D.Blocks* term are shown in table 4.11. The symbolic forms of the maximal models for this experiment, derived according to the rules given in table 2.5,

are as follows:

$$\begin{aligned} \mathrm{E}[Y] &= C.D \\ \mathrm{Var}[Y] &= G + Blocks + Blocks.Plots + Blocks.Plots.Subplots + D.Blocks \end{aligned}$$

Table 4.11: Structure set and analysis of variance table for the standard split-plot experiment, modified to include the *D.Blocks* interaction

STRUCTURE SET

Tier	Structure
1	b *Blocks*/c *Plots*/d *Subplots*
2	d *D*$*$(c *C*+*Blocks*)

ANALYSIS OF VARIANCE TABLE

SOURCE	DF	EXPECTED MEAN SQUARES Coefficients of ϕ_{BPS}	ϕ_{BP}	ϕ_{DB}	ϕ_B	$\boldsymbol{\mu}$
Blocks	$(b-1)$	1	d	c	cd	
Blocks.Plots	$b(c-1)$					
C	$(c-1)$	1	d			$f_C(\boldsymbol{\mu})$
Residual	$(b-1)(c-1)$	1	d			
Blocks.Plots.Subplots	$bc(d-1)$					
D	$(d-1)$	1		c		$f_D(\boldsymbol{\mu})$
C.D	$(c-1)(d-1)$	1				$f_{CD}(\boldsymbol{\mu})$
D.Blocks	$(b-1)(d-1)$	1		c		
Residual	$(c-1)(d-1)(b-1)$	1				

The inclusion of this term means that the conditions laid down in section 2.2.5 are no longer satisfied; the set of terms from the second tier do not include a term to which all other terms in the tier are marginal. However, this can be overcome by

making *Blocks* crossed with both C and D; having determined the expected mean squares with the additional terms *C.Blocks* and *C.D.Blocks* included, ϕ_{CB} and ϕ_{CDB} are set to zero and the additional terms removed from the analysis. Although, leaving them in would make no substantial difference to the analysis.

A number of authors, including Anderson and Bancroft (1952), Federer (1955 and 1975), Harter (1961) and Yates (1965), have discussed the advisability of isolating the *D.Blocks* term. Federer (1955, p.274) asserts that, while it is arithmetically possible to partition out the *D.Blocks* interaction (his replicate $\times B$ interaction), this should not be done as it is 'confounded' with *C.D.Blocks* interaction (his replicates $\times A \times B$ interaction). The other authors and Federer (1975) suggest that it should be isolated in certain circumstances. In fact, it is the *Blocks.Subplots* term (an unrandomized term) which cannot be isolated as it is nonorthogonal to the D effects, since the levels of D are not balanced across the levels of *Subplots*. On the other hand, in contrast to Federer (1955), I assert that the *D.Blocks* term (being an intertier interaction which is a generalized term for block-treatment or unit-treatment interaction) can be partitioned out if this is desirable.

4.3.2 Experiments with two or more classes of replication factors

This group of experiments includes series-of-experiments (Kempthorne, 1952, chapter 28; Federer, 1955, chapter X, section 1.4.4; Cochran and Cox, 1957, chapter 14), repeated measurements (Winer, 1971 chapters 4 and 7) and change-over experiments (Cochran and Cox, 1957, section 4.6a; John and Quenouille, 1977, section 11.4). They all involve at least two classes of replication factors, for example, field and time.

The experiments will be subdivided into those that have only one class of replication factors in the bottom tier and those that have two or more such classes. Experiments with two or more classes of replication in the bottom tier are further subdivided into three categories on the basis of the randomization of factors to the classes of replication factors in the bottom tier.

These experiments, while they exhibit many similarities, differ from each other in an

analogous way to the three experiments discussed in section 6.6.1 and in other ways. These differences have not always been taken into account in the analyses performed but are brought to the fore when the proposed approach is employed.

4.3.2.1 Single class in bottom tier

Because there is more than one class of replication factors in the experiments of this category but only one class can occur in the bottom tier, replication factors must be randomized to those in the bottom tier. This type of experiment is typified by the series-of-experiments experiment mentioned above. A **series-of experiments experiment** is one that involves repetition, usually in time and/or space, and which involves a different set of experimental units at each repetition (Cochran and Cox, 1957, chapter 14). That is, replication factors, such as *Times*, are randomized to the levels combinations of factors in the bottom tier. Their analysis is the same as for a split-plot experiment.

Times randomized. Suppose an agronomist wishes to investigate the effect on crop yield of different amounts of nitrogen fertilizer and the way in which these effects vary over time. An experiment is set up in which the nitrogen treatments are arranged in a randomized complete block design. The whole plots are subdivided into subplots and one subplot from each whole plot is randomly selected to be harvested at one time, harvesting being performed on several occasions. For this experiment, *Levels* of nitrogen and *Times* of harvesting are the randomized factors. The analysis of the experiment would follow the analysis of the standard split-plot experiment (table 4.10), *Levels* of nitrogen corresponding to factor C and *Times* of harvesting to factor D. This is not a repeated measurements experiment as only one measurement is made on each physical unit, that is, on each subplot. However, it involves two classes of replication factors, field and time factors.

Times randomized and sites unrandomized. The classic experiment of this type is the one analysed by Yates and Cochran (1938). It involves a randomized complete block design of three blocks and five varieties, replicated at each of six sites. Observations were recorded in two successive years, the experiment being performed

on different tracts of land within each site each year. The overall analysis of variance table given by Yates and Cochran (1938) is reproduced, in essentially the same form, in table 4.12; the *Residual* mean square is different from the Experimental error of Yates and Cochran as it is based on just the five varieties analysed, rather than the ten for which data were available.

Table 4.12: Yates and Cochran (1938) analysis of variance table for an experiment involving sites and years

SOURCE	DF		MSq
	General	Example	
Sites	$(s-1)$	5	1414.73
Years	$(y-1)$	1	1266.17
Sites.Years	$(s-1)(y-1)$	5	459.59
Varieties	$(v-1)$	4	442.50
Varieties.Sites	$(v-1)(s-1)$	20	73.88
Varieties.Years	$(v-1)(y-1)$	4	24.32
Varieties.Sites.Years	$(v-1)(s-1)(y-1)$	20	46.40
Blocks.Sites.Years	$sy(b-1)$	24	72.28
Residual	$sy(b-1)(v-1)$	96	23.90

However, the unrandomized factors are *Sites*, *Tracts*, *Blocks* and *Plots*; *Varieties* and *Years* are the randomized factors, the *Varieties* being randomized to *Plots* and the *Years* to *Tracts*. The structure set for the experiment, which includes the interaction of the randomized factors with *Sites*, is shown in table 4.13.

The structure set is identical to that for a split-split-plot experiment in which some of the intertier interactions are of interest. As for the last example, this experiment is not a repeated measurements experiment, although it involves the two classes of replication factors, field factors and time factors. The classification of *Sites* as a variation factor and *Years* as an expectation factor in this experiment is not a foregone conclusion. However, experience shows that it is unlikely that results from different sites and different years would exhibit the necessary symmetry for them to be regarded

Table 4.13: Structure set and analysis of variance table for an experiment involving sites and years

STRUCTURE SET

Tier	Structure
1	*s Sites/y Tracts/b Blocks/v Plots*
2	*v Varieties*Sites*y Years*

ANALYSIS OF VARIANCE TABLE

SOURCE	DF		EXPECTED MEAN SQUARES Coefficients of					MSq	F
	General	Example	ϕ_{STBP}	ϕ_{STB}	ϕ_{ST}		$\boldsymbol{\mu}$		
Sites	$(s-1)$	5		1	v	bv	$f_S(\boldsymbol{\mu})$	1414.73	
Sites.Tracts	$s(y-1)$	6							
Years	$(y-1)$		1	1	v	bv	$f_Y(\boldsymbol{\mu})$	1266.17	
Sites.Years	$(s-1)(y-1)$		5	1	v	bv	$f_{SY}(\boldsymbol{\mu})$	459.59	
Sites.Tracts.Blocks	$sy(b-1)$	24		1	v			72.28	3.02
Sites.Tracts.Blocks.Plots	$syb(v-1)$	144							
Varieties	$(v-1)$		4	1			$f_V(\boldsymbol{\mu})$	442.50	18.51
Varieties.Sites	$(v-1)(s-1)$		20	1			$f_{VS}(\boldsymbol{\mu})$	73.88	3.09
Varieties.Years	$(v-1)(y-1)$		4	1			$f_{VY}(\boldsymbol{\mu})$	24.32	1.02
Varieties.Sites.Years	$(v-1)(s-1)(y-1)$		20	1			$f_{VSY}(\boldsymbol{\mu})$	46.40	1.94
Residual	$sy(b-1)(v-1)$		96	1				23.90	

as variation factors. The expected mean squares will be based on treating *Sites* and *Years* as expectation factors. The symbolic forms of the maximal models for this experiment, derived according to the rules given in table 2.5, are as follows:

$$\begin{aligned} \mathrm{E}[Y] &= \mathit{Varieties.Sites.Years} \\ \mathrm{Var}[Y] &= G + \mathit{Sites.Tracts} + \mathit{Sites.Tracts.Blocks} + \mathit{Sites.Tracts.Blocks.Plots} \end{aligned}$$

Table 4.13 also gives the analysis of variance table derived from the structure for the study. The decomposition of the *Total* sum of squares for this analysis is equivalent to that of Yates and Cochran, but the modified analysis reflects more accurately the types of variability (section 6.6.2) contributing to each subspace. *Sites.Years* is totally and exhaustively confounded (section 6.3) with *Sites.Tracts* and so assumptions are required to test the significance of the *Sites.Years* term. This has not been recognized previously.

4.3.2.2 Two or more classes in bottom tier, factors randomized to only one

Many repeated measurements experiments are included in the category investigated in this section. **Repeated measurements experiments** are ones in which observations are repeated over several times, with *Times* being an unrandomized factor (Winer, 1971).

Repetitions in time. Consider a randomized complete block experiment in which several clones of some perennial crop are to be compared. The yield for each plot is measured in successive years without any change in the experimental layout. Generated data for such an experiment are given in appendix A.3.

This type of experiment is often referred to as a split-plot-in-time, the years being regarded as a split-plot treatment randomized to hypothetical subplots (Bliss, 1967, p.392). Thus the analysis of variance often used to analyse such experiments is the standard split-plot analysis (table 4.10). This analysis for the generated set of data is presented in table 4.14. Again, *Years* is taken to be an expectation factor as in the times-randomized-and-sites-unrandomized experiment of section 4.3.2.1. From this analysis we conclude that there is no interaction between *Clones* and *Years* and no

overall differences between the *Years* but that there are overall differences between the *Clones*.

Table 4.14: Analysis of variance table for the split-plot analysis of a repeated measurements experiment involving only repetitions in time

SOURCE	DF		EXPECTED MEAN SQUARES Coefficients of				MSq	F
	General	Example	ϕ_{BPY}	ϕ_{BP}	ϕ_B	$\boldsymbol{\mu}$		
Blocks	$(b-1)$	4	1	d	cd		75.38	
Blocks.Plots	$b(c-1)$	10						
Clones	$(c-1)$	2	1	d		$f_C(\boldsymbol{\mu})$	490.52	8.77
Residual	$(b-1)(b-1)$	8	1	d			55.96	
Blocks.Plots.Subplots	$bc(y-1)$	45						
Years	$(y-1)$	3	1			$f_Y(\boldsymbol{\mu})$	105.57	2.84
Clones.Years	$(c-1)(y-1)$	6	1			$f_{CY}(\boldsymbol{\mu})$	48.52	1.30
Residual	$c(b-1)(y-1)$	36	1				37.22	

However, the set of factors actually involved is *Blocks*, *Plots*, *Years* and *Clones*. An observational unit is a plot during a particular year. *Clones* is the only randomized factor, it being randomized to the *Plots* within *Blocks*. Thus, the structure set is as shown in table 4.15. It differs from the structure set for the standard split-plot experiment in that

1. *Years* arises in the bottom tier (being innate to an observational unit),
2. there are no hypothetical subplots, and
3. the *Clones.Years* interaction is seen to be an intertier interaction.

The analysis of variance table corresponding to the revised structure set is also given in table 4.15. The symbolic forms of the maximal models for this experiment,

Table 4.15: Structure set and analysis of variance table for a repeated measurements experiment involving only repetitions in time

STRUCTURE SET

Tier	Structure
1	*(b Blocks/c Plots)∗y Years*
2	*c Clones∗Years*

ANALYSIS OF VARIANCE TABLE

SOURCE	General DF	Example	EXPECTED MEAN SQUARES Coefficients of ϕ_{BPY}	ϕ_{BP}	ϕ_{BY}	ϕ_B	$\boldsymbol{\mu}$	MSq	F
Blocks	$(b-1)$	4	1	y	c	cy		75.38	
Blocks.Plots	$b(c-1)$	10							
Clones	$(c-1)$	2	1	y			$f_C(\boldsymbol{\mu})$	490.52	
Residual	$(b-1)(b-1)$	8	1	y				55.96	14.77
Years	$(y-1)$	3	1		c		$f_Y(\boldsymbol{\mu})$	105.57	
Blocks.Years	$(b-1)(y-1)$	12	1		c			104.07	27.47
Years.Blocks.Plots	$b(c-1)(y-1)$	30							
Clones.Years	$(c-1)(y-1)$	6	1				$f_{CY}(\boldsymbol{\mu})$	48.52	12.80
Residual	$(b-1)(c-1)(y-1)$	24	1					3.79	

derived according to the rules given in table 2.5, are as follows:

$$\begin{aligned} \mathrm{E}[Y] &= \mathit{Clones.Years} \\ \mathrm{Var}[Y] &= G + \mathit{Blocks} + \mathit{Blocks.Plots} + \mathit{Blocks.Years} + \mathit{Blocks.Plots.Years} \end{aligned}$$

The analysis of variance table includes a source for *Blocks.Years*, about the inclusion of which there has been some confusion in the literature. The usual justification has been that this interaction often occurs (see, for example, Anderson and Bancroft, 1952; Steel and Torrie, 1980). However, it is seen to be generally appropriate, in the light of the structure set, to partition it out; to omit it, in any particular instance, requires one to argue that it will not occur. Indeed, the analysis presented in table 4.15 reveals that for the generated data, *Blocks.Years* is a significant source of variation. As a result, the conclusions from the analysis given in table 4.15 differ markedly from those in table 4.14 in that a rather large interaction between *Clones* and *Years* has been detected. This interaction was not detected in the split-plot analysis because the *Subplot Residual* was inflated by the *Blocks.Years* component included in it.

Repetitions in time and space. Suppose that the experiment described in the previous example was repeated at each of several sites. At first sight, one might be tempted to think one had an experiment of the type described by Yates and Cochran (see section 4.3.2.1) and, for an overall analysis of the data, to use that given in table 4.13. However, the unrandomized factors in the experiment are *Sites*, *Reps*, *Plots* and *Years* (that is, *Years* has not been randomized to *Tracts* of ground as in the Yates-Cochran experiment). *Clones* is the only randomized factor. The structure set for the experiment, a reflection of the experimental population and procedures, and including a number of intertier interactions, is shown in table 4.16. Again, *Sites* and *Years* are taken to be expectation factors as in the times-randomized-and-sites-unrandomized experiment of section 4.3.2.1. The symbolic forms of the maximal models for this experiment, derived according to the rules given in table 2.5, are as follows:

$$\begin{aligned} \mathrm{E}[Y] &= \mathit{Clones.Sites.Years} \\ \mathrm{Var}[Y] &= G + \mathit{Sites.Blocks} + \mathit{Sites.Blocks.Plots} + \mathit{Sites.Blocks.Years} \\ &\quad + \mathit{Sites.Blocks.Plots.Years} \end{aligned}$$

Table 4.16: Structure set and analysis of variance table for an experiment involving repetitions in time and space

STRUCTURE SET

Tier	Structure
1	*(s Sites/b Blocks/c Plots)∗y Years*
2	*c Clones∗Sites∗Years*

ANALYSIS OF VARIANCE TABLE

SOURCE	DF	EXPECTED MEAN SQUARES Coefficients of ϕ_{SBPY}	ϕ_{SBP}	ϕ_{SBY}	ϕ_{SB}	$\boldsymbol{\mu}_{CSY}$
Sites	$(s-1)$	1	y	c	cy	$f_S(\boldsymbol{\mu}_{CSY})$
Sites.Blocks	$s(b-1)$	1	y	c	cy	
Sites.Blocks.Plots	$sb(c-1)$					
Clones	$(c-1)$	1	y			$f_C(\boldsymbol{\mu}_{CSY})$
Clones.Sites	$(c-1)(s-1)$	1	y			$f_{CS}(\boldsymbol{\mu}_{CSY})$
Residual	$s(b-1)(c-1)$	1	y			
Years	$(y-1)$	1		c		$f_Y(\boldsymbol{\mu}_{CSY})$
Sites.Years	$(s-1)(y-1)$	1		c		$f_{SY}(\boldsymbol{\mu}_{CSY})$
Sites.Blocks.Years	$(s-1)(b-1)(y-1)$	1		c		
Sites.Blocks.Plots.Years	$sb(c-1)(y-1)$					
Clones.Years	$(c-1)(y-1)$	1				$f_{CY}(\boldsymbol{\mu}_{CSY})$
Clones.Sites.Years	$(c-1)(s-1)(y-1)$	1				$f_{CSY}(\boldsymbol{\mu}_{CSY})$
Residual	$s(b-1)(c-1)(y-1)$	1				

The analysis of variance table for this experiment (also given in table 4.16) is different from the table given in table 4.13 in that the *Residual* of the latter has been partitioned into two *Residuals* for the former. Thus the terms used for testing the various hypotheses are different for the two analyses.

Table 4.17: Experimental layout for a repeated measurements experiment involving split plots and split blocks (Federer, 1975)[†]

Block	Herbicide	Development Stage																					
		3							1							2							
	I	7	6	3	5	2	1	4	1	4	6	2	7	3	5	5	6	3	1	7	2	4
A	II	7	6	3	5	2	1	4	1	4	6	2	7	3	5	5	6	3	1	7	2	4
	III	7	6	3	5	2	1	4	1	4	6	2	7	3	5	5	6	3	1	7	2	4
		3							2							1							
	III	3	2	1	6	4	5	7	5	4	2	3	7	6	1	6	2	4	3	7	5	1
B	I	3	2	1	6	4	5	7	5	4	2	3	7	6	1	6	2	4	3	7	5	1
	II	3	2	1	6	4	5	7	5	4	2	3	7	6	1	6	2	4	3	7	5	1
		1							2							3							
	III	3	6	2	5	1	4	7	6	3	7	5	4	2	1	1	2	6	4	7	3	5
C	II	3	6	2	5	1	4	7	6	3	7	5	4	2	1	1	2	6	4	7	3	5
	I	3	6	2	5	1	4	7	6	3	7	5	4	2	1	1	2	6	4	7	3	5
		1							3							2							
	II	7	2	3	5	1	4	6	7	6	3	2	4	1	5	1	4	5	6	3	2	7
D	III	7	2	3	5	1	4	6	7	6	3	2	4	1	5	1	4	5	6	3	2	7
	I	7	2	3	5	1	4	6	7	6	3	2	4	1	5	1	4	5	6	3	2	7

[†]The levels of T are given inside the boxes.

Measurement of the several parts of a pasture. Federer (1975, example 7.4) discusses a repeated measurements experiment involving repetitions in time and space and for which the basic design is obtained by combining split-block and split-plot

design principles. There are three whole plot herbicide preconditioning treatments (H) arranged in a randomized complete block design of four blocks each with three rows. The blocks are further subdivided into three columns and the three levels of a development stage factor (D) randomized to the columns within a block. Each column is subdivided into seven subplots and a third factor (T) randomized to them. The experimental layout is shown in table 4.17. The produce of each of the 63 plots in the experiment is divided into three parts (grass, legumes and weeds) and the weight of each part for each plot recorded, giving 189 measurements.

The structure set for this experiment is as follows:

Tier	Structure
1	*(4 Blocks/(3 Rows∗(3 Cols/7 Subplots)))∗3 Parts*
2	*3 H∗3 D∗7 T∗Parts*

Table 4.18: Analysis of variance table for a repeated measurements experiment involving split plots and split blocks

SOURCE	DF	EXPECTED MEAN SQUARES Coefficients of												
		ϕ_{BRCSP}	ϕ_{BRCP}	ϕ_{BCSP}	ϕ_{BCP}	ϕ_{BRP}	ϕ_{BP}	ϕ_{BRCS}	ϕ_{BRC}	ϕ_{BCS}	ϕ_{BC}	ϕ_{BR}	ϕ_{B}
Blocks	3	1	7	3	21	21	63	3	21	9	63	63	108
Blocks.Rows	8												
H	2	1	7			21		3	21			63	
Residual	6	1	7			21		3	21			63	
Blocks.Cols	8												
D	2	1	7	3	21			3	21	9	63		
Residual	6	1	7	3	21			3	21	9	63		
Blocks.Cols.Subplots	72												
T	6	1		3				3		9			
D.T	12	1		3				3		9			
Residual	54	1		3				3		9			
Blocks.Rows.Cols	16												
H.D	4	1	7					3	21				
Residual	12	1	7					3	21				
Blocks.Rows.Cols.Subplots	144												
H.T	12	1						3					
H.D.T	24	1						3					
Residual	108	1						3					
Parts	2	1	7	3	21	21	63						
Parts.Blocks	6	1	7	3	21	21	63						
Parts.Blocks.Rows	16												
Parts.H	4	1	7			21							
Residual	12	1	7			21							
Parts.Blocks.Cols	16												
Parts.D	4	1	7	3	21								
Residual	12	1	7	3	21								
Parts.Blocks.Cols.Subplots	144												
Parts.T	12	1		3									
Parts.D.T	24	1		3									
Residual	108	1		3									
Parts.Blocks.Rows.Cols	32												
Parts.H.D	8	1	7										
Residual	24	1	7										
Parts.Blocks.Rows.Cols.Subplots	288												
Parts.H.T	24	1											
Parts.H.D.T	48	1											
Residual	216	1											

†Variation contribution only to expected mean squares.

The analysis of variance is given in table 4.18.

In this experiment the unrandomized factor *Parts* is clearly an expectation factor. The symbolic forms of the maximal models for this experiment, derived according to the rules given in table 2.5, are as follows:

$$\begin{aligned}
\mathrm{E}[Y] &= \mathit{Parts.H.D.T} \\
\mathrm{Var}[Y] &= G + \mathit{Blocks} + \mathit{Blocks.Rows} + \mathit{Blocks.Columns} \\
&\quad + \mathit{Blocks.Columns.Subplots} + \mathit{Blocks.Rows.Columns} \\
&\quad + \mathit{Blocks.Rows.Columns.Subplots} \\
&\quad + \mathit{Blocks.Parts} + \mathit{Blocks.Rows.Parts} + \mathit{Blocks.Columns.Parts} \\
&\quad + \mathit{Blocks.Columns.Subplots.Parts} + \mathit{Blocks.Rows.Columns.Parts} \\
&\quad + \mathit{Blocks.Rows.Columns.Subplots.Parts}
\end{aligned}$$

The analysis given by Federer (1975) is given in table 4.19.

There are two major differences between the two analyses. First, the sources designated 'error (HT)' and 'error (HDT)' by Federer are not separated in the analysis given in table 4.18; they are combined in the *Residual* source for *Blocks.Rows.Cols.-Subplots*. Because of the sampling employed, their separation is not justified. Second, the source 'error (Parts)' of Federer (1975, section 7.4), has been partitioned into the *Residual* sources for the interactions involving *Parts.Blocks* in table 4.18. The analysis presented in table 4.18 is quite different from that obtained within the conventional split-plot framework by Federer.

Table 4.19: Federer (1975) Analysis of variance table for a repeated measurements experiment involving split plots and split blocks

SOURCE	DF
Blocks	3
H	2
Blocks.H = error (H)	6
D	2
Blocks.D = error(D)	6
T	6
D.T	12
Blocks.T.S = error(T)	54
H.D	4
Blocks.H.D = error(HD)	12
H.T	12
Blocks.H.T = error(HT)	36
H.D.T	24
Blocks.H.D.T = error(HDT)	72
Parts	2
Parts.H	4
Parts.D	4
Parts.T	12
Parts.D.T	24
Parts.H.D	8
Parts.H.T	24
Parts.H.D.T	48
Blocks.Parts.H.D.T = error (Parts)	378

4.3.2.3 Factors randomized to two or more classes in bottom tier, no carry-over

Subjects with repetitions in time. In a psychological experiment four subjects of each sex participated in three blocks of four trials. In each block the subjects were given two pairs of synonyms and two pairs of words unrelated in meaning. One word of the pair was played through a headphone to the left ear and the other to the right ear. The experimenter used three different interstimulus intervals; that is, three different times between when the first word was played to the left ear and when the second word was played. These were randomly assigned to the blocks of trials for each subject. The order of the four word pairs used in the experiment was randomized and this order used for all the interstimulus intervals and subjects. The subjects were asked to press one of two buttons if the two words were synonyms and the other button if they were unrelated. Two subjects of each sex chosen at random were asked to use their left hand and the others to use their right hand (all subjects were right-handed). The time taken from when the second word was played to when the buzzer was pressed (the reaction time) was measured.

The unrandomized factors in this experiment are *Sex*, *Subjects*, *Blocks* and *Trials*; the randomized factors are *Hand*, *ISI* (interstimulus interval), *Relation* and *Pairs*. The structure set for the experiment is as follows:

Tier	Structure
1	*(2 Sex/4 Subjects/3 Blocks)∗4 Trials*
2	*2 Hand∗3 ISI∗(2 Relation/2 Pairs)∗Sex*

The resulting analysis table is given in table 4.20. The symbolic forms of the maximal models for this experiment, derived according to the rules given in table 2.5, are as follows:

$$\begin{aligned} \mathrm{E}[Y] &= \mathit{Relations.Pairs.Hand.ISI.Sex} \\ \mathrm{Var}[Y] &= G + \mathit{Sex.Subjects} + \mathit{Sex.Subjects.Blocks} + \mathit{Trials} \\ &\quad + \mathit{Sex.Trials} + \mathit{Sex.Subjects.Trials} \\ &\quad + \mathit{Sex.Subjects.Blocks.Trials} \end{aligned}$$

Table 4.20: Analysis of variance table for a repeated measurements experiment with factors randomized to two classes of replication factors, no carry-over effects

SOURCE	DF	EXPECTED MEAN SQUARES† Coefficients of ϕ_{XSBT}	ϕ_{XST}	ϕ_{XT}	ϕ_T	ϕ_{XSB}	ϕ_{XS}
Sex	1	1	3	12		4	12
Sex.Subjects	6						
Hand	1	1	3			4	12
Hand.Sex	1	1	3			4	12
Residual	4	1	3			4	12
Sex.Subjects.Blocks	16						
ISI	2	1				4	
ISI.Sex	2	1				4	
Hand.ISI	2	1				4	
Hand.ISI.Sex	2	1				4	
Residual	8	1				4	
Trials	3						
Relation	1	1	3	12	24		
Relation.Pairs	2	1	3	12	24		
Sex.Trials	3						
Relation.Sex	1	1	3	12			
Relation.Pairs.Sex	2	1	3	12			
Sex.Subjects.Trials	18						
Relation.Hand	1	1	3				
Relation.Hand.Sex	2	1	3				
Relation.Pairs.Hand	1	1	3				
Relation.Pairs.Hand.Sex	2	1	3				
Residual	12	1	3				
Sex.Subjects.Blocks.Trials	48						
Relation.ISI	2	1					
Relation.ISI.Sex	2	1					
Relation.Hand.ISI	2	1					
Relation.Hand.ISI.Sex	2	1					
Relation.Pairs.ISI	4	1					
Relation.Pairs.ISI.Sex	4	1					
Relation.Pairs.Hand.ISI	4	1					
Relation.Pairs.Hand.ISI.Sex	4	1					
Residual	24	1					

†Variation contribution only to the expected mean squares.

In the analysis, the intertier interactions between *Sex* and the other randomized factors are to be partitioned out. Also, the factor *Blocks*, which is intrinsically crossed with the other factors in the bottom tier, is nested within *Subjects* and *Sex* because the order in which the interstimulus intervals were used was randomized for each subject. However, *Trials* remains crossed with the other factors because the order of presentation of the four word pairs was the same for all blocks and subjects.

The analysis given in table 4.20 differs from what would be obtained by analogy with those given by Winer (1971) in that i) the randomized and unrandomized factors (for example, *Sex* and *Hand* respectively) are distinguished, ii) the structure in the time factors (*Blocks* and *Trials*) is fully recognized and iii) intertier interactions between *Subjects* and *ISI*, *Relation* and *Pairs* are not included. Clearly, the randomization procedures are reflected in the confounding pattern evident in the analysis table in table 4.20.

4.3.2.4 Factors randomized to two or more classes in bottom tier, carry-over

The experiments in this category are based on the **change-over design**, which is a design in which measurements on experimental units are repeated and the treatments are changed between measurements in such a way that the carry-over effects of treatments can be estimated (Cochran and Cox, 1957, section 4.6a; John and Quenouille, 1977, section 11.4). The analysis described in this section is based on joint work with W.B. Hall; this involved discussions during which the analysis for experiments without preperiod, such as the animals-with-repetitions-in-time experiment, was formulated. It was available in a manuscript submitted for publication in 1979 but Payne and Dixon (1983) have since indicated how the analysis can be performed with GENSTAT 4.

Animals with repetitions in time. Cochran and Cox (1957, sections 4.61a and 4.62a) analyse the results from part of an experiment on feeding dairy cows. They analysed the milk yield from a 6-week period for six cows that were fed a different diet in each of three periods. The order of the diets for each cow was obtained by

using two 3×3 Latin square designs. The original experiment involved 18 cows and utilized 6 squares; the 18 cows were divided into 6 sets so that the 3 cows in each set were as similar as possible in respect to milk yielding ability (Cochran, Autrey and Cannon, 1941). The pair of Latin squares used in the part of the experiment analysed allows one to estimate the carry-over (or residual effects) of treatments in the period immediately after they are applied. However, because there is no preperiod, carry-over effects are not estimated from the first period.

Cochran and Cox point out that, in change-over experiments based on sets of Latin squares, treatments are to be randomized to letters and rows and columns of the squares are randomized. The experimenter has to decide whether to remove period effects separately in each square, as is best if period effects are likely to differ from square to square; on the other hand, the experimenter might elect to remove overall period effects. In the former case the squares are kept separate and the rows and columns randomized separately in each square; in the latter, all columns are randomized and the rows are randomized across squares.

However, randomization of the rows of a single square can only be used when the residual effects are balanced across a single square, as may be the case for an even number of treatments. In the example from Cochran and Cox, a pair of squares is required to achieve balance so that rows must be randomized across this pair of squares.

The unrandomized factors are *Sets*, *Cows* and *Periods*. The structure for the randomized factors is complicated by the fact that carry-over effects cannot occur in measurements taken in the first period. This is overcome by introducing a factor for no carry-over effect versus carry-over effect. That is, a factor (*First*) which is 1 for the first period and 2 for other periods. The factor for carry-over effects (*Carry*) then has four levels: 1 for no carry-over and 2, 3 and 4 for carry-over of the first, second and third diets, respectively; however, the order of this factor is 3. The structure set for the experiment is as follows:

Tier	Structure
1	*(2 Sets/3 Cows)∗3 Periods*
2	*2 First/3 Carry+3 Direct*

Table 4.21: Analysis of variance table for the change-over experiment from Cochran and Cox (1957, section 4.62a)

SOURCE	DF	EXPECTED MEAN SQUARES† Coefficients of ϕ_{SCP}	ϕ_{SP}	ϕ_P	ϕ_{SC}	ϕ_S	MSq	F
Sets	1	1	3		3	9	18.00	
Sets.Cows	4							
First.Carry‡	2	1			3		2112.06	2.74
Residual	2	1			3		769.50	
Periods	2							
First	1	1	3	6			8311.36	2.62
Residual	1	1	3	6			3168.75	
Sets.Periods	2	1	3				4.50	
Sets.Cows.Periods	8							
First.Carry§	2	1					19.21	0.39
Direct¶	2	1					1427.28	28.65
Residual	4	1					49.81	

†Variation contribution only to the expected mean squares.
‡*First.Carry* is partially confounded with the *Sets.Cows* with efficiency 0.167.
§*First.Carry* is partially confounded with *Sets.Cows.Periods* with efficiency 0.833.
¶*Direct* is partially aliased with *First.Carry* with efficiency 0.800.

The relationship between *First* and *Carry* must be nested as it is impossible to have no carry-over (level 1 of *First*) with carry-over from a dietary treatment (levels 2, 3 and 4 of *Carry*). The relationship between the carry-over factors and *Direct* (dietary effect) must be independent because of the combinations of one diet following another.

This example does not fulfil the conditions given in section 2.2.5; there is no term

derived from the structure from the second tier to which all other terms from that tier are marginal and, as *Direct* is not orthogonal to *First.Carry*, the experiment is not structure balanced. However, with randomized factors being designated as expectation factors, it is possible to use the approach to formulate an analysis, albeit not a unique analysis. The symbolic forms of the maximal models for this experiment, derived according to the rules given in table 2.5, are as follows:

$$\begin{aligned} \mathrm{E}[Y] &= \mathit{First.Carry} + \mathit{Direct} \\ \mathrm{Var}[Y] &= G + \mathit{Sets} + \mathit{Sets.Cows} + \mathit{Periods} + \mathit{Sets.Periods} \\ &\quad + \mathit{Sets.Cows.Periods} \end{aligned}$$

The analysis of variance table is given in table 4.21; it differs from that specified by Payne and Dixon (1983), and from that given by Cochran and Cox (1957), in that here *Periods* is crossed with all first tier factors.. The *First.Carry* source in the analysis table gives the differences between carry-over effects as it is orthogonal to *First*. The analysis of variance was performed in GENSTAT 4 (Alvey *et al.*, 1977). Because the algorithm used to perform the analysis in GENSTAT 4 is sequential in nature, the effect of having *First* and *Carry* before *Direct* in the structure is that *Direct* is adjusted for *First.Carry* but not vice versa. By repeating the analysis with *Direct* first in the formula, the analysis in which *First.Carry* is adjusted for *Direct* will be obtained.

Experiment with preperiod. Kunert (1983) gives examples of change-over experiments in which there is a preperiod so that residual effects are estimated from all periods of the experiment. Such experiments have a somewhat simpler analysis than those without preperiod, such as the animals-with-repetitions-in-time experiment just discussed. For example, consider Kunert's (1983) example 4.7. The layout for this experiment is given in table 4.22.

The unrandomized factors for this experiment are *Units* and *Periods* and the randomized factors are *Direct* and *Carry*. The structure set is as follows:

Tier	Structure
1	*4 Units*12 Periods*
2	*3 Carry+3 Direct*

Table 4.22: Experimental layout for a change-over experiment with preperiod(Kunert, 1983)

			Periods											
		Preperiod	1	2	3	4	5	6	7	8	9	10	11	12
	1	3	1	2	3	1	2	3	1	2	3	1	2	3
	2	2	1	2	3	3	2	1	1	1	3	3	2	2
Units	3	3	2	3	1	1	3	2	2	2	1	1	3	3
	4	1	3	1	2	2	1	3	3	3	2	2	1	1

The analysis of variance table is given in table 4.23. Again, this example does not fulfil the conditions given in section 2.2.5; as for the previous example, there is no term derived from the structure for the second tier to which all other terms derived from that tier are marginal and, as *Direct* is not orthogonal to *Carry*, the experiment is not structure balanced. But, with randomized factors again being designated as expectation factors, it has been possible to use the approach to formulate a nonunique analysis. The symbolic forms of the maximal models for this experiment, derived according to the rules given in table 2.5, are as follows:

$$\begin{aligned} \mathrm{E}[Y] &= \mathit{Carry} + \mathit{Direct} \\ \mathrm{Var}[Y] &= G + \mathit{Units} + \mathit{Periods} + \mathit{Units.Periods} \end{aligned}$$

Table 4.23: Analysis of variance table for the change-over experiment with preperiod from Kunert (1983)

SOURCE	DF	EXPECTED MEAN SQUARES[†] Coefficients of ϕ_{UP}	ϕ_P	ϕ_U
Units	3	1		12
Periods	11			
Carry[‡]	2	1	4	
Residual	9	1	4	
Units.Periods	33			
Carry[§]	2	1		
Direct[¶]	2	1		
Residual	29	1		

[†] Variation contribution only to the expected mean squares.
[‡] *Carry* is partially confounded with the *Periods* with efficiency 0.062.
[§] *Carry* is partially confounded with *Units.Periods* with efficiency 0.938.
[¶] *Direct* is partially aliased with *Carry* with efficiency 0.938.

Chapter 5

Analysis of three-tiered experiments

5.1 Introduction

In this chapter the analysis of three-tiered experiments is examined to illustrate how the method described in chapter 2 facilitates their analysis. As is candidly acknowledged in section 2.1, a satisfactory analysis for many studies can be formulated without utilizing the proposed paradigm. However, it was suggested that the analysis of complex experiments would be assisted if the approach is employed. This is particularly the case for multitiered experiments; indeed, the full analysis of the experiment presented in section 5.2.4 can only be achieved with it. The analyses presented herein differ from those produced by other published methods so that, in some cases, I put forward analyses that more closely follow generally accepted principles for the analysis of designed experiments. Again, it will be assumed that the analyses discussed will only be applied to data that conform to the assumptions necessary for them to be valid.

5.2 Two-phase experiments

Two-phase experiments were introduced by McIntyre (1955). They are commonly used in the evaluation of wine (Ewart, Brien, Soderlund and Smart, 1985; Brien, May and Mayo, 1987).

5.2.1 A sensory experiment

To introduce the analysis of two-phase experiments using the method presented herein, the analysis of an orthogonal two-phase experiment is given in this section; the analysis has been previously discussed by Brien (1983).

Consider an experiment to evaluate a set of wines made from the produce of a field trial in order to test the effects of several viticultural treatments. Suppose that, in the field trial, the treatments are assigned to plots according to a randomized complete block design. The produce from each plot was separately made into wine which was evaluated at a tasting in which several judges are given the wines over a number of sittings. One wine is presented for scoring to each judge at a sitting and each wine is presented only once to a judge. The order of presentation of the wines is randomized for each judge. This experiment is then a two-phase experiment. In the first phase the field trial is conducted, and in the second phase the wine made from the produce of each plot in the field trial is evaluated by several judges.

The factors in the experiment are *Blocks*, *Plots* and *Treatments* from the field phase of the experiment, and *Judges* and *Sittings* from the tasting phase. An observational unit (of which there are jbt) is the wine given to a judge at a particular sitting.

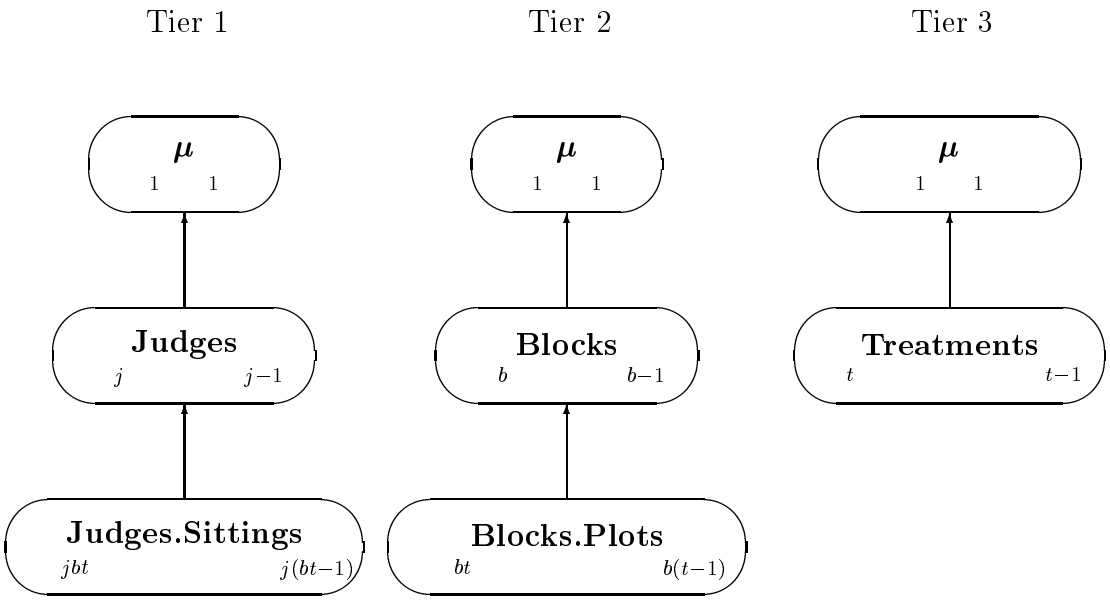
The structure set is derived as described in section 2.2.4. *Judges* and *Sittings* are the factors that would index the observational unit if no randomization had occurred, and so these form the bottom tier of unrandomized factors. The field units, and hence the wines, are uniquely identified by the factors *Blocks* and *Plots* and they would do so even if no randomization had been carried out in the field phase. As the combinations of these factors were randomized to the sittings for each judge, they form the second tier. The levels of *Treatments* were randomized to the plots within

each block and so *Treatments* forms the third or top tier. The structure set, assuming no intertier interaction, is as follows:

Tier	Structure
1	*j Judges/bt Sittings*
2	*b Blocks/t Plots*
3	*t Treatments*

The degrees of freedom of terms derived from the structure for a tier are computed, as outlined in table 2.2, using the Hasse diagrams of term marginalities; the diagrams for this example are given in figure 5.1

Figure 5.1: Hasse diagram of term marginalities for a sensory experiment



The analysis of variance table for this example, derived according to the rules given in table 2.1, is given in table 5.1. The indentation of the *Treatments* source indicates

that *Treatments* is confounded with *Blocks.Plots*. The *Residual* source immediately below the *Treatments* source corresponds to the unconfounded *Blocks.Plots* subspace, that is, the unconfounded differences between plots within a block. Similarly, the *Blocks* and *Blocks.Plots* sources are confounded with the *Judges.Sittings* source and the second *Residual* source provides the unconfounded *Judges.Sittings* subspace.

Table 5.1: Analysis of variance table for a two-phase wine-evaluation experiment

SOURCE	DF	EXPECTED MEAN SQUARES Coefficients of ϕ_{JS}	ϕ_J	ϕ_{BP}	ϕ_B	$\boldsymbol{\mu}_T$
Judges	$j-1$	1	bt			
Judges.Sittings	$j(bt-1)$					
Blocks	$(b-1)$	1		j	jt	
Blocks.Plots	$b(t-1)$					
Treatments	$(t-1)$	1		j		$f(\boldsymbol{\mu}_T)$
Residual	$(b-1)(t-1)$	1		j		
Residual	$(j-1)(bt-1)$	1				
Total	$jbt-1$					

For the purpose of determining the maximal expectation and variation models, all factors, except for *Treatments*, are assumed to contribute to variation. The maximal models for this experiment are derived as described in table 2.5 and, assuming the data are lexicographically ordered on *Judges* and *Sittings*, are as follows:

$$\begin{aligned} \mathrm{E}[\boldsymbol{y}] &= \boldsymbol{\mu}_T \\ \mathrm{Var}[\boldsymbol{y}] &= \mathbf{V}_1 + \mathbf{V}_2 \end{aligned}$$

where

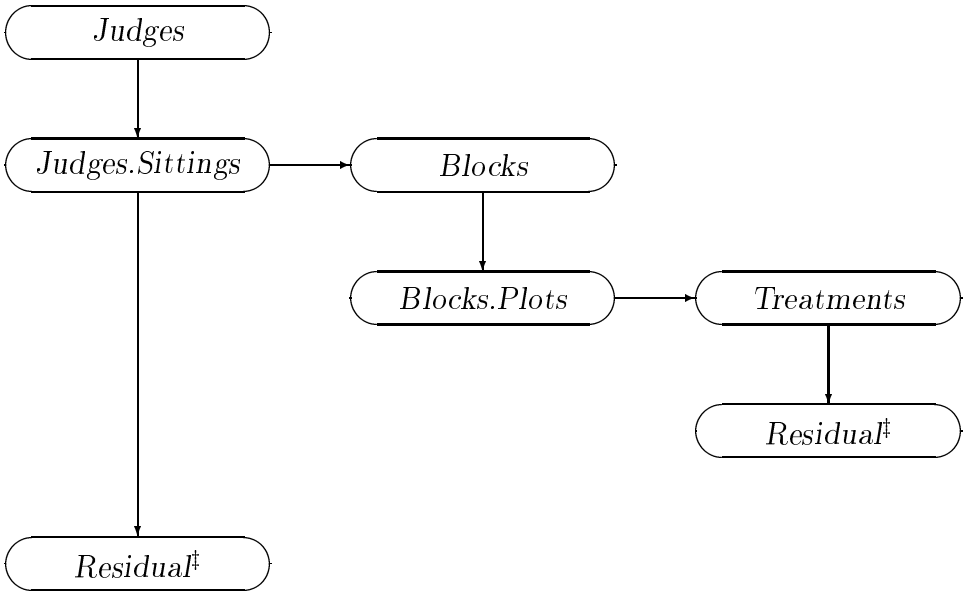
$$\mathbf{V}_1 = \phi_G \mathbf{J} \otimes \mathbf{J} + \phi_J \mathbf{I} \otimes \mathbf{J} + \phi_{JS}\, \mathbf{I} \otimes \mathbf{I},$$

$$\mathbf{V}_2 = \mathbf{U}_2(\phi_B \mathbf{I} \otimes \mathbf{J} \otimes \mathbf{J} + \phi_{BP} \mathbf{I} \otimes \mathbf{I} \otimes \mathbf{J})\mathbf{U}_2', \text{ and}$$

$\mathbf{U}_2$ is the permutation matrix of order jbt reflecting the assigning of levels combinations of *Blocks* and *Plots* to the sittings in which they were presented to each judge.

The expected mean squares under this model, derived as described in table 2.8, are also as given in table 5.1.

Figure 5.2: Minimal sweep sequence for a two-phase sensory experiment†



†Lines originating below a term signify a residual sweep and lines originating alongside a term signify a pivotal sweep (section 3.3.1.1).
‡*Residual* does not involve a sweep but merely serves to indicate the origin of the residuals for a residual source.

The minimal sweep sequence for performing the analysis as prescribed in section 3.3.1.1 is given in figure 5.2.

Table 5.2: Analysis of variance table, including intertier interactions, for a two-phase wine-evaluation experiment

SOURCE	DF	EXPECTED MEAN SQUARES Coefficients of							
		ϕ_{JS}	ϕ_J	ϕ_{BPJ}	ϕ_{BJ}	ϕ_{BP}	ϕ_B	ϕ_{TJ}	$\boldsymbol{\mu}_T$
Judges	$j-1$	1	bt	1	t			b	
Judges.Sittings	$j(bt-1)$								
Blocks	$(b-1)$	1		1	t	j	jt		
Blocks.Plots	$b(t-1)$								
Treatments	$(t-1)$	1		1		j		b	$f(\boldsymbol{\mu}_T)$
Residual	$(b-1)(t-1)$	1		1		j			
Blocks.Judges	$(b-1)(j-1)$	1		1	t				
Blocks.Plots.Judges	$b(t-1)(j-1)$								
Treatments.Judges	$(t-1)(j-1)$	1		1				b	
Residual	$(b-1)(t-1)(j-1)$	1		1					
Total	$jbt-1$								

It might be considered desirable to modify the structure set for the example to include intertier interactions likely to arise. For this purpose, factors from lower tiers have to be included in the structures for some higher tiers. An alternative structure set for the example, involving such intertier interaction, is as follows:

Tier	Structure
1	*j Judges/bt Sittings*
2	*(b Blocks/t Plots)∗Judges*
3	*t Treatments∗Judges*

The analysis derived from this structure set is given in table 5.2. This analysis is quite different from that presented in table 5.1; in particular, the test for *Treatments* now involves a ratio of linear combinations of mean squares, whereas only a ratio

of mean squares is involved in table 5.1. Thus, it is possible that quite different conclusions will be reached depending on which analysis is performed.

5.2.2 McIntyre's experiment

In this section the method presented herein is applied to the nonorthogonal, but structure-balanced, three-tiered experiment presented by McIntyre (1955). This illustrates the application to a more complicated experiment which results in an analysis of variance table that is more informative than previously presented analysis tables in that it reflects the randomization employed in the experiment. Further, there is some clarification of which terms should be included in the analysis.

The object of the experiment was to investigate the effects of four light intensity treatments on the synthesis of tobacco mosaic virus in the leaves of *Nicotiana tabacum*. In the first phase of the experiment, *Nicotiana* leaves, inoculated with virus, were subjected to the four different light intensities. The experimental arrangement for the first phase was obtained using two 4×4 Latin square designs, the rows and columns of these squares corresponding to *Nicotiana* plants and position of the leaves on these plants; the two Latin squares corresponded to different sets of *Nicotiana* plants. The layout is illustrated in figure 5.3.

In the second phase sap from each of the leaves of the first phase was injected into a half-leaf of the assay plant, *Datura stramonium*. The assignment of first-phase leaves to the half-leaves of the assay plants was accomplished using four Graeco-Latin squares; the rows and columns of the squares corresponded to *Datura* plants and position of the leaf on the assay plants, respectively. Within a Graeco-Latin square, the four leaves from one *Nicotiana* plant from each set were assigned to the half-leaves of the assay plant using the one alphabet for each plant. The layout is illustrated in figure 5.4.

Figure 5.3: Layout for the first phase of McIntyre's (1955) experiment†

Nicotiana Plants

Leaf Position	1	2	3	4
1	a 1	b 5	c 9	d 13
2	b 2	a 6	d 10	c 14
3	c 3	d 7	a 11	b 15
4	d 4	c 8	b 12	a 16

Leaf Position	1	2	3	4
1	a 17	b 21	c 25	d 29
2	c 18	d 22	a 26	b 30
3	d 19	c 23	b 27	a 31
4	b 20	a 24	d 28	c 32

†The letter in each cell refers to the light intensity to be applied to the unit and the number to the unit.

Figure 5.4: Layout for the second phase of McIntyre's (1955) experiment†

Datura Plants

Assay Leaf Position	1	2	3	4	5	6	7	8
1	1 17	2 20	3 18	4 19	5 23	6 22	7 24	8 21
2	2 18	1 19	4 17	3 20	8 22	7 23	6 21	5 24
3	3 19	4 18	1 20	2 17	7 21	8 24	5 22	6 23
4	4 20	3 17	2 19	1 18	6 24	5 21	8 23	7 22

Datura Plants

Assay Leaf Position	9	10	11	12	13	14	15	16
1	9 28	10 25	11 27	12 26	13 30	14 31	15 29	16 32
2	10 27	9 26	12 28	11 25	16 31	15 30	14 32	13 29
3	11 26	12 27	9 25	10 28	15 32	16 29	13 31	14 30
4	12 25	11 28	10 26	9 27	14 29	13 32	16 30	15 31

†The numbers in the cell refer to the units from the first phase to be assigned to the two half-leaves of the assay plant.

The observational unit is a half leaf of an assay plant and the factors in the experiment are *Reps*, *Datura*, *APosition*, *Halves*, *Sets*, *Nicotiana*, *Position* and *Treatments*. The structure set for this experiment, derived using the steps given in section 2.2.4, is as follows:

Tier	Structure
1	*((4 Reps/4 Datura)∗4 APosition)/2 Halves*
2	*(2 Sets/4 Nicotiana)//Nicotiana*
	+(Sets/Nicotiana)∗4 Position
3	*4 Treatments*

The structures derived from the factors in tiers two and three correspond to the structure set for the first phase of the experiment, while the structure derived from bottom tier factors corresponds to the structure of the units from the second phase. Note that *Nicotiana* has to be included as a pseudoterm to *Sets.Nicotiana* for the correct degrees of freedom to be obtained using the method described in table 2.2. The pseudofactor indexes which *Nicotiana* plants from the first phase were assigned to the same *Datura* plant in the second phase.

The analysis of variance for the experiment, obtained using the rules given in table 2.1, is given in table 5.3. The Hasse diagrams of term marginalities, used in obtaining the degrees of freedom of the terms in the analysis table as prescribed in table 2.2, are presented in figure 5.5.

For the purpose of deriving the maximal expectation and variation models for the experiment, it is likely that all factors in the experiment, other than *Treatments*, will be classified as variation factors. Thus, the application of the steps given in table 2.5 yields the following models for the experiment, assuming the data are lexicographically ordered on *Reps*, *Datura*, *APosition*, and *Halves*:

$$\begin{aligned} \mathrm{E}[\boldsymbol{y}] &= \boldsymbol{\mu}_T \\ \mathrm{Var}[\boldsymbol{y}] &= \mathbf{V}_1 + \mathbf{V}_2 \end{aligned}$$

where

Figure 5.5: Hasse diagram of term marginalities for McIntyre's experiment

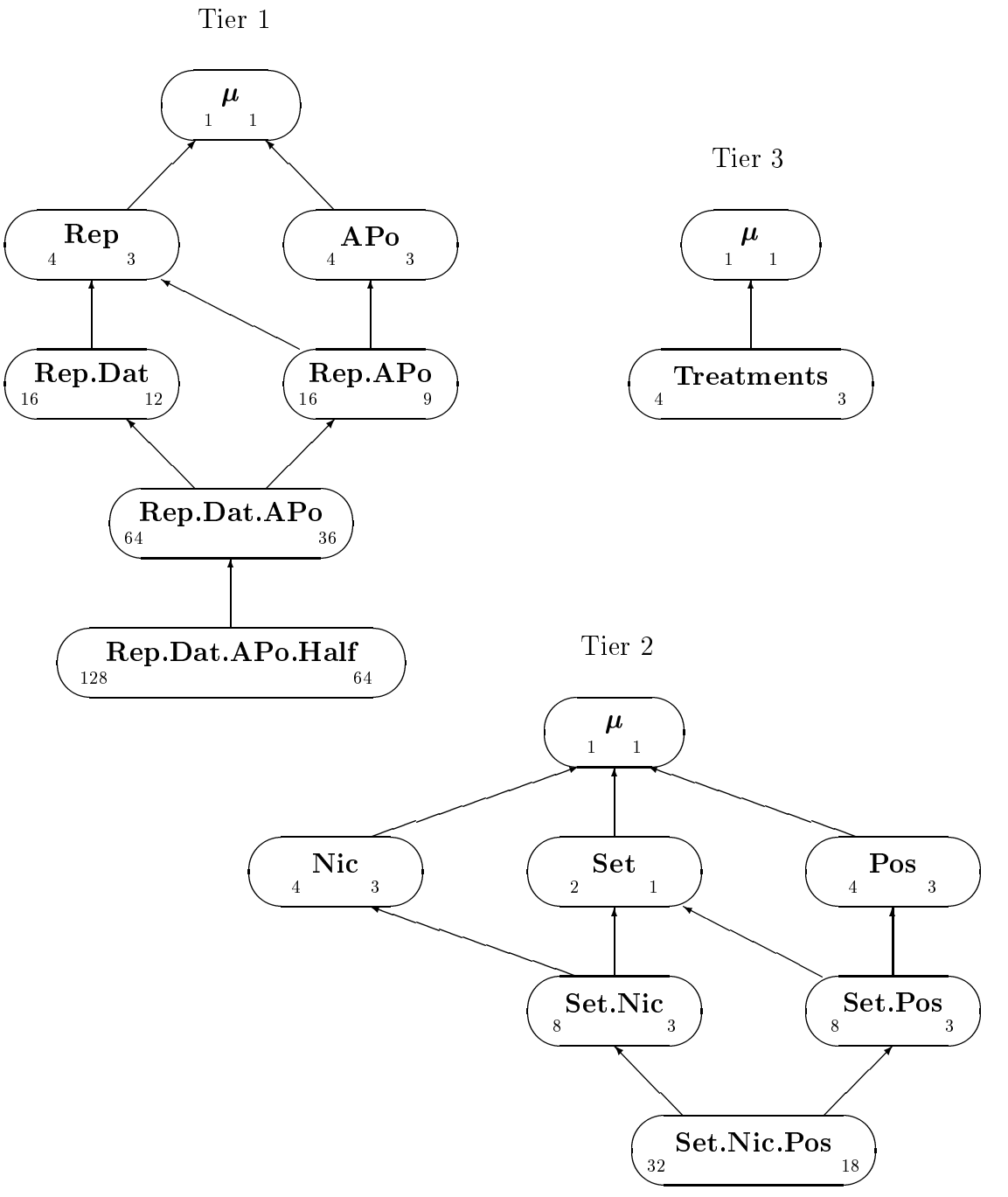


Table 5.3: Analysis of variance table for McIntyre's two-phase experiment

SOURCE	DF	EXPECTED MEAN SQUARES Coefficients of ϕ_{RADH}	ϕ_{RDA}	ϕ_{RA}	ϕ_A	ϕ_{RD}	ϕ_R	ϕ_{SNP}	ϕ_{SN}	ϕ_{SP}	ϕ_S	ϕ_P	$\boldsymbol{\mu}_T$	MSq	F
Reps	3														
Sets.Nicotiana	3	1	2	8		8	32	4	16					182.58	
Reps.Datura	12	1	2			8								75.12	6.37
APosition	3	1	2	8	32									119.07	14.87
Reps.APosition	9	1	2	8										8.01	0.68
Reps.Datura.APosition	36														
Position†	3	1	2					2		8		16		36.95	0.91
Sets.Position†	3	1	2					2		8				40.47	1.30
Sets.Nicotiana.Position†	18														
Treatments†	3	1	2					2					$f(\boldsymbol{\mu}_T)$	74.12	2.38
Residual	15	1	2					2						31.14	2.64
Residual	12	1	2											11.80	
Reps.Datura.APosition.Halves	64														
Sets	1	1						4	16	16	64			41.40	
Sets.Nicotiana‡	3	1						4	16					10.30	
Position†	3	1						2		8		16		23.38	0.54
Sets.Position†	3	1						2		8				43.31	4.31
Sets.Nicotiana.Position†	18														
Treatments†	3	1						2					$f'(\boldsymbol{\mu}_T)$	31.23	3.11
Residual	15	1						2						10.04	
Residual	36	1												7.60	
Total	127														

†These sources are partially confounded with efficiency 0.50.
‡The restrictions placed on randomization result in the subspace of *Sets.Nicotiana* confounded with *Reps* being orthogonal to that confounded with *Reps.Datura.APosition.Halves*. *Sets.Nicotiana* is thus orthogonal to all first tier sources.

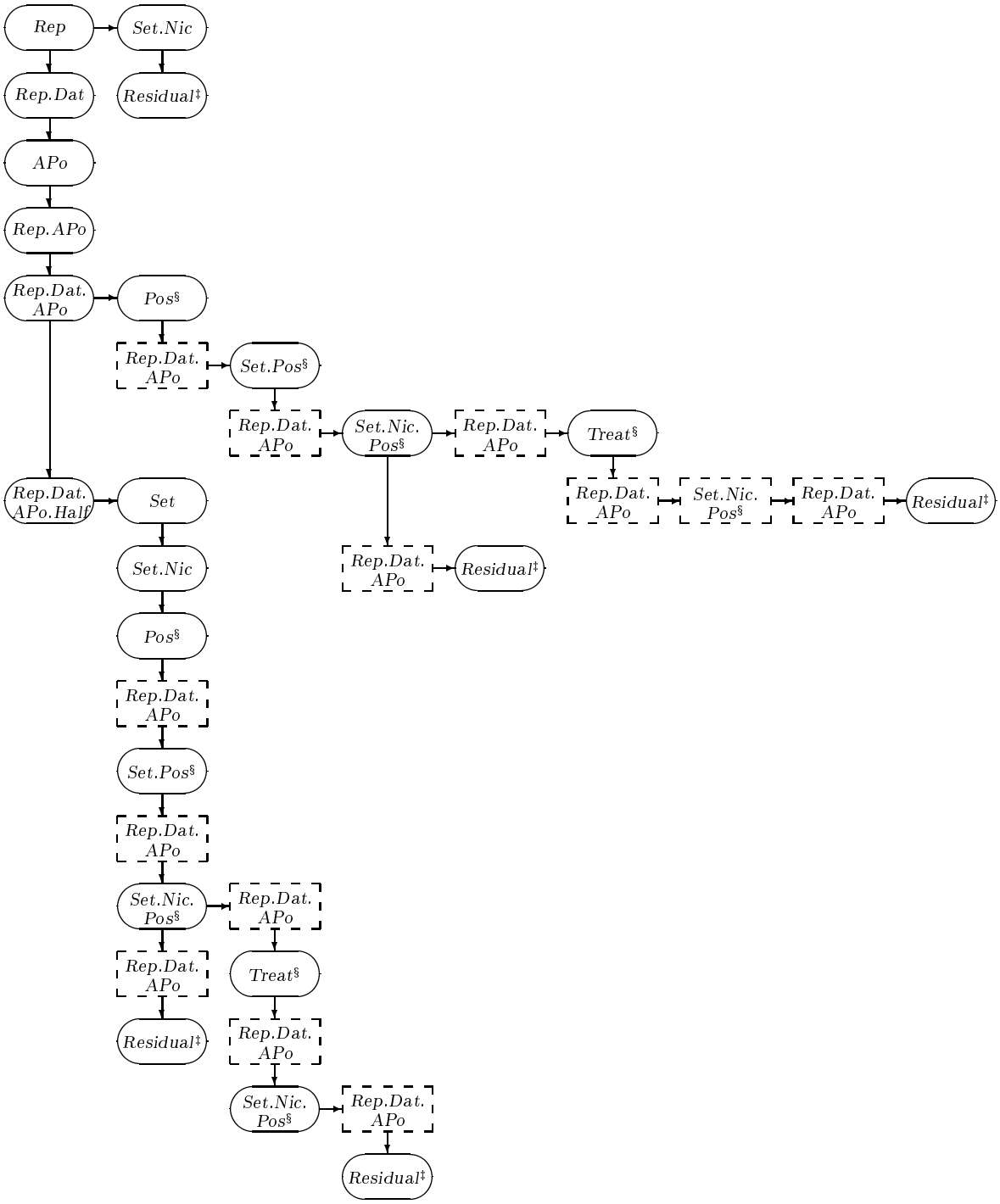
$$
\begin{aligned}
\mathbf{V}_1 &= \phi_G\mathbf{J}\otimes\mathbf{J}\otimes\mathbf{J}\otimes\mathbf{J} + \phi_R\mathbf{I}\otimes\mathbf{J}\otimes\mathbf{J}\otimes\mathbf{J} + \phi_{RD}\mathbf{I}\otimes\mathbf{I}\otimes\mathbf{J}\otimes\mathbf{J} \\
&\quad + \phi_A\mathbf{J}\otimes\mathbf{J}\otimes\mathbf{I}\otimes\mathbf{J} + \phi_{RA}\mathbf{I}\otimes\mathbf{J}\otimes\mathbf{I}\otimes\mathbf{J} + \phi_{RDA}\mathbf{I}\otimes\mathbf{I}\otimes\mathbf{I}\otimes\mathbf{J} \\
&\quad + \phi_{RDAH}\mathbf{I}\otimes\mathbf{I}\otimes\mathbf{I}\otimes\mathbf{I}, \\
\mathbf{V}_2 &= \mathbf{U}_2(\phi_P\mathbf{J}\otimes\mathbf{J}\otimes\mathbf{I}\otimes\mathbf{J} + \phi_S\mathbf{I}\otimes\mathbf{J}\otimes\mathbf{J}\otimes\mathbf{J} + \phi_{SP}\mathbf{I}\otimes\mathbf{J}\otimes\mathbf{I}\otimes\mathbf{J} \\
&\quad + \phi_{SN}\mathbf{I}\otimes\mathbf{I}\otimes\mathbf{J}\otimes\mathbf{J} + \phi_{SNP}\mathbf{I}\otimes\mathbf{I}\otimes\mathbf{I}\otimes\mathbf{J})\mathbf{U}_2', \text{ and} \\
\mathbf{U}_2 &\text{ is a permutation matrix of order 128 reflecting the assignment of the} \\
&\quad \text{levels combinations of } \textit{Set}, \textit{Nicotiana} \text{ and } \textit{Position} \text{ to the halves.}
\end{aligned}
$$

Based on these models, the expected mean squares, which are also given in table 5.3, are derived using the steps given in table 2.8.

The analysis differs from that given by Curnow (1959) only in its layout and in that the *Reps.APosition* interaction has been isolated. The advantage of the layout of the analysis table presented in table 5.3 is that the confounding between sources in the table is obvious. For example, *Treatments* has been confounded with *Sets.Nicotiana.Position* which, in turn, is confounded with both *Reps.Datura.APosition* and *Reps.Datura.APosition.Halves*. In respect, of the *Reps.APosition* interaction, Curnow (1959) has combined this source with the *Reps.Datura.APosition Residual* source in the 'Residual (2)' of his Sums analysis. Also, the *Reps.APosition* interaction is not 'of the character of a treatment and block interaction' as suggested by Curnow, but is a source contributing to variation that can be separated from the *Residual*.

The sums of squares were computed using the sweep sequence presented in figure 5.6. The directly nonorthogonal terms in the experiment are *Positions*, *Sets.Positions* and *Sets.Nicotiana.Positions* and these terms are structure balanced. In addition, the nonorthogonality of the last term induces nonorthogonality in the *Treatments* term which must be taken into account in the analysis sequence. Since most terms are orthogonal, most backsweeps are redundant and the sequence shown in figure 5.6 is the minimal sequence.

Figure 5.6: Minimal sweep sequence for McIntyre's two-phase experiment†



†Lines originating below a term signify a residual sweep and lines originating alongside a term signify a pivotal sweep (section 3.3.1.1). Terms placed in dashed boxes signify a backsweep (section 3.3.1.1).
‡*Residual* does not involve a sweep but merely serves to indicate the origin of the residuals for a residual source.
§For these sources effective means are calculated by dividing computed means by an efficiency factor of 0.5.

5.2.3 Taste-testing experiment from Wood, Williams and Speed (1988)

Wood, Williams and Speed (1988) in their discussion of two-phase experiments claim that they provide an analysis of variance table which is very similar to that put forward by Brien (1983). In this section, I illustrate how the analysis of variance table produced using the method outlined herein differs from that presented by Wood *et al.* (1988). As a result, it will become clear that their partition of the *Total* sum of squares may not be correct and that a more informative analysis of variance table can be produced. Also, from the discussion of this example, it will be evident how differences in the layout of an experiment might affect the analysis and, hence, be reflected in the analysis of variance table. The analyses presented in this section are all structure balanced.

The Wood *et al.* (1988) experiment with which we are concerned is their second example, a taste-testing experiment the purpose of which was to investigate the effects of six storage treatments on milk drinks. The experiment was a two-phase experiment; in the first or storage phase, the milk drinks were subjected to the storage treatments, whilst in the second or tasting phase, tasters scored the produce from the storage phase. The storage treatments were the six combinations of two types of container (plastic, glass) and three temperatures (-20°C, 1°C, 30°C).

A problem encountered at the outset in deriving the analysis for this semiconstructed example, is that, as I shall elaborate later in this section, the design used in the first phase could not have been as described by Wood *et al.* (1988). However, the following scenario does fit with the Wood *et al.* (1988) description in that a randomized complete block design is utilized in the assignment of treatment combinations in the first phase.

Suppose that the first phase of the experiment involved treating milk rather than storing it. In each of two periods six runs were performed; at each run the milk was treated at one of the three temperatures mentioned above while contained in either the plastic or glass container. After processing, six samples, corresponding to the six type-temperature combinations, were randomly presented to 8 judges in each of two

sessions. This experiment will be referred to as the *Wood, Williams and Speed (1988) processing experiment*. The data from the experiment are presented in table 5.4.

Table 5.4: Scores from the Wood, Williams and Speed (1988) processing experiment[†]

Session	1						2					
Type	Plastic			Glass			Plastic			Glass		
Temperature	-20	1	30	-20	1	30	-20	1	30	-20	1	30
Judge												
1	4	5	5	**6**	**3**	**5**	**5**	**6**	**7**	7	4	7
2	**6**	**6**	**7**	5	6	7	4	7	6	**5**	**6**	**6**
3	4	**7**	8	**8**	2	**8**	**2**	8	**3**	8	**7**	7
4	**6**	6	**7**	5	**3**	4	2	**5**	1	**6**	2	**3**
5	7	7	**7**	**7**	**7**	7	**7**	**7**	8	7	8	**8**
6	**7**	**8**	8	6	5	**7**	8	6	**7**	**7**	**8**	8
7	7	**7**	**7**	**6**	6	6	**6**	6	6	8	**8**	**6**
8	**7**	7	7	6	**6**	**6**	6	**6**	**6**	**8**	8	6

[†]The bolded scores are from the second period

The observational unit for this experiment is a unit scored by a judge in a session. The factors are *Judge*, *Session*, *Unit*, *Period*, *Run*, *Type* and *Temperature*. The factors that would index the observational unit if no randomization had occurred are *Judge*, *Session* and *Unit* so these form the bottom or unrandomized tier. The factors *Period* and *Run* index uniquely the first-phase units and would index the first-phase units if no randomization had occurred in that phase. Hence, these factors form the second tier of factors. The third tier is comprised of *Type* and *Temperature* as these were assigned randomly to runs within each period. The structure set derived from these tiers is as follows, it being necessary to include pseudofactors to obtain a structure-balanced set of terms:

Tier	Structure
1	*(8 Judge∗2 Session)/6 Unit*
2	*(2 Period/6 Run)//(2 Pseudo*Temperature)*
3	*2 Type∗3 Temperature*

The pseudofactor *Pseudo* is a factor of two levels. Observations that take level 1 of *Pseudo* are those with the levels combinations 1,1 and 2,2 of *Period* and *Type*, otherwise an observation takes level 2 of *Pseudo*. The pseudoterms identify the various subspaces of *Period.Run* that have the same efficiency factors relative to the tier 1 structure (see table 5.5).

The degrees of freedom of terms derived from the structure for a tier are computed, as outlined in table 2.2, using the Hasse diagrams of term marginalities; the diagrams for this example are given in figure 5.7. The analysis of variance table for this example, derived according to the rules given in table 2.1, is given in table 5.5.

Assume all factors in the experiment, except *Type* and *Temperature*, are to be designated as variation factors. The symbolic form of the maximal models for this experiment, derived according to the rules given in table 2.5, is as follows:

$$\begin{aligned} \mathrm{E}[Y] &= \mathit{Type.Temperature} \\ \mathrm{Var}[Y] &= G + \mathit{Judge} + \mathit{Session} + \mathit{Judge.Session} + \mathit{Judge.Session.Unit} \\ &\quad + \mathit{Period} + \mathit{Period.Run} \end{aligned}$$

Note that it may not be appropriate to designate *Judge* as a variation factor. This is because judges evaluate in an individualistic manner and it will be important to compare one judge's evaluation with another's; this is certainly the case with wine evaluation (Brien, May and Mayo, 1987). However, in order to conform with Wood *et al.* (1988), *Judge* will remain a variation factor.

The expected mean squares based on the above model are also given in table 5.5. In computing these, one had first to derive the expectation for each of the mean squares that would have been obtained if terms arising from pseudoterms had not been combined. The expectation of a combined mean square was then obtained as the weighted average of the expectation of the mean squares comprising it, the weights being the degrees of freedom of the mean squares. Thus, the expectation of

Figure 5.7: Hasse diagram of term marginalities for the Wood, Williams and Speed (1988) processing experiment

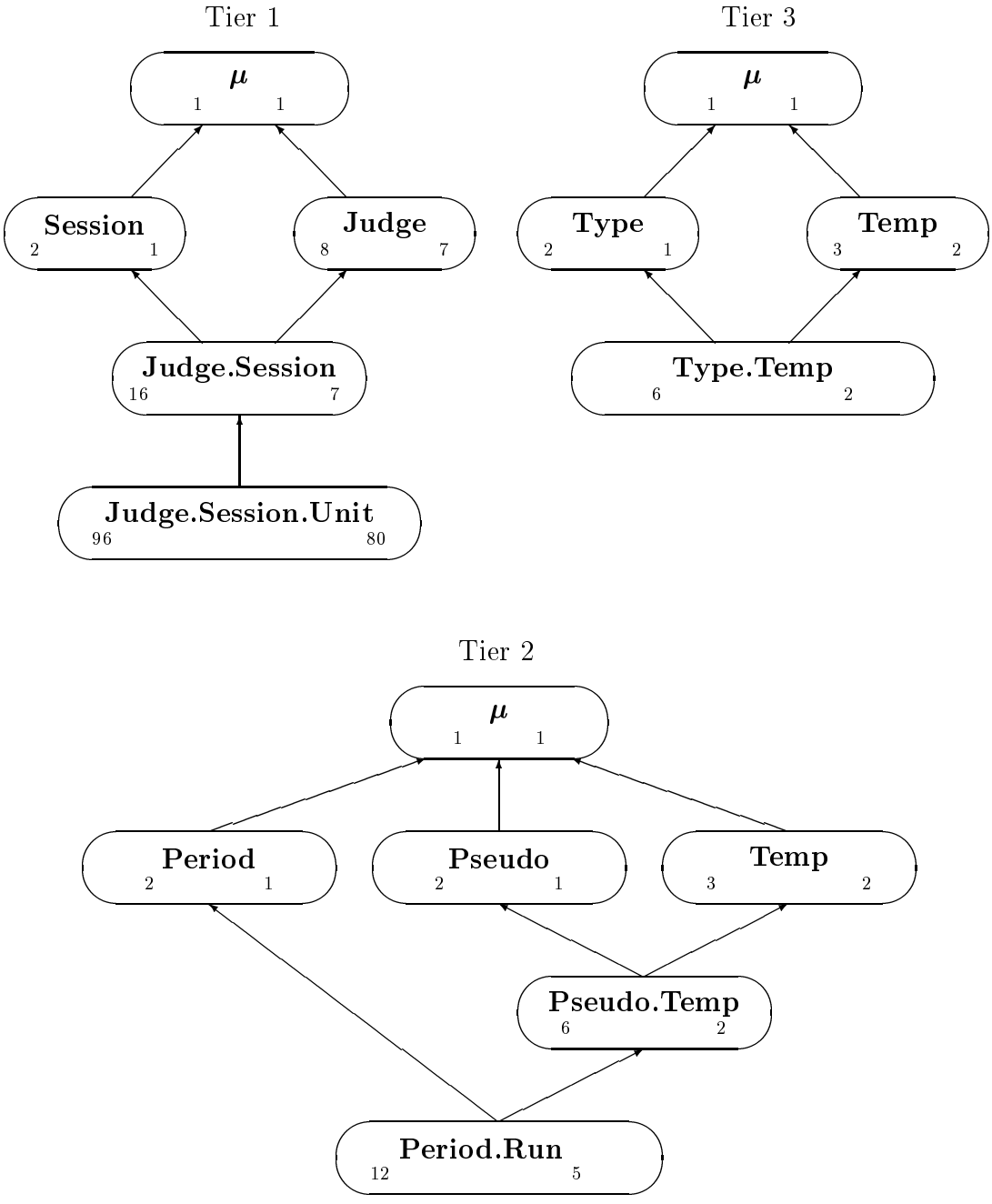


Table 5.5: Analysis of variance table for Wood, Williams and Speed (1988) processing experiment

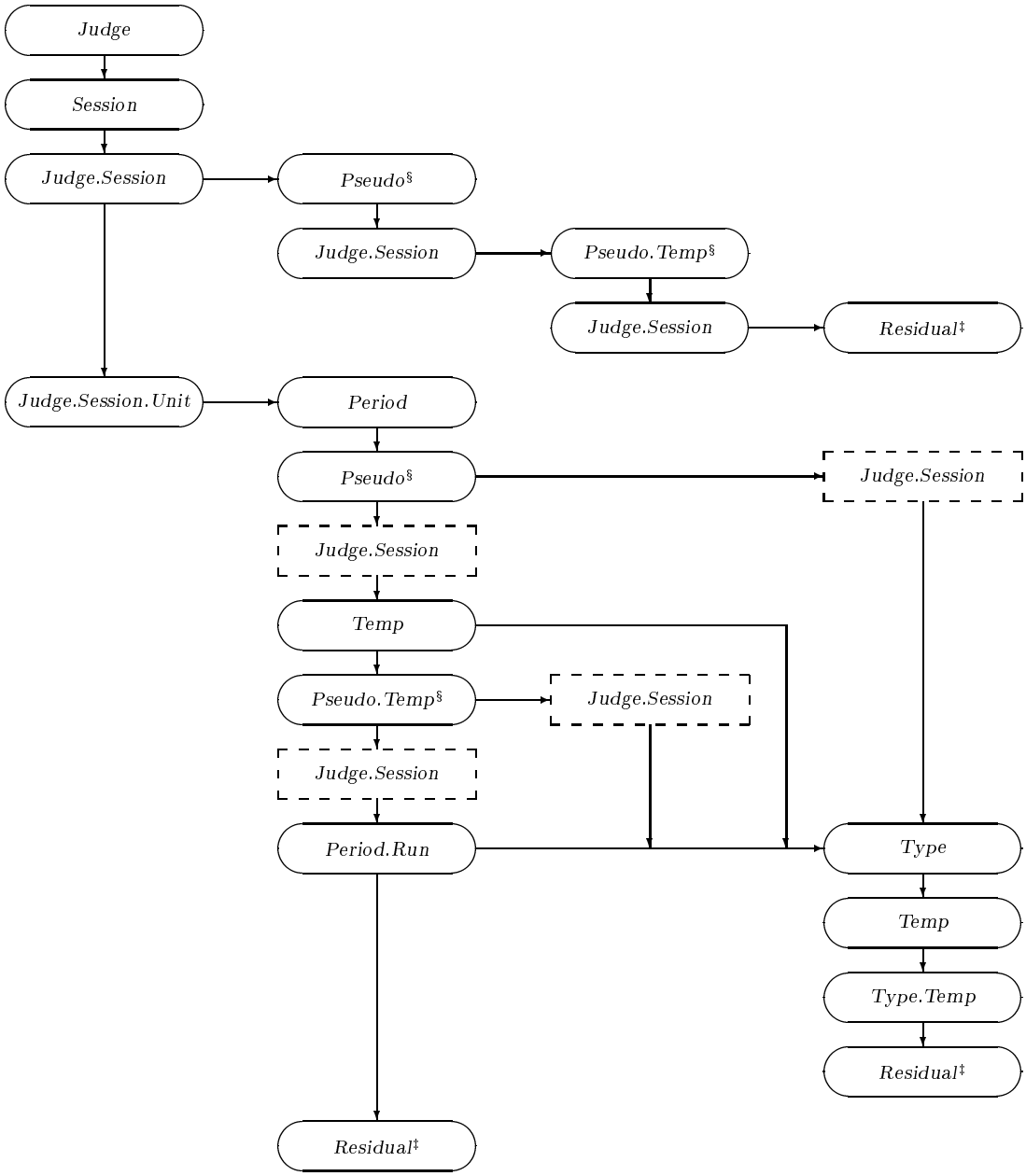
ANALYSIS OF VARIANCE TABLE

SOURCE	DF	EXPECTED MEAN SQUARES Coefficients of ϕ_{JSU}	ϕ_{JS}	ϕ_S	ϕ_J	ϕ_{PR}	ϕ_P	MSq
Judge	7	1	6		12			12.213
Session	1	1	6	48				0.010
Judge.Session	7							
Period.Run	3	1	6			$\frac{8}{3}$		3.066
Residual	4	1	6					2.719
Judge.Session.Unit	80							
Period	1	1				8	48	1.260
Period.Run	10							
Type	1	1				8		0.094
Temperature	2	1				8		0.667
Type.Temperature	2	1				8		8.000
Residual	5	1				$\frac{32}{5}$		0.909
Residual	69	1						1.735
Total	95							

INFORMATION SUMMARY

Model term	Efficiency
Judge.Session	
Pseudo	$\frac{1}{3}$
Pseudo.Temp	$\frac{1}{3}$
Judge.Session.Unit	
Pseudo	$\frac{2}{3}$
Pseudo.Temp	$\frac{2}{3}$

Figure 5.8: Minimal sweep sequence for Wood, Williams and Speed (1988) processing experiment†



†Lines originating below a term signify a residual sweep and lines originating alongside a term signify a pivotal sweep (section 3.3.1.1). Where there are multiple inputs, the original effects are added together to form the input for the sweep to be performed at the destination. Terms placed in dashed boxes signify a backsweep (section 3.3.1.1).
‡*Residual* does not involve a sweep but merely serves to indicate the origin of the residuals for a residual source.
§For this source effective means are calculated by dividing computed means by an efficiency factor which is given in table 5.5.

the *Period.Run Residual* mean square is

$$\frac{2(\phi_{JSU} + 8\phi_{PR}) + 3(\phi_{JSU} + \frac{16}{3}\phi_{PR})}{2+3} = \phi_{JSU} + \frac{32}{5}\phi_{PR}$$

The sums of squares were computed using the sweep sequence presented in figure 5.8.

As I mentioned earlier in this section, the actual physical conduct of the experiment will mean that it is unlikely that the assignment of treatment combinations in the first phase could have been achieved using a randomized complete block design with replicates corresponding to the blocks. This is because it was a storage experiment, with the milk being stored in either plastic or glass containers; thus, there would have to have been several containers of each type (3 if there were no replicates or 6 otherwise) and types could not have been randomly assigned to containers. On the other hand, Temperatures would have been randomized to the different containers which may or may not have been blocked into two replicates. We will presume that they were blocked and refer to this experiment as the *Wood, Williams and Speed (1988) storage experiment*.

The factors are *Judge*, *Session*, *Unit*, *Rep*, *Type*, *Container* and *Temperature*. The factors that would index the observational unit if no randomization had been performed are *Judge*, *Session* and *Unit* so these form the bottom or unrandomized tier. The factors *Rep*, *Type* and *Container* index uniquely the first-phase units and would index the first-phase units if no randomization had been performed in that phase. Hence, these factors form the second tier of factors. The third tier is comprised of *Temperature* as this was assigned randomly to containers within each rep-type combination. The structure set derived from these tiers is as follows, it again being necessary to include the pseudoterms to obtain a balanced analysis:

Tier	Structure
1	*(8 Judge∗2 Session)/6 Unit*
2	*(2 Rep∗2 Type)//2 Pseudo/6 Container)//(Pseudo*Temperature)*
3	*Type∗3 Temperature*

Table 5.6: Analysis of variance table for the Wood, Williams and Speed (1988) storage experiment

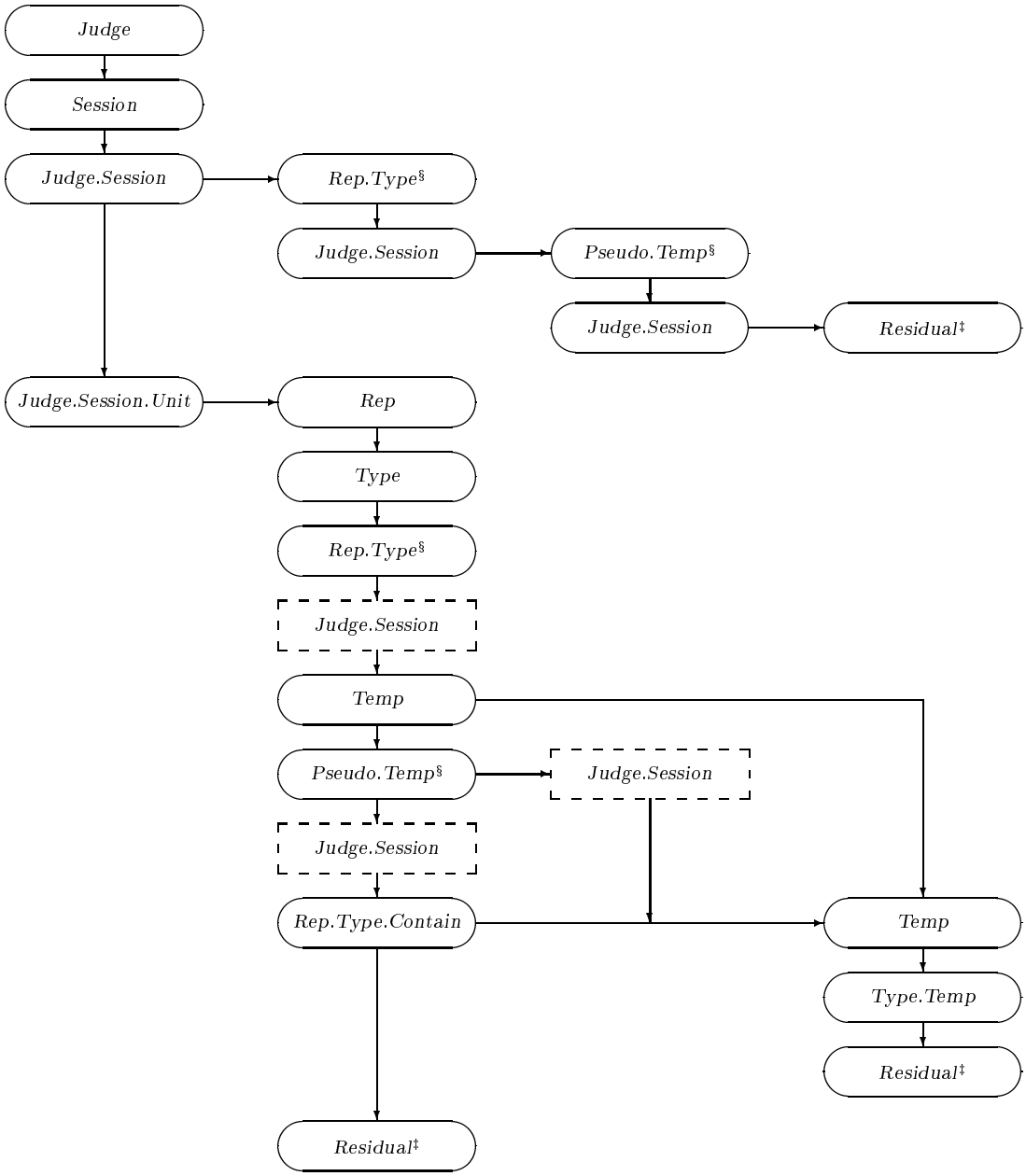
ANALYSIS OF VARIANCE TABLE

SOURCE	DF	EXPECTED MEAN SQUARES Coefficients of ϕ_{JSU}	ϕ_{JS}	ϕ_S	ϕ_J	ϕ_{RTC}	ϕ_{RT}	ϕ_R	MSq
Judge	7	1	6		12				12.213
Session	1	1	6	48					0.010
Judge.Session	7								
Rep.Type	1	1	6			$\frac{8}{3}$	$\frac{24}{3}$		6.420
Rep.Type.Container	2	1	6			$\frac{8}{3}$			1.389
Residual	4	1	6						2.719
Judge.Session.Unit	80								
Rep	1	1				8	24	48	1.260
Type	1	1				8	24		0.094
Rep.Type	1	1				$\frac{16}{3}$	$\frac{48}{3}$		2.778
Rep.Type.Container	8								
Temperature	2	1				8			0.667
Type.Temperature	2	1				8			8.000
Residual	4	1				$\frac{20}{3}$			0.441
Residual	69	1							1.735
Total	95								

INFORMATION SUMMARY

Model term	Efficiency
Judge.Session	
Pseudo	$\frac{1}{3}$
Pseudo.Temp	$\frac{1}{3}$
Judge.Session.Unit	
Pseudo	$\frac{2}{3}$
Pseudo.Temp	$\frac{2}{3}$

Figure 5.9: Minimal sweep sequence for the Wood, Williams and Speed (1988) storage experiment†



†Lines originating below a term signify a residual sweep and lines originating alongside a term signify a pivotal sweep (section 3.3.1.1). Where there are multiple inputs, the original effects are added together to form the input for the sweep to be performed at the destination. Terms placed in dashed boxes signify a backsweep (section 3.3.1.1).
‡*Residual* does not involve a sweep but merely serves to indicate the origin of the residuals for a residual source.
§For this source effective means are calculated by dividing computed means by an efficiency factor which is given in table 5.6.

The analysis of variance table for this example, derived according to the rules given in table 2.1, is given in table 5.6.

Again, assume all factors in the experiment, except *Type* and *Temperature*, are to be designated as variation factors. The symbolic form of the maximal models for the storage experiment, derived according to the rules given in table 2.5, is as follows:

$$\begin{aligned} \mathrm{E}[Y] &= \mathit{Type.Temperature} \\ \mathrm{Var}[Y] &= G + \mathit{Judge} + \mathit{Session} + \mathit{Judge.Session} + \mathit{Judge.Session.Unit} \\ &\quad + \mathit{Rep} + \mathit{Rep.Type} + \mathit{Rep.Type.Container} \end{aligned}$$

The expected mean squares based on the above model are also given in table 5.6. Again, the expectation of the *Rep.Type.Container Residual* mean square had to be obtained as the weighted average of the expectations of the mean squares of which it is comprised. It is calculated as follows:

$$\frac{2(\phi_{JSU} + 8\phi_{RTC}) + 2(\phi_{JSU} + \frac{16}{3})}{2+2} = \phi_{JSU} + \frac{20}{3}\phi_{RTC}$$

The sums of squares were computed using the sweep sequence presented in figure 5.9.

Comparison of the tables that I have produced (tables 5.5 and 5.6) with that presented by Wood *et al.* (1988) (see table 5.7) reveals a number of differences.

Firstly, their table gives no indication of the first phase units to which the types and temperatures were randomized. Consequently, the term with which *Type*, *Temperature* and *Type.Temperature* is confounded has been omitted from each of the tables, whereas in table 5.5 it is clear that these terms are confounded with *Period.Run* and, in table 5.6, that the last two terms are confounded with *Rep.Type.Container*.

Secondly, there is no suggestion in the Wood *et al.* (1988) table of the *Replicate* interactions with *Type* and *Temperature* being intertier interactions, which they are, except for *Rep.Type* in the storage experiment. However, it is usual to assume there are not such interactions and, if required to facilitate the analysis, they are only included as pseudoterms or terms with no scientific interpretation. Further, as Brien (1983) suggests the intertier interactions of *Type* and *Temperature* with *Judge* are more likely to be important in taste-testing experiments. But, if it is thought that the

Table 5.7: Analysis of variance table after that presented by Wood, Williams and Speed (1988) for a taste-testing experiment

ANALYSIS OF VARIANCE TABLE

STRATUM	DF	EXPECTED MEAN SQUARES Coefficients of ϕ_{JSU}	ϕ_{JS}	ϕ_S	ϕ_J	ϕ_{RTyTe}	ϕ_{RTy}	ϕ_{RTe}	ϕ_R	MSq
Judge	7	1	6	12						12.213
Session	1	1	6	48						0.010
Judge.Session										
replicate.type	1	1	6		$\frac{8}{3}$	$\frac{24}{3}$				6.420
replicate.type.temperature	2	1	6		$\frac{8}{3}$					1.389
residual	4	1	6							2.719
Judge.Session.Unit										
replicate	1	1			8	24	16	48		1.260
type	1	1			8	24				0.094
temperature	2	1			8		16			0.667
type.temperature	2	1			8					8.000
replicate.type	1	1			$\frac{16}{3}$	$\frac{48}{3}$				2.778
replicate.temperature	2	1			8		16			0.542
replicate.type.temperature	2	1			$\frac{16}{3}$					0.340
residual	69	1								1.753

INFORMATION SUMMARY

Model term	Efficiency factor
Judge.Session stratum	
replicate.type	$\frac{1}{3}$
replicate.type.temperature	$\frac{1}{3}$
Judge.Session.Unit stratum	
replicate.type	$\frac{2}{3}$
replicate.type.temperature	$\frac{2}{3}$

Replicate interactions might occur, one can include them, in addition to *Period.Run* or *Rep.Type.Container*. Wood *et al.* (1988) provide no such rationale and it would seem that they included them as full terms merely as a device to obtain a balanced analysis. In these circumstances, they are more correctly designated as pseudoterms.

An important consequence of not including the *Replicate* interactions is that the partition of the *Total* sum of squares differs so that divisors for F-test and estimates of standard errors will differ. In particular, the *Period.Run Residual* mean square from the storage experiment can be obtained by pooling the *replicate.type, replicate.temperature* and *replicate.type.temperature* mean squares from the Wood *et al.* (1988). The *Rep.Type.Container Residual* mean square from the processing experiment can be obtained by pooling the *replicate.temperature* and *replicate.type.temperature* mean squares from the Wood *et al.* (1988) analysis.

Finally, Wood *et al.* (1988) assert that a problem in using the analysis-of-variance method to obtain estimates of the canonical covariance components is that there are usually more equations than parameters to estimate. This is not the case for this example, nor for any of the other examples presented in the thesis.

In summary, of the analyses I have presented, the one most like that of Wood *et al.* (1988) is surprisingly not that for the experiment employing the same design as theirs, that is, the processing experiment based on a randomized complete block design in the first phase. Rather, it is most like the storage experiment. Table 5.6 contains almost the same set of mean squares as those in the Wood *et al.* (1988) table. The differences are that the *Rep.Type.Container Residual* mean square consists of two mean squares from the Wood *et al.* (1988) analysis and that the mean squares are labelled differently to those in the Wood *et al.* (1988) table so that the types of variability (section 6.6.2) contributing to the subspace are more accurately portrayed.

I believe this example demonstrates the advantage of employing the paradigm I have proposed in the case of complex experiments. It provides a framework for deciding which terms to include in the analysis that has to do with the behaviour expected in the data rather than basing the decision on which terms are required to achieve a balanced analysis.

5.2.4 Three structures required

In this section, a constructed structure-balanced example is presented, the experiment being one that requires three structures for a complete analysis.

Consider a two-phase experiment (McIntyre, 1955) consisting of field and wine evaluation phases. Suppose that the field phase involved a viticultural experiment to investigate differences between four types of trellising and two methods of pruning. The design consisted of two adjacent Youden squares of three rows and four columns, the plots of which were each split into two subplots (or halfplots). Trellis was assigned to main plots as shown in table 5.8 and methods of pruning were assigned at random independently to the two halfplots within each main plot.

Table 5.8: Assignment of the trellis treatment to the main plots in the field phase of the experiment.

	Squares							
	1				2			
Columns	1	2	3	4	1	2	3	4
Rows								
1	4	1	2	3	2	1	4	3
2	1	2	3	4	3	2	1	4
3	2	3	4	1	4	3	2	1

For the evaluation phase, there were six judges all of whom took part in 24 sittings. In the first 12 of these sittings the wines made from the halfplots of one square were evaluated; the final 12 sittings were to evaluate the wines from the other square. At each sitting, each judge assessed two glasses of wine from each of the two halfplots of one of the main plots. The main plots allocated to the judges at each sitting are shown in table 5.9, and were determined as follows. For the allocation of rows, each occasion was subdivided into 3 intervals of 4 consecutive sittings. During each interval, each judge examined plots from one particular row, these being determined

Table 5.9: Assignment of the main plots (*Row* and *Column* combinations) from the field experiment to the judges at each sitting in the evaluation phase.

	Occasion 1											
Intervals	1				2				3			
Sittings	1	2	3	4	1	2	3	4	1	2	3	4
Judges												
1	13	12	11	14	31	34	32	33	22	23	24	21
2	23	22	21	24	11	14	12	13	32	33	34	31
3	33	32	31	34	21	24	22	23	12	13	14	11
4	31	34	33	32	22	23	21	24	13	12	11	14
5	11	14	13	12	32	33	31	34	23	22	21	24
6	21	24	23	22	12	13	11	14	33	32	31	34

	Occasion 2											
Intervals	1				2				3			
Sittings	1	2	3	4	1	2	3	4	1	2	3	4
Judges												
1	24	21	22	23	31	33	32	34	11	13	12	14
2	14	11	12	13	21	23	22	24	31	33	32	34
3	34	31	32	33	11	13	12	14	21	23	22	24
4	33	32	31	34	13	11	14	12	24	22	23	21
5	23	22	21	24	33	31	34	32	14	12	13	11
6	13	12	11	14	23	21	24	22	34	32	33	31

using two 3×3 Latin square designs, one for judges 1–3 and the other for judges 4–6. Thus, for example, judge 1 examined plots from row 1 during interval 1 of the first occasion, plots from row 3 during interval 2, and from row 2 during interval 3. As a result, differences between judges and intervals could be eliminated from row differences. At each sitting judges 1–3 examined wines from one particular column and judges 4–6 examined wines from another column. Taking the 12 sittings from each occasion, the ordered pairs of columns allocated to the two sets of judges were chosen to ensure, firstly, that each possible ordered combination of two out of four columns occurred exactly once, and, secondly, that each judge examined a plot from every column during each interval. Thus, judge differences could be eliminated from column and row-column comparisons, and hence trellis differences; also, the amount of information on row-column comparisons, and hence trellis differences, remaining after sitting differences are eliminated is maximized. For clarity, table 5.9 shows the plan in unrandomized order; in reality there would be a random permutation of the numberings of the intervals within each occasion, the sittings within each interval, and the judges on each occasion. Likewise, for each judge-sitting combination, the positions (on the table) of the four glasses containing the two replicate wines from the two halfplots were also randomized. Appendix A.4 contains such a randomized plan together with a set of computer-generated scores. These scores are based on sum of a set of effects, each of which is generated from a normal distribution; the sum was then rounded to the nearest multiple of 0.5. This produces scores that take similar values to those that would be obtained in practice. It is presumed that their distribution is sufficiently close to being normal so that the analysis of variance is approximately valid.

The observational unit for the experiment is a glass of wine in a position at a sitting to be evaluated by an evaluator. The factors in the experiment are *Occasions*, *Intervals*, *Sittings*, *Judges*, *Positions*, *Rows*, *Squares*, *Columns*, *Halfplots*, *Trellis* and *Method*.

The structure set is derived as described in section 2.2.4. Three tiers are required for this experiment and the structure set based on these is as follows:

Tier	Structure
1	*((2 Occasions/3 Intervals/4 Sittings)∗6 Judges)/4 Positions*
2	*(3 Rows∗(2 Squares/4 Columns))/2 Halfplots*
3	*4 Trellis∗2 Method*

The structure derived from the factors in the first tier describes the underlying structure of the units (glasses of wine) of the evaluation phase and reflects the permutations to be employed (for example, intervals within occasions). The second gives the inherent structure of the units (halfplots) of the field phase and the third defines the structure of treatments applied in the field.

Assuming that the necessary assumptions hold for a joint analysis of the scores produced by the judges, the analysis of variance for the experiment, obtained using the rules given in section 2.2.4, would be as shown in table 5.10. The Hasse diagrams of term marginalities, used in obtaining the degrees of freedom of the terms in the analysis table as prescribed in table 2.2, are presented in figure 5.10.

A crucial aspect of this experiment is that, in both phases, it involves the randomization of factors such that terms derived from the same tier are confounded with different terms from lower tiers. The second crucial aspect is that a term derived from the third tier is nonorthogonal to terms from the second tier which are themselves nonorthogonal to terms derived from the first tier; efficiency factors for the nonorthogonal terms are given in table 5.11. The full decomposition for this example cannot be achieved with less than three structures.

Figure 5.10: Hasse diagram of term marginalities for an experiment requiring three tiers

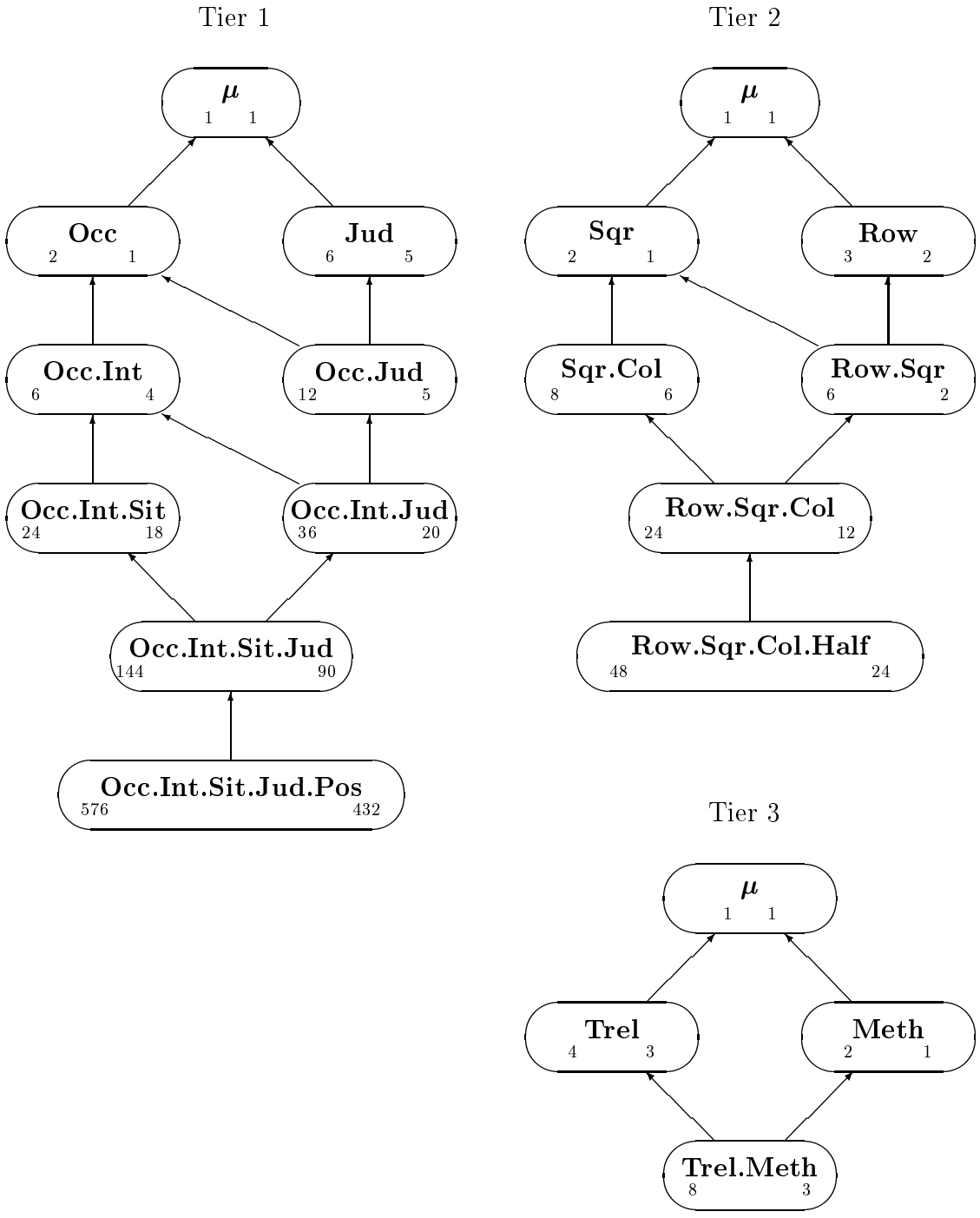


Table 5.10: Analysis of variance table for an experiment requiring three tiers

		VARIATION CONTRIBUTION TO EXPECTED MEAN SQUARES Coefficients of																
SOURCE	DF	ϕ_{OISJP}	ϕ_{OISJ}	ϕ_{OIJ}	ϕ_{OIS}	ϕ_{OJ}	ϕ_J	ϕ_{OI}	ϕ_O	ϕ_{RQCH}	ϕ_{RQC}	ϕ_{RQ}	ϕ_{QC}	ϕ_Q	ϕ_R	MSq	F	$\nu_1^\dagger$	$\nu_c^\dagger$
Occ	1																		
Sqr	1	1	4	16	48		24	96	288	12	24	96	72	288		1.0851	0.32	19.3	12.6
Occ.Int	4		1	4	16		24	96								3.8585	1.94	4.7	10.1
Occ.Int.Sit	18																		
Sqr.Col	6																		
Trel	3	1	4				24			4	8		24			1.1450			
Residual	3	1	4				24			4	8		24			1.2300	2.88	3.6	18.4
Residual	12	1	4				24									0.3524	1.07		
Jud	5		1	4	16	48	96									4.5924	0.43		
Occ.Jud	5		1	4	16	48										10.7549	5.97		
Occ.Int.Jud	20																		
Row	2	1	4	16						12	24	96		192		16.7192	19.68		
Row.Sqr	2	1	4	16						12	24	96				0.8494	0.55	3.8	9.9
Residual	16	1	4	16												1.8002	5.49		
Occ.Int.Sit.Jud	90																		
Sqr.Col	6																		
Trel	3	1	4							8	16		48			0.7037			
Residual	3	1	4							8	16		48			0.3867	1.15	3.0	19.3
Row.Sqr.Col	12																		
Trel	3	1	4							12	24					4.5600			
Residual	9	1	4							12	24					0.3386	0.93	40.9	51.6
Residual	72	1	4													0.3280	0.83		
Occ.Int.Sit.Jud.Pos	432																		
Row.Sqr.Col.Half	24																		
Meth	1	1								12						0.1111			
Trel.Meth	3	1								12						2.3323	5.10		
Residual	20	1								12						0.4571	1.16		
Residual	408	1														0.3943			
Total	575																		

†The numerator and denominator degrees of freedom, ν_1 and ν_2 respectively, for the F-ratios for which the degrees of freedom have to be computed using Satterthwaite's (1946) approximation as the F-ratios are the ratios of linear combinations of mean squares.

Table 5.11: Information summary for an experiment requiring three tiers

Sources	Efficiency
Occ.Int.Sit	
Sqr.Col	$\frac{1}{3}$
Trel	$\frac{1}{27}$
Occ.Int.Sit.Jud	
Sqr.Col	$\frac{2}{3}$
Trel	$\frac{2}{27}$
Row.Sqr.Col	
Trel	$\frac{8}{9}$

Assuming all factors in the experiment, except *Trellis* and *Method*, are to be designated as variation factors, the maximal models for this experiment, derived according to the rules given in table 2.5 and presuming the data are lexicographically ordered on *Occasions*, *Intervals*, *Sittings*, *Judges* and *Positions*, is as follows:

$$\begin{aligned} \mathrm{E}[\boldsymbol{y}] &= \boldsymbol{\mu}_{TM} \\ \mathrm{Var}[\boldsymbol{y}] &= \mathbf{V}_1 + \mathbf{V}_2 \end{aligned}$$

where

$$\begin{aligned} \mathbf{V}_1 = {} & \phi_G \mathbf{J} \otimes \mathbf{J} \otimes \mathbf{J} \otimes \mathbf{J} \otimes \mathbf{J} + \phi_O \mathbf{I} \otimes \mathbf{J} \otimes \mathbf{J} \otimes \mathbf{J} \otimes \mathbf{J} \\ & + \phi_{OI} \mathbf{I} \otimes \mathbf{I} \otimes \mathbf{J} \otimes \mathbf{J} \otimes \mathbf{J} + \phi_{OIS} \mathbf{I} \otimes \mathbf{I} \otimes \mathbf{I} \otimes \mathbf{J} \otimes \mathbf{J} \\ & + \phi_J \mathbf{J} \otimes \mathbf{J} \otimes \mathbf{J} \otimes \mathbf{I} \otimes \mathbf{J} + \phi_{OJ} \mathbf{I} \otimes \mathbf{J} \otimes \mathbf{J} \otimes \mathbf{I} \otimes \mathbf{J} \\ & + \phi_{OIJ} \mathbf{I} \otimes \mathbf{I} \otimes \mathbf{J} \otimes \mathbf{I} \otimes \mathbf{J} + \phi_{OISJ} \mathbf{I} \otimes \mathbf{I} \otimes \mathbf{I} \otimes \mathbf{I} \otimes \mathbf{J} \\ & + \phi_{OISJP} \mathbf{I} \otimes \mathbf{I} \otimes \mathbf{I} \otimes \mathbf{I} \otimes \mathbf{I}, \\ \mathbf{V}_2 = {} & \mathbf{U}_2 (\phi_R \mathbf{I} \otimes \mathbf{J} \otimes \mathbf{J} \otimes \mathbf{J} \otimes \mathbf{J} + \phi_Q \mathbf{J} \otimes \mathbf{I} \otimes \mathbf{J} \otimes \mathbf{J} \otimes \mathbf{J} \\ & + \phi_{QC} \mathbf{J} \otimes \mathbf{I} \otimes \mathbf{I} \otimes \mathbf{J} \otimes \mathbf{J} + \phi_{RQ} \mathbf{I} \otimes \mathbf{I} \otimes \mathbf{J} \otimes \mathbf{J} \otimes \mathbf{J} \\ & + \phi_{RQC} \mathbf{I} \otimes \mathbf{I} \otimes \mathbf{I} \otimes \mathbf{J} \otimes \mathbf{J} + \phi_{RQCH} \mathbf{I} \otimes \mathbf{I} \otimes \mathbf{I} \otimes \mathbf{I} \otimes \mathbf{J}) \mathbf{U}_2', \text{ and} \end{aligned}$$

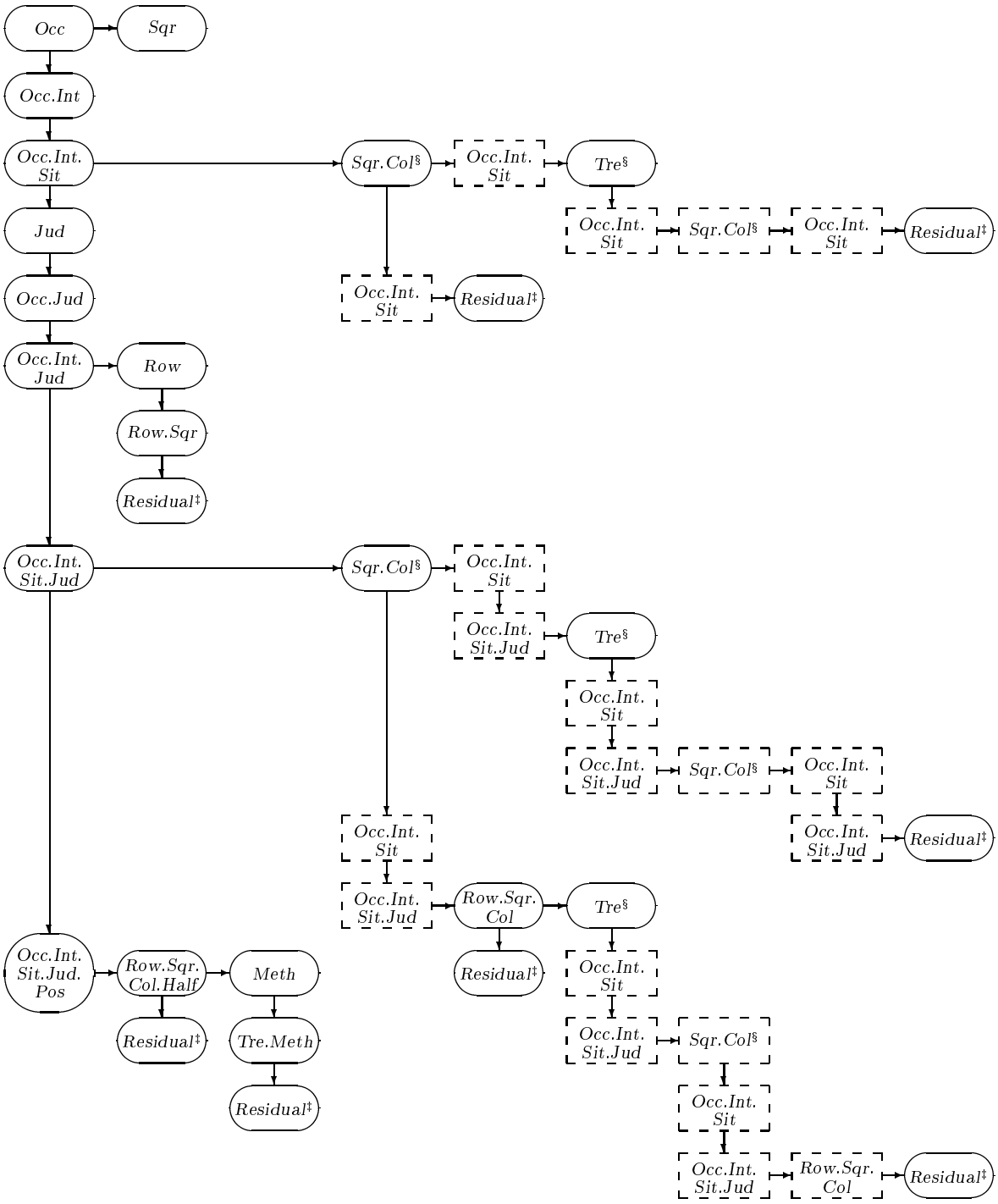
$\mathbf{U}_2$ is the permutation matrix of order 576 reflecting the assigning of the levels combinations of *Rows*, *Squares*, *Columns* and *Halfplots* to positions in which they were presented to each judge at each sitting in each interval on an occasion.

The steps set out in table 2.8 are used to obtain the contribution of this variation model to the expected mean squares which are given in table 5.10.

The minimal sweep sequence for performing the analysis is given in figure 5.11.

The analysis presented in table 5.10 indicates that the significant canonical covariance components are those for the terms *Occasions.Judges*, *Occasions.Intervals.Judges* and *Rows* and that there is an interaction between the factors *Trellis* and *Method*; because this interaction is significant no F-ratios for the main effects of *Trellis* and *Method* are presented.

Figure 5.11: Minimal sweep sequence for an experiment requiring three tiers†



†Lines originating below a term signify a residual sweep and lines originating alongside a term signify a pivotal sweep (section 3.3.1.1). Terms placed in dashed boxes signify a backsweep (section 3.3.1.1).

‡*Residual* does not involve a sweep but merely serves to indicate the origin of the residuals for a residual source.

§For this source effective means are calculated by dividing computed means by an efficiency factor which is given in table 5.11.

5.3 Superimposed experiments

Superimposed experiments are those in which an initial experiment is to be extended to include one or more extra randomized factors. They provide another type of experiment whose analysis is elucidated when the proposed method is utilized. However, the utilization of the steps given in chapter 2 will be left implicit.

Superimposed experiments provide further examples of experiments in which the division of the factors into two classes based on their randomization is inadequate. This is the case for superimposed experiments that involve a second randomization requiring knowledge of the results of the first randomization, such as those described by Preece, Bailey and Patterson (1978).

5.3.1 Conversion of a completely randomized design

One method of superimposing a new set of treatments on a completely randomized design (Preece *et al.*, 1978) is to randomize the new set of treatments within those plots receiving the same original treatment. The observational unit in this experiment is a plot. The factors are *Plots* and *Ftreats* from the original experiment and *Streats* from the modified experiment. The structure set and analysis of variance for such an experiment are given in table 5.12. It is most likely that *Plots* would be designated a variation factor and *Ftreats* and *Streats* expectation factors. Hence, the symbolic form of the maximal models for this experiment, derived according to the rules given in table 2.5, is as follows:

$$\begin{aligned} \mathrm{E}[Y] &= Ftreats + Streats \\ \mathrm{Var}[Y] &= G + Plots \end{aligned}$$

The expected mean squares under these models are given in table 5.12.

To obtain this analysis does not require the device of 'regarding the first set of treatments as a block factor' as is done by Preece *et al.* (1978). Furthermore, the analysis more accurately portrays the randomization that has occurred in the experiment. That *Streats* is indented under the *Residual* source for *Ftreats* indicates that,

Table 5.12: Structure set and analysis of variance table for a superimposed experiment based on a completely randomized design

STRUCTURE SET

Tier	Structure
1	*rt Plots*
2	*t Ftreats*
3	*r Streats*

ANALYSIS OF VARIANCE TABLE

SOURCE	DF	EXPECTED MEAN SQUARES
Plots	$rt-1$	
Ftreats	$t-1$	$\phi_P + f_F(\boldsymbol{\mu})$
Residual	$t(r-1)$	
Streats	$r-1$	$\phi_P + f_S(\boldsymbol{\mu})$
Residual	$(r-1)(t-1)$	ϕ_P
Total	$rt-1$	

in the second experiment, *Streats* was randomized to plots such that it is orthogonal to *Ftreats*.

5.3.2 Conversion of a randomized complete block design

To superimpose a new set of treatments on a randomized complete block design with t treatments in t blocks, take a $t \times t$ Latin square and label its rows with the *Blocks* labels of the first experiment and its columns using the original treatment labels (Preece *et al.*, 1978). The observational unit in this experiment is a plot. The factors are *Blocks*, *Plots* and *Ftreats* from the original experiment and *Streats* in the modified

Table 5.13: Structure set and analysis of variance table for a superimposed experiment based on a randomized complete block design

STRUCTURE SET

Tier	Structure
1	t *Blocks*/t *Plots*
2	t *Ftreats*
3	t *Streats*

ANALYSIS OF VARIANCE TABLE

SOURCE	DF	EXPECTED MEAN SQUARES Coefficients of ϕ_{BP}	ϕ_B	$\boldsymbol{\mu}$
Blocks	$t-1$	1	t	
Blocks.Plots	$t(t-1)$			
Ftreats	$t-1$	1		$f_F(\boldsymbol{\mu})$
Residual	$(t-1)^2$			
Streats	$t-1$	1		$f_S(\boldsymbol{\mu})$
Residual	$(t-1)(t-2)$	1		
Total	t^2-1			

experiment. The structure set and analysis of variance for such an experiment are given in table 5.13. *Blocks* and *Plots* will be classified as variation factors and *Ftreats* and *Streats* as expectation factors. Hence, the symbolic form of the maximal models for this experiment, derived according to the rules given in table 2.5, is as follows:

$$\begin{aligned} \mathrm{E}[Y] &= \mathit{Ftreats} + \mathit{Streats} \\ \mathrm{Var}[Y] &= G + \mathit{Blocks} + \mathit{Blocks.Plots} \end{aligned}$$

The expected mean squares under these models are given in table 5.13.

Comments similar to those made in the case of the superimposed experiment based on a completely randomized design apply here also. In particular, that *Streats* is indented under both *Blocks.Plots* and the *Residual* source for *Ftreats* indicates that, in the second experiment:

1. *Streats* was randomized to plots so that it is orthogonal to *Blocks* and *Ftreats*, and
2. *Streats* was confounded with *Blocks.Plots*.

5.3.3 Conversion of Latin square designs

Preece *et al.* (1978, section 5) give three methods of superimposing a new set of t treatments on a $t \times t$ Latin square. They are:

1. simultaneously randomize the first and second experiments by choosing any Graeco-Latin square and randomly permuting its rows and its columns;
2. take any Latin square orthogonal to that in the original experiment; permute the rows and columns of the second square in such a way that the original Latin square remains unchanged apart from a possible permutation of the letters; and
3. provided that the original Latin square is one of a complete set of mutually orthogonal Latin squares, choose at random any other member of the set; randomly allocate the second set of treatments to the letters of the second square.

In the first method, the two sets of treatments are randomized simultaneously, while in the last two they are randomized separately.

The analysis for a superimposed experiment, in which the treatments are randomized simultaneously, would follow that for a standard Graeco-Latin square. The observational unit for such an experiment is a row-column combination. The factors are *Rows*, *Columns*, *Ftreats* and *Streats*. The structure set and analysis of variance are given in table 5.14A.

Table 5.14: Structure set and analysis of variance table for superimposed experiments based on Latin square designs

A) SIMULTANEOUS RANDOMIZATION

B) SEPARATE RANDOMIZATION

STRUCTURE SETS

Tier	Structure
1	t *Rows*$*$$t$ *Columns*
2	t *Ftreats* + t *Streats*

Tier	Structure
1	t *Rows*$*$$t$ *Columns*
2	t *Ftreats*
3	t *Streats*

ANALYSIS OF VARIANCE TABLES

SOURCE	DF	EXPECTED MEAN SQUARES Coefficients of ϕ_{RC}	ϕ_C	ϕ_R	$\boldsymbol{\mu}$
Rows	$t-1$	1		t	
Columns	$t-1$	1	t		
Rows.Columns	$(t-1)^2$				
Ftreats	$t-1$	1			$f_F(\boldsymbol{\mu})$
Streats	$t-1$	1			$f_S(\boldsymbol{\mu})$
Residual	$(t-1)(t-3)$	1			
Total	t^2-1				

SOURCE	DF	EXPECTED MEAN SQUARES Coefficients of ϕ_{RC}	ϕ_C	ϕ_R	$\boldsymbol{\mu}$
Rows	$t-1$	1		t	
Columns	$t-1$	1	t		
Rows.Columns	$(t-1)^2$				
Ftreats	$t-1$	1			$f_F(\boldsymbol{\mu})$
Residual	$(t-1)(t-2)$				
Streats	$t-1$	1			$f_S(\boldsymbol{\mu})$
Residual	$(t-1)(t-3)$	1			
Total	t^2-1				

The model-based analysis of superimposed experiments, in which the treatments are randomized separately, is the same irrespective of the method used. The observational unit for such an experiment is a row-column combination. The factors are *Rows*, *Columns* and *Ftreats* from the original experiment and *Streats* in the modified experiment. The structure set and analysis of variance for such an experiment are given in table 5.14B. This is different to the situation for a randomization-based analysis where the appropriate analysis may be different for the two methods (Preece *et al.*, 1978 and Bailey, 1991).

For all methods of randomization, the *Rows* and *Columns* will be classified as variation factors and *Ftreats* and *Streats* as expectation factors. Hence, the symbolic form of the maximal models for this experiment, derived according to the rules given in table 2.5, is as follows:

$$\begin{aligned} \mathrm{E}[Y] &= Ftreats + Streats \\ \mathrm{Var}[Y] &= G + Rows + Columns + Rows.Columns \end{aligned}$$

The expected mean squares under these models are given in table 5.14.

The analysis for the experiments involving separate randomization is similar to that for the other such superimposed experiments in that *Streats* is confounded with a *Residual* source, namely that for *Rows.Columns*. From this, it is concluded that:

1. *Streats* was randomized to row-column combinations so that it is orthogonal to *Rows*, *Columns* and *Ftreats*, and
2. *Streats* is confounded with *Rows.Columns*.

5.4 Single-stage experiments

Both two-phase (section 5.2) and superimposed (section 5.3) experiments involve two stages in their experimentation and it might therefore be supposed that multiple stages characterize multitiered experiments. However, this is not so and in this section we present examples of single-stage experiments that are three-tiered. Again, the utilization of the steps presented in chapter 2 will be left implicit.

5.4.1 Plant experiments

Suppose an experiment has been conducted to investigate differences in first-year growth between six Eucalyptus species when the plots on which they have been planted are prepared using three different methods. There are five blocks of land available for the experiment and each block of land has 18 plots. Thus there are three plants of each species in a block. The three methods of plot preparation are assigned at random to the three plots containing the same species. All told, there are 15 plants of each species used in the experiment and these are allocated, one to a plot, at random. The observational unit is a plot and the factors in the experiment are *Blocks*, *Plots*, *Species*, *Plants*, and *Methods*. The factors *Blocks*, *Plots* and *Plants* will be designated variation factors and *Species* and *Methods* expectation factors.

In respect of the tiers, *Blocks* and *Plots* are the factors that would index the observational units if no randomization had been performed and so they form the bottom tier of unrandomized factors. Next, the factors *Species* and *Plants* were randomized to the observational units and these form the second tier. As *Methods* is randomized to the plants within a blocks-species combination, the species on a particular plot must be known prior to randomizing *Methods*. As a result, *Methods* must be in the third tier.

The structure set, derived from the tiers as described in section 2.2.4, is given in table 5.15. To obtain the correct degrees of freedom for all terms, it is necessary to specify that *Sets* is a pseudoterm to *Species.Plants*. This reflects the assignment of different sets of plants to the different blocks. Also, *Species* is included in the third tier because of the interest in its interaction with *Methods*.

The analysis of variance table, derived as described in table 2.1, is given in table 5.15. This table makes it clear that *Species* and *Methods* are both confounded with *Blocks.Plots*.

It is likely that *Blocks*, *Plots* and *Plants* will be classified as variation factors and *Species* and *Methods* as expectation factors. Hence, the symbolic forms of the maximal models for this experiment, derived according to the rules given in table 2.5,

Table 5.15: Structure set and analysis of variance table for a three-tiered plant experiment

STRUCTURE SET

Tier	Structure
1	*5 Blocks/18 Plots*
2	*(6 Species/15 Plants)//5 Sets*
3	*3 Methods∗Species*

ANALYSIS OF VARIANCE TABLE

SOURCE	DF	EXPECTED MEAN SQUARES Coefficients of ϕ_{BP}	ϕ_B	ϕ_{SP}	$\boldsymbol{\mu}$
Blocks					
Species.Plants	4	1	18	1	
Blocks.Plots	85				
Species	5	1		1	$f_S(\boldsymbol{\mu})$
Species.Plants	80				
Methods	3	1		1	$f_M(\boldsymbol{\mu})$
Methods.Species	15	1		1	$f_{MS}(\boldsymbol{\mu})$
Residual	62	1		1	
Total	89				

are as follows:

$$\begin{aligned} \mathrm{E}[Y] &= \mathit{Methods.Species} \\ \mathrm{Var}[Y] &= G + \mathit{Blocks} + \mathit{Blocks.Plots} + \mathit{Species.Plants} \end{aligned}$$

The expected mean squares under these models are given in table 5.15.

A point that arises in connection with this experiment is the inclusion of the factor *Plants* which is nested within *Species*. It is required to fully describe the randomiza-

tion that occurred in this experiment. However, in many experiments such as this, this factor is ignored. Most often, the levels combinations of the factors *Species* and *Methods* would be randomized to the levels combinations of *Plots* within *Blocks*; there would be no specific allocation of plants of different species. However, the disadvantage of this is that *Methods* differences are not protected by randomization from systematic differences between *Plants* of the same species. Further, from the analysis table presented in table 5.15, it is evident that the sources *Blocks* and *Species.Plants* confounded with *Blocks* are associated with the same subspace of the sample space. Thus there are two type of variability, namely experimental unit variability and treatment error (section 6.6.2), contributing to this subspace.

5.4.2 Animal experiments

Animal experiments, although not two-phase experiments, represent a group of commonly occurring three-tiered experiments. This is because they typically involve animals, units to which animals are assigned and treatments.

For example, consider a sheep experiment conducted to investigate the effects of four levels of pasture availability and four stocking rates on the intake of herbage. [This example is a simplified version of an experiment reported by Whittaker (1965).] These treatment combinations were randomized according to a randomized complete block design to the 16 plots in each of four blocks. The size of the plots was adjusted so that the correct stocking rate would be obtained if four sheep were assigned to the plot. Thus, there were altogether 256 sheep required for the experiment and these were divided into 4 groups of 64 according to body weight; 64 flocks of four sheep were then formed by selecting four sheep from the same body weight class, the four sheep from a body weight class being selected so that the different flocks from the same body weight class had as similar weights as possible. The flocks were then assigned at random to the plots so that all flocks from the same body weight class were in the same block. The weight gain of each sheep over the period of the experiment was determined, as was the pasture production of each plot. The latter was measured as the dry weight of clippings produced in an enclosed area.

Table 5.16: Structure set and analysis of variance table for a grazing experiment

STRUCTURE SET

Tier	Structure
1	*4 Classes/16 Flocks/4 Sheep*
2	*4 Blocks/16 Plots*
3	*4 Avail*4 Rate*

ANALYSIS OF VARIANCE TABLE

SOURCE	DF	EXPECTED MEAN SQUARES Coefficients of ϕ_{CFS}	$\phi_{CF}+\phi_{BP}$	ϕ_B	$\boldsymbol{\mu}$
Classes	3				
Blocks	3	1	4	64	$f_C(\boldsymbol{\mu})$
Classes.Flocks	60				
Blocks.Plots	60				
Avail	3	1	4		$f_A(\boldsymbol{\mu})$
Rate	3	1	4		$f_R(\boldsymbol{\mu})$
Avail.Rate	9	1	4		$f_{AR}(\boldsymbol{\mu})$
Residual	45	1	4		
Classes.Flocks.Sheep	192	1			
Total	255				

The observational unit in respect of the weight gain measurements is a sheep. The factors in the experiment are *Classes*, *Sheep*, *Flocks*, *Blocks*, *Plots*, *Avail* and *Rate*. In determining the structure set for this study, it will be assumed that *Classes* is independent of *Avail* and *Rate*; it is necessary to assume at least that the three factor interaction between them is zero, otherwise there would be no *Blocks.Plots Residual*. The structure set for the study and analysis of variance table are shown in table 5.16.

The factors *Sheep*, *Flocks*, *Blocks* and *Plots* will be designated variation factors and *Classes*, *Avail* and *Rate* expectation factors. Hence, the symbolic forms of the maximal models for this experiment, derived according to the rules given in table 2.5, are as follows:

$$\begin{aligned} \mathrm{E}[Y] &= \mathit{Classes} + \mathit{Avail.Rate} \\ \mathrm{Var}[Y] &= G + \mathit{Blocks} + \mathit{Blocks.Plots} + \mathit{Classes.Flocks} + \mathit{Classes.Flocks.Sheep} \end{aligned}$$

The expected mean squares under these models are given in table 5.16.

A particular problem that arises in these experiments is that one often has insufficient animals to enable one to replicate the treatments as described in the above experiment (Conniffe, 1976; Blight and Pepper, 1984). Thus we may have several flocks of sheep assigned to plots to which treatments are also assigned. The revised experimental structure set and analysis of variance table would then be as given in table 5.17. The revised models are:

$$\begin{aligned} \mathrm{E}[Y] &= \mathit{Avail.Rate} \\ \mathrm{Var}[Y] &= G + \mathit{Plots} + \mathit{Flocks} + \mathit{Flocks.Sheep} \end{aligned}$$

The expected mean squares under these models are given in table 5.17.

It is clear from this table that there is no test available for *Availability* and *Rate* differences without assuming that both *Flocks* and *Plots* canonical covariance components are zero; that is, that the covariance of observations with the same *Flocks* (*Plots*) level is now the same as the covariance of observations with different *Flocks* (*Plots*) levels. The use of the proposed method displays the problem in such a manner that its essence is readily appreciated. The problem of determining the experimental unit, which greatly perplexed Blight and Pepper (1984), is avoided. The application

Table 5.17: Structure set and analysis of variance table for the revised grazing experiment

STRUCTURE SET

Tier	Structure
1	*16 Flocks/4 Sheep*
2	*16 Plots*
3	*4 Avail*4 Rate*

ANALYSIS OF VARIANCE TABLE

SOURCE	DF	EXPECTED MEAN SQUARES Coefficients of ϕ_{FS}	$\phi_F + \phi_P$	$\boldsymbol{\mu}$
Flocks	15			
Plots	15			
Avail	3	1	4	$f_A(\boldsymbol{\mu})$
Rate	3	1	4	$f_R(\boldsymbol{\mu})$
Avail.Rate	9	1	4	$f_{AR}(\boldsymbol{\mu})$
Flocks.Sheep	48	1		
Total	63			

of the method, which is based on determining the observational unit, will reveal the confounding relationships between sources.

The analyses I have described are for the weight gain of the individual sheep; that is, the observational unit is a sheep. If one wanted to analyse measurements taken on the plots in the original experiment, pasture production for example, then the structure set for the study would be as follows:

Tier	Structure
1	*4 Blocks/16 Plots*
2	*4 Classes/16 Flocks*
3	*4 Avail∗4 Rate*

While there is no doubt about the composition of the three tiers given above, there is uncertainty about the order of the tiers I have nominated as the second and third tiers. This is because the levels combinations of the factors in both the second and third tiers were randomized to the levels combinations of the factors in the first tier. The order given seems reasonable on the grounds that:

1. together *Classes* and *Flocks* uniquely index the observational units, whereas *Avail* and *Rate* do not; and
2. *Avail* and *Rate* have been designated expectation factors whereas *Flocks* has been designated a variation factor.

Further examples of three-tiered animal experiments are provided by the chick experiment described by John and Quenouille (1977, section 4.9) and the pig experiment described by Free (1977). Both of these experiments involve assigning animals and treatments to cages/pens. The second experiment described in section 6.6.1 is also a three-tiered animal experiment.

5.4.3 Split plots in a row-and-column design

Federer (1975, example 5.1) presents an experiment in which the split plots are arranged in a row-and-column design. It is another example that requires three tiers to adequately represent its randomization. The experiment consists of three whole plot treatments (C) arranged in a randomized complete block design having five blocks. There are four split-plot treatments (D) arranged in a four-row by five-column design. Different rectangles are used for each whole-plot treatment. For each rectangle, the columns are randomized to blocks and the rows of the rectangle randomized to the rows of the subplots for each C treatment. The experimental layout is shown in

table 5.18. The experiment is unusual in that the subplot treatments are randomized within the levels of the whole-plot treatments.

Table 5.18: Experimental layout for a split-plot experiment with split plots arranged in a row-and-column design (Federer, 1975)

c_2	c_1	c_3	c_1	c_3	c_2	c_2	c_3	c_1	c_2	c_1	c_3	c_3	c_2	c_1
d_2	d_3	d_1	d_4	d_1	d_3	d_4	d_4	d_1	d_1	d_1	d_2	d_3	d_1	d_2
d_4	d_4	d_3	d_1	d_2	d_2	d_1	d_2	d_2	d_4	d_4	d_4	d_1	d_3	d_3
d_3	d_2	d_4	d_3	d_3	d_1	d_2	d_1	d_4	d_3	d_3	d_3	d_2	d_4	d_1
d_1	d_1	d_2	d_2	d_4	d_4	d_3	d_3	d_3	d_2	d_2	d_1	d_4	d_2	d_4

The observational unit for the experiment is a row within a plot. The unrandomized factors in the experiment are *Blocks*, *Plots* and *Rows*; C and D are the randomized factors. However, the levels of C must be known, before the levels of D can be assigned to the observational units. That is, there are two classes of randomized factors, and hence three classes or tiers for the experiment. The tiers are: {*Block, Plots, Rows*}, $\{C\}$ and $\{D\}$. The structure set for the study is given below and the analysis table is given in table 5.19. Note that the structure for the second tier involves both *Blocks* and *Rows* as these two factors were taken into account in randomizing D.

Because the rows of the row-and-column design are randomized within each whole-plot treatment, it is not appropriate to include the *Rows* and *Rows.Blocks* terms in the specification. Any meaningful connection between rows within a block is nullified by the randomization. However,subplots must, in actual fact, be connected across whole plots because all the subplots in a single row have the same chance of being included in the row of subplots within any one whole plot treatment. The restrictions on randomization have made it possible to estimate the *C.Rows* term (*Rows* nested within C), which will eliminate any overall *Rows* effects.

To determine the maximal expectation and variation models for the experiment, it will be assumed that *Blocks*, *Plots* and*Rows* contribute to the variation and that C

Table 5.19: Structure set and analysis of variance table for a split-plot experiment with split plots arranged in a row-and-column design (Federer, 1975)

STRUCTURE SET

Tier	Structure
1	*5 Blocks/3 Plots/4 Rows*
2	*Blocks*(3 C/Rows)*
3	*C*4 D*

ANALYSIS OF VARIANCE TABLE

SOURCE	DF	EXPECTED MEAN SQUARES Coefficients of ϕ_{BPR}	ϕ_{BP}	ϕ_B	ϕ_{BCR}	ϕ_{CR}	ϕ_{BC}	$\boldsymbol{\mu}$
Blocks	4	1	4	12	1			
Blocks.Plots	10							
C	2	1	4		1	5	4	$f_C(\boldsymbol{\mu})$
Blocks.C	8	1	4		1		4	
Blocks.Plots.Rows	45							
C.Rows	9							
$D^\dagger$	3	1			1	5		$f_D^1(\boldsymbol{\mu})$
$C.D^\dagger$	6	1			1	5		$f_{CD}^1(\boldsymbol{\mu})$
Blocks.C.Rows	36							
$D^\dagger$	3	1			1			$f_D^2(\boldsymbol{\mu})$
$C.D^\dagger$	6	1			1			$f_{CD}^2(\boldsymbol{\mu})$
Residual	27	1						

†The nonorthogonal terms D and $C.D$ are confounded with *C.Rows* with efficiency 0.04 and with *Blocks.C.Rows* with efficiency 0.96.

Table 5.20: Information summary for a split-plot experiment with split plots arranged in a row-and-column design (Federer, 1975)

Sources	Efficiency
C.Rows	
D	0.04
C.D	0.04
Blocks.C.Rows	
D	0.96
C.D	0.96

and D contribute to the expectation. Thus, the symbolic form of the maximal models for this experiment, derived according to the rules given in table 2.5, is as follows:

$$\begin{aligned} \mathrm{E}[Y] &= C.D \\ \mathrm{Var}[Y] &= G + Blocks + Blocks.Plots + Blocks.Plots.Rows \\ &\quad + Blocks.C + C.Rows + Blocks.C.Rows \end{aligned}$$

The expected mean squares under this model, derived as described in table 2.8, are also as given in table 5.19. The analysis presented in table 5.19 is the same as that presented by Federer (1975) except that D and $C.D$ are estimated from two sources and that it is seen that the expected mean square for C involves ϕ_{CR} so that tests will have to involve *C.Rows*.

Chapter 6

Problems resolved by the present approach

In section 1.4, I specified a number of issues that would need to be dealt with adequately if a strategy for factorial linear model analysis is to be adjudged as satisfactory. In this chapter, I address the manner in which the method presented in this thesis deals with each of these issues. An earlier version of much of this material is contained in Brien (1989) which is reproduced in appendix C. I believe that the insights outlined below demonstrate that the view of analysis of variance provided by the approach is useful. It provides a paradigm for the analysis of a wide range of studies and clarifies a number of issues.

6.1 Extent of the method

As prescribed in section 2.2.5 and provided the assumptions underlying the analysis are met, the approach as outlined in this thesis is applicable to randomized experiments and unrandomized studies — unrandomized experiments, purely observational studies and sample surveys (Cox and Snell, 1981) — in which:

1. there is a term in each structure, the maximal term for the structure, to which every other term in that structure is marginal,

2. any two terms from the same structure are orthogonal in the sense that the orthogonal complements, in their model spaces, of their intersection subspace are orthogonal (Wilkinson, 1970; Tjur, 1984, section 3.2);
3. the set of terms in each structure is closed under the formation of minima;
4. the structures in which there are variation terms are regular;
5. the maximal term for Tier 1 uniquely indexes the observational units;
6. expectation and variation factors are randomized only to variation factors; and
7. terms in the analysis satisfy the requirements for structure balance as outlined in section 3.3.1.

All structures in the study must satisfy the first three of the above conditions and hence must be Tjur structures; some of the structures must also satisfy some of the other conditions.

It is clear that the proposed framework covers multiple-error experiments, including multitiered experiments, and may include intertier interactions. The structure-balance condition above can be relaxed to become: the terms in the study must exhibit structure balance after those involving only expectation factors have been omitted. Thus, the approach outlined can also be employed with experiments whose expectation terms exhibit first-order balance such as the carry-over experiment of section 4.3.2.4, or those with completely nonorthogonal expectation models such as the two-factor completely randomized design with unequal replication presented in section 4.2.2.

While nonorthogonal expectation factors can be dealt with, the ability to deal with nonorthogonality between variation factors is limited to situations in which the terms derived from the structures from different tiers are at least structure balanced. The limitations presented here, such as the inability to deal with nonorthogonality between variation terms arising in the same tier and irregular variation terms, would appear to be limitations of this calculus, rather than of the approach's broad philosophy.

Chapters 2 and 3 contain a set of rules that provides a calculus for obtaining the expected mean squares, given the division of the factors into tiers and the expecta-

tion/variation dichotomy, for the entire range of studies outlined here.

6.2 The basis for inference

The approach put forward in this thesis is a model comparison approach to linear model analysis; inference is via the analysis-of-variance method and so is a least squares procedure. The terms in the models are those found in the accompanying analysis of variance table, these having been derived from the randomization-based tiers.

The use of model-based versus randomization-based inference is discussed in section 1.3. Our emphasis on general linear models derives from the philosophy propounded by Fisher (1935, 1966, section 21.1; 1956) and Yates (1965). They suggest that the aim of the analysis should be to use one's knowledge of the situation to formulate a realistic, parsimonious model. As a result the analysis will be more efficient because it incorporates more of the investigator's knowledge. Their view, with which we have much sympathy, is that the role of the randomization test is secondary to model-based tests. It is used to confirm the robustness of model-based tests to departures from normality.

Further motivation for using model-based analysis is that, not uncommonly, situations arise in which scientifically interesting questions cannot be addressed by a randomization test. Some examples are tests to determine the relative magnitudes of various canonical covariance components, tests involving randomized variation factors, and tests to determine whether certain intertier interactions have to be taken into account in inferences from the experiment (section 6.7). Another example is that described by Yates (1965) and Harville (1975) where supplementary information becomes available and needs to be taken into account by, for example, analysis of covariance.

In particular, it is often asserted that in using the analysis of variance to analyse experiments one must make the assumption of intertier additivity. This will clearly be the case if randomization analysis is being employed as this assumption is essential to it. However, there are situations in which it is desirable, where possible, to include

intertier interactions in models. The sensory experiment (section 4.2.1) provides an example in which an intertier interaction should be included in the maximal variation model as one of them ($A.B.E$) is significant; others ($A.E$) may have been. Nearly all the examples in section 4.3.2 provide further instances where intertier interactions are involved.

While randomization does provide support for the robustness of model-based tests, this is not its primary role in the proposed approach. Here, its major roles are:

- to hold the investigator's view of the material under investigation; this is used at the model identification stage to assist in determining the models, and hence the form of the analysis of variance table; and
- to provide insurance against bias in the allocation process and, hence, against the formulation of an inadequate model.

As far as determining the models is concerned, the aspects of the randomization that are relevant are the sets of factors involved in the randomization and the restrictions placed on randomization. These aspects contain important information about how the experimenter viewed the factors in the experiment. In particular, which terms are likely to contribute to differences between the observational units. Thus, if one wishes to ensure that the relevant physical features of the study are taken into account in the models used for it, then the models should reflect the randomization that was carried out. The proposed paradigm ensures that the models reflect it by deriving the models from the randomization-based tiers. The manner in which it does this is summarized in the analysis of variance table, in the form of the particular sources that end up being included and the confounding relationships between them.

As suggested above, a second role for randomization is in providing insurance against bias in the allocation process. In particular, it affords some justification for concluding that differences associated with terms consisting only of randomized factors are not the result of the terms to which they are randomized. Thus, while Harville (1975) explains how randomization can be dispensed with, I agree with Kempthorne (1977) that it is useful as an insurance against model inadequacy. An investigation of the analysis of unrandomized studies illustrates this point.

Consider an observational study planned to investigate the effect of treatment on blood cholesterol by observing patients and recording whether they smoke tobacco and measuring their blood cholesterol. A general feature of such studies, relevant to model identification, is that all the factors will be unrandomized so that only a single structure is required to describe the study. Thus, the only dichotomy required for this stage is the expectation/variation dichotomy. In the example, the unrandomized structure, determined as described in section 2.2.4, is *2 Smoking/p Patients*. Further, suppose *Smoking* is designated to be an expectation factor and *Patients* a variation factor. The analysis of variance table, based on this grouping of factors and derived as prescribed in chapter 2, is given in table 6.1A. Model selection is trivial for this example.

Table 6.1: Analysis of variance for an observational study

A) UNRANDOMIZED ANALYSIS		B) QUASIRANDOMIZED ANALYSIS	
SOURCE	EXPECTED MEAN SQUARES	SOURCE	EXPECTED MEAN SQUARES
Smoking	$\phi_{SP} + f_S(\boldsymbol{\mu})$	*Patients*	
		Smoking	$\phi_P + f_S(\boldsymbol{\mu})^\dagger$
Smoking.Patients	ϕ_{SP}	*Residual*	ϕ_P

$^\dagger f(\boldsymbol{\mu}_S) = p(\mu_1 - \mu_2)^2/2$ where μ_i is the expectation for the ith *Smoking* level.

If, on the other hand, smoking was to be regarded as having been randomized to patients, the structure set would be:

Tier	Structure
1	*2p Patients*
2	*2 Smoking*

The analysis of variance table, based on this structure set and the expectation/-variation dichotomy as before, is given in table 6.1. The sum of squares for the *Residual* in this analysis is the same as that for *Smoking.Patients* from the previous analysis and the *Smoking* sums of squares in the two analyses are equal. The essential difference between the two analyses is that, in the unrandomized analysis, *Smoking* is marginal to *Smoking.Patients*, whereas, in the quasirandomized analysis, *Smoking* is confounded with *Patients*.

The form of the analysis for the unrandomized example symbolizes the fact that grouping of the patients according to smoking behaviour cannot be considered arbitrary as there is a substantial probability of systematic differences between groups irrespective of the effects of smoking. That is, patients are nested within smoking and there are recognizable subsets of patients. A comparison, at model testing, of the *Smoking* and *Smoking.Patients* mean squares from this analysis investigates the question 'Are differences between patients from different smoking groups greater than within group differences?'. That is, the question does not address the cause of the difference between the groups, which, as has already been recognized, may not be due to smoking differences.

However, it is conceivable that there is interest in regarding smoking as having been randomized to patients, which amounts to regarding groupings of the patients according to smoking as arbitrary. The form of the analysis in this case incorporates the assumption of arbitrary grouping of patients according to *Smoking* as there is no factor nesting *Patients*.

Associated with the difference in arbitrariness, and hence forms of the analyses, is a difference between the questions examined by equivalent mean square comparisons from the two analyses. A comparison of the *Smoking* and *Residual* mean squares in the second analysis, where groupings are arbitrary, examines the question 'Has smoking caused differences greater than can be expected from patient differences?'. Clearly, the crucial difference is that one is able to draw causal inferences when groupings according to smoking can be regarded as arbitrary.

It is a matter for those expert in the subject area in which the study is set as to whether or not groupings can be considered arbitrary and, hence, which analysis is

appropriate. However, to regard them as arbitrary in this instance is somewhat more dangerous than in randomized experiments. In randomized experiments, randomization provides an objective mechanism which makes it more likely (and, indeed, it is routinely assumed) that groupings based on randomized factors are arbitrary. Thus, in the sensory example (section 4.2.1), inferences about batches are unlikely to be affected by systematic position differences.

So randomization does have a role, albeit restricted, to play in model-based analysis and it is important that the full details of the randomization employed are accurately recorded when the study is reported.

6.3 Factor categorizations

It has been asserted herein that the division of the factors into tiers and the expectation/variation dichotomy are the factor categorizations fundamental to model identification. The division of the factors into tiers generates a structure set for a study which, as Brien (1983) argues, is based on the factor relationships and incidences arising from the design used in the study and the assumptions made about the occurrence of terms (section 2.2.4). As such it leads to an inventory of the identifiable, physical features of the study that might affect the response, just what is required given the class of models under consideration. The expectation/variation dichotomy specifies the parameters of the distribution through which the factors affect the response. In this it is driven by subject matter considerations, namely, the type of inference desired and the parameters thought best to reflect the anticipated behaviour of the factors. The predictive/standardizing dichotomy is central to prediction.

Other commonly used dichotomies are the fixed/random and block/treatment dichotomies. It is argued below that the fixed/random dichotomy has no role to play in linear model analysis, although it should be considered in determining the relevant population for inferences. Further, it will be suggested that the division of the factors into tiers, and the accompanying unrandomized/randomized dichotomy, is a more satisfactory nomenclature than block/treatment dichotomy.

From the discussion in section 1.2.2, it would appear that the consensus among authors is that fixed factors are those for which the levels of the factor represent a complete sample of the levels about which inferences are to be drawn. Random factors are those which represent an incomplete sample of the levels of interest. The terms fixed/random are often taken to be identical to expectation/variation, possibly because it is usual to parametrize effects arising from only fixed factors in terms of expectation and those involving random factors in terms of variation. That is, the difference between expectation/variation factors in parametrization parallels the difference between fixed/random. However, as outlined here, there is clearly a distinction between the bases of the two dichotomies.

The fixed/random dichotomy is synonymous with complete/incomplete sampling. Thus, for the sensory example presented in section 4.2.1, the random factors are *Occasion*, *Evaluator* and *Batch*; the fixed factors are *Area* and *Position*. This grouping of the factors is different to that given in section 4.2.1 for the expectation/variation dichotomy. The implication of this is that the maximal expectation and variation models will differ between the two groupings.

The basis of the expectation/variation dichotomy is whether or not the terms arising from a factor display symmetry but this is not the basis of the fixed/random dichotomy. While some statisticians may base the fixed/random dichotomy on this distinction and the fixed/random dichotomy could be suitably redefined on this basis, I advocate the adoption of the expectation/variation dichotomy to avoid the potential double-usage inherent in redefinition. In any case as Yates (1965) points out, the fixed/random dichotomy, as defined here, does have a role to play in considering 'the relevant population for inferences'. It needs to be retained for this purpose. However, as suggested in section 1.2.2.3, it has no part to play in determining models where the variation is parametrized in terms of canonical covariance components; that is, it is superfluous in determining the analysis table and the expected mean squares based on canonical components. These are determined by the division of the factors into tiers and the expectation/variation dichotomy.

As discussed in section 1.2.1.2, the distinction between block and treatment factors is considered by many statisticians to be fundamental to determining the appropriate

analysis of variance for a particular experiment. However, it was also pointed out that the basis for classifying the factors has not usually been spelt out as it is taken to be intuitively obvious. It was suggested that this is not always the case, especially in animal, psychological and industrial experiments, and that in the literature this problem typically arises in the form 'Is *Sex* a block or a treatment factor?' (for example, Preece, 1982, section 6.2). The sensory example presented in section 4.2.1 provides a further instance of the problem in that some confusion is likely to surround the classification of the factor *Batch*; the issue also arises in connection with experiments involving a *Time* factor such as those discussed in section 4.3.2 involving the factor *Years*.

Further, there has been some divergence between authors in their usage of the terms. As argued in section 1.2.1.2, it would appear that Nelder (1965a, 1977) and Bailey (1981, 1982a) intended that the distinction corresponds to the unrandomized/-randomized dichotomy (see also Bailey, 1985). Thus, these authors would see block factors as corresponding to what I have called unrandomized factors. On the other hand, Houtman and Speed (1983) and Tjur (1984) seem to regard the distinction as corresponding to the expectation/variation dichotomy, with block factors corresponding to variation factors.

In the context of randomization analysis, the unrandomized/randomized and expectation/variation (under randomization) dichotomies are equivalent for two-tiered experiments and it is irrelevant to consider to which dichotomy the block/treatment dichotomy is equivalent. All three dichotomies are equivalent.

However, in linear model-based analysis of two-tiered experiments, the expectation/variation and unrandomized/randomized dichotomies are not always equivalent; they are not in the sensory example presented in section 4.2.1 nor are they in situations described by Nelder (1977, section 2.3). To equate the expectation/variation dichotomy to the unrandomized/randomized dichotomy will, in such instances, result in inappropriate tests of hypotheses or estimates of standard errors since, as we shall see, these depend on the former dichotomy. To dispense with the unrandomized/randomized dichotomy, and generate separate structures for the expectation and variation factors, is to shift the focus away from the central issue of identifying the physical

sources of differences taken into account by the investigator. The result of this will be an inaccurate description of the pertinent physical features of the study and there is a risk that not all relevant sources will be identified. That is, as Fisher (1935, 1966) began pointing out, the analysis must reflect what was actually done in the study, or at least what was intended to be done. A more detailed examination of this matter is not possible here, but some insight can be gained by considering the problems which arise in generating the structure set for the sensory example (section 4.2.1) from its expectation/variation partition.

In linear model-based analysis for two-tiered experiments, it seems that the block/-treatment dichotomy most naturally corresponds to the unrandomized/randomized dichotomy; indeed, it could be argued that the usage of the terms block/treatment, suitably defined, be substituted for unrandomized/randomized. I recommend against this as the latter terms embody the operational basis of the distinction between the two types of factors. The failure of the former terms to do this has perhaps led to the divergence of usage in the literature mentioned above and is likely to be perpetuated if continued. For example, calling *Batch* a treatment factor appears incongruous; however, it is a randomized factor and so, as outlined in section 6.2, there is some justification for assuming that there are no systematic position differences affecting differences between batches.

Neither nomenclature is entirely adequate for three-tiered experiments (chapter 5; Brien, 1983), such as the two-phase experiments of McIntyre (1955), and to refer to the sets of factors as tiers 1, 2 and 3 avoids the problem. Although the sets might be referred to as unrandomized$_2$/unrandomized$_1$/randomized for two-phase experiments, with the subscripts referring to the phase (section 5.2), there are experiments for which the appropriate designation would appear to be unrandomized/randomized$_2$/randomized$_1$ (sections 5.3 and 5.4).

In respect of the question 'Is *Sex* a block or treatment factor?', the answer is clearly that there is no universal prescription; it will be a randomized factor when individuals of different sexes are randomized to the observational units and an unrandomized factor when the observational units consist of individuals of different sexes. In the latter case, it is likely that there would be interest in interactions between the unrandom-

ized factor *Sex* and the randomized factors (as in the example of section 4.3.2.3). The examples discussed in section 4.3.2 also demonstrate that a factor may in one instance be a randomized factor, yet in a superficially similar experiment be an unrandomized factor; compare the times-randomized (-and-sites-unrandomized) experiments (section 4.3.2.1) with the repetitions-in-time (-and-space) experiments (section 4.3.2.2). The use of the structure set for determining the analysis in these cases results in analyses that reflect differences in the procedures employed in them (section 6.6.1) and as a result differ, at least in type of variability (section 6.6.2) involved and perhaps in the partitioning of the *Total* sum of squares.

6.4 Model composition and the role of parameter constraints

In respect of expectation model selection, the proposed approach is a model comparison, rather than a parametric interpretation, approach (see section 1.2.2). However, it differs from the usual model comparison treatment in its parametrization of an expectation model. Here an expectation model is based on the minimal set of marginal terms for that model rather than consisting of all terms, including all marginal terms, appropriate to the model being considered. The proposed approach is in agreement with that advocated by Nelder (1977) to the extent that it does not necessarily involve the imposition of constraints on the parameters of the expectation model. However, whereas Nelder holds that it is undesirable to place constraints on the parameters, here the imposition of constraints leads to an inconsequential reparametrization of the model. For example, consider the dependence and additive independence models for the two factors V and T in the split-plot experiment used as an example in section 2.2 (see section 2.2.6.2).

Two alternative parametrizations of the additive independence model are:

$$\begin{aligned} \mathrm{E}[y_{klm}] &= \zeta_i + \tau_j, \text{ and} \\ \mathrm{E}[y_{klm}] &= \mu' + \zeta_i' + \tau_j' \end{aligned}$$

where

$$\begin{aligned} \mu' &= \overline{\zeta}_{\cdot} + \overline{\tau}_{\cdot}, \\ \zeta_i' &= \zeta_i - \overline{\zeta}_{\cdot}, \text{ and} \\ \tau_j' &= \tau_j - \overline{\tau}_{\cdot}. \end{aligned}$$

Two alternative parametrizations of the dependence model are:

$$\begin{aligned} \mathrm{E}[y_{klm}] &= (\zeta\tau)_{ij}, \text{ and} \\ \mathrm{E}[y_{klm}] &= \mu^\star + \zeta_i^\star + \tau_j^\star + (\zeta\tau)_{ij}^\star \end{aligned}$$

where

$$\begin{aligned} \mu^\star &= (\overline{\zeta\tau})_{\cdot\cdot}, \\ \zeta_i^\star &= (\overline{\zeta\tau})_{i\cdot} - (\overline{\zeta\tau})_{\cdot\cdot}, \\ \tau_j^\star &= (\overline{\zeta\tau})_{\cdot j} - (\overline{\zeta\tau})_{\cdot\cdot}, \text{ and} \\ (\zeta\tau)_{ij}^\star &= (\zeta\tau)_{ij} - (\overline{\zeta\tau})_{i\cdot} - (\overline{\zeta\tau})_{\cdot j} + (\overline{\zeta\tau})_{\cdot\cdot}. \end{aligned}$$

For each model, the alternative parametrizations are mathematically equivalent and it has been the usual practice to use the second parametrization in each case, although without the qualifiers I have included. As a result the dependence model is often regarded as being the same as the additive model except for the interaction term. However, superficially similar terms, such as ζ_i' and $\zeta_i^\star$, are quite different: ζ_i' is the effect of V independent of the level of T, whereas $\zeta_i^\star$ is the average response of V over the levels of T. This distinction is especially important in unbalanced studies, since whereas $\zeta_i' = \zeta_i^\star$ in orthogonal studies, this is not the case in unbalanced studies.

Of the parametrizations given above, the most natural is that involving the minimal set of marginal terms since it relates directly to the mechanism hypothesized to generate the data. The second parametrization in each case would seem most useful for obtaining an expression for the interaction that measures the difference between these two models (Darroch, 1984). The use of the saturated parametrization of the

models also has the advantage that the sequence of testing models cannot ignore the marginality between expectation models (for example, testing for V will not be attempted given $V.T$ has been accepted).

In employing the approach to analyse experiments with nonorthogonal expectation models, such as the two-factor completely randomized design with unequal replication, the hypotheses tested will depend on the observed cell frequencies. However, Nelder (1982) points out that from an information-theoretic viewpoint this is appropriate. It reflects the differences in information among the various contrasts in the parameter space. The advantage of the approach presented here, over that relying on parametric functions of cell means, is that the possible nondetection of significant results is avoided (Burdick and Herr, 1980).

Clearly, expectation model selection involves the comparison of a series of distinct models, rather than choosing between terms to include in a model. On the other hand, comparison of models in variation model selection is equivalent to deciding which terms are to be included in the model.

6.5 Appropriate mean square comparisons

A major consequence of the approach outlined here is that the uniformity of mean squares hoped for by Nelder (1977) unfortunately does not obtain. Nelder (1977) obtains uniformity by modelling all terms as random variables uncorrelated with each other; I believe this strategy is flawed as the homogeneity properties associated with random variables may not always be appropriate. Instead, I designate some terms as contributing to expectation, for which homogeneity assumptions are not required, and the others to variation. The expected mean squares for a study, and hence mean square comparisons and hypotheses tested (or, equivalently, standard errors), depend on the expectation/variation classification of the factors, parallelling the effect of the fixed/random classification of mixed model analysis. For example, in the sensory experiment (section 4.2.1), it would not be relevant to consider the hypothesis that area differences are greater than could be expected from $A.B$ and $A.E$ variability combined, even if $A.E$ is significant. This is because $A.E$ has not been hypothesized

to be a source of variation in the experiment. If it were, then the hypothesis would be relevant. The aforementioned dependence is not the result of imposing constraints on the parameters as is sometimes argued. Rather, it is the result of the fundamental differences between expectation and variation models in respect of the behaviour of marginal terms. In expectation models, the inclusion of a marginal term amounts to an alternative parametrization of the same model (section 6.4), whereas for a variation model a similar inclusion adds to the complexity of the variance matrix model.

There is considerable discussion on the testing of main effects in the presence of interaction in the literature (see for example Nelder (1977) and accompanying discussion). The approach presented here makes it explicit that the testing of expectation main effects in the presence of expectation interaction is seen to be illogical, *at the model identification stage* (section 6.4); it involves an attempt to use two different models to describe the same data. Of course, in situations such as those described by Elston and Bush (1964) and Tukey (1977), estimates of main effects for expectation factors may be required at the prediction stage even if the fitted model involves interactions to which they are marginal. As Kempthorne (1975a) states, the desirability of estimating main effects in these circumstances depends on 'a forcing specification of the target population'. However, the situation in respect of variation terms differs from that for expectation terms; it is appropriate to test variation terms whether or not terms to which they are marginal are significant. The sensory example (section 4.2.1) provides a case in point. In this example, it is necessary to test a variation term ($A.B$) which is marginal to significant variation terms with the result that $A.B$ is judged to be not significant. Hence, the covariance of wine scores from the same $A.B$ combination is the same as that of scores from different $A.B$ combinations; that is, *Area.Batches* does not contribute to the variability of the scores. The difference between expectation and variation terms, essentially recognized by Fisher (1935, 1966) in a section added to the sixth edition (1951, section 65), is a consequence of the different nature of the models noted in section 6.3.

Also, Nelder (1977, section 2.3) suggests that sources corresponding to 'random' (variation) terms should occur only in the numerator of F-ratios when they are randomized terms and only in the denominator when they are unrandomized. However,

the sensory example (section 4.2.1) provides a case in which it is relevant to use a source corresponding to a randomized variation term in the denominator. As the $A.E$ interaction is not significant, the randomized main effect A is to be tested and this involves using the randomized variation interaction $A.B$. The A main effect is not significant, indicating that the difference between the wines from different areas is no greater than could be expected between those from two different batches in the same area.

6.6 Form of the analysis of variance table

The method described in chapter 2 involves the specification of the models for a study from the terms derived from the structure sets formed from the randomization-based tiers. Accompanying this model will be an analysis of variance table incorporating the same set of terms as the model and summarizing the confounding relationships between the terms. That is not to say that the analysis of variance table is derived from the models; rather they have a common origin: the structure sets. However, as Cox (1984) suggests, the analysis of variance table is in many cases easier to assimilate than the bare linear model as the analysis table incorporates information not contained in the model. In my view, this is particularly so if it is of the form advocated in this thesis.

The form of the analysis of variance tables for the two-tiered experiments presented herein will be the same as those produced from the statistical programming language GENSTAT 4 (Alvey *et al.*, 1977), that implements Nelder's (1965a,b) approach to deriving the structure sets for an experiment. This will be the case for the many standard two-tiered designs such as randomized complete block, balanced and partially balanced incomplete block, lattice, confounded factorial and split-plot designs. The structure sets for many of these are discussed by Nelder (1965a,b) and Alvey *et al.* (1977). The form of the analysis of variance table for multitiered experiments, presented in Brien (1983), is an extension of that for the two-tiered experiments.

In sections 6.6.1–6.6.3, we investigate the benefits that lead one to recommend the use of the particular form of analysis of variance table advocated herein.

One of these benefits is that it results in models and analysis of variance tables that reflect the randomization employed in the study. As a result it differentiates between studies which, although they involve different randomization procedures, traditionally have the same model and analysis of variance applied to them.

A second benefit is that the types of variability contributing to various subspaces are portrayed in the analysis of variance table. One is able to determine readily which combination of experimental unit variability, variability separated from experimental error, treatment error, sampling error and intertier interaction is contributing to a subspace.

A third benefit is that, when the inadequate replication underlying what I have termed total and exhaustive confounding occurs, it is evident in tables derived using the method.

6.6.1 Analyses reflecting the randomization

Structure sets have been used by a number of authors as a basis for specifying the analysis of variance table appropriate to a study (Bennett and Franklin, 1954; Schultz, 1955; Zyskind, 1962a; Nelder, 1965a,b; Alvey *et al.*, 1977; Brien, 1983, 1989). A particular issue about which these authors differ is the number of structures necessary to obtain the analysis of variance table and specify the linear model.

As an example, authors such as Bennett and Franklin (1954) and Schultz (1955) would use the single structure $Blocks*Treatments$ to specify the analysis for a randomized complete block design. This would generate the analysis of variance given in table 6.2A. However, this formulation does not properly represent the way in which the design was set up, with *Plots* nested within *Blocks*, and *Treatments* randomized independently onto *Plots* within a *Block*. Consequently, Nelder (1965), Wilkinson and Rogers (1973), Brien (1983, 1989) and Payne *et al.* (1987) prefer to specify the inherent structure of the design separately from the treatments imposed on it, and would thus use the two structures $Blocks/Plots$ and *Treatments*. The analysis of variance tables generated by these structures is shown in table 6.2B. Of course, both formulations lead ultimately to an equivalent partition of the *Total* sum of squares and

hence analysis. However, only the second table portrays the randomization employed in the experiment by exhibiting the confounding relationships between terms.

Table 6.2: Randomized complete block design analysis of variance tables for two alternative structure sets

A) SINGLE FORMULA		B) TWO FORMULÆ	
SOURCE	DF	SOURCE	DF
Blocks	$b-1$	*Blocks*	$b-1$
Treatments	$t-1$	*Blocks.Plots*	$b(t-1)$
		Treatments	$t-1$
Blocks.Treatments	$(b-1)(t-1)$	*Residual*	$(b-1)(t-1)$

It has also been demonstrated herein that three tiers are necessary to portray the randomization that has occurred in some experiments. However, it is clear that for the example presented in section 5.2.1, for example, the correct sample variance partition can be obtained by replacing *Plots* in the second tier with *Treatments*, in a manner analogous to the randomized complete block design. The structure set for obtaining the analysis then becomes:

Tier	Structure
1	*j Judges/bt Sittings*
2	*b Blocks∗t Treatments*

But again this table will not adequately portray the randomization performed.

Another shortcut sometimes employed in the specification of experiments is to replace a factor in a tier by factors from higher tiers; for example, for a randomized complete block experiment, the structure set could be specified as follows:

Tier	Structure
1	*Blocks/Treatments*
2	*Treatments*

While this may be more efficient from the viewpoint of computer storage, the structure set no longer adequately reflects the way in which the experiment was carried out. Hence, the analysis table may no longer exhibit the confounding relationships between terms. The same effect is produced by a rule followed in GENSTAT 4, namely that terms included in both unrandomized ('block') and randomized ('treatment') models will be deleted from the block model. This also contradicts rule 4 of table 2.1. These departures from tables based on structure sets can be particularly confusing in more complicated experiments.

So an important feature of the proposed approach is that it results in different analysis of variance tables for studies that vary in their randomization procedures. It seems desirable that this occur. For example, Kempthorne (1955) and Anderson and Maclean (1974) suggest there should be a distinction made between the randomized complete block design and the two-factor completely randomized design with no interaction. Wilk and Kempthorne (1957) also mention the Latin square design and the superficially similar $(1/t)$th fraction of a t^3 factorial experiment (where the fraction is chosen using a Latin square arrangement). In general, as outlined in section 6.2, there can be substantive differences in the inferences applicable to experiments that differ in their randomization.

To investigate in more detail the manner in which the proposed method results in different analysis of variance tables for studies that differ in their layout, I apply the proposed method to the three experiments discussed by White (1975) and to a multistage survey; a similar exercise carried out for the 'two-factor' studies described by Graybill (1976, section 14.9) would provide similar insights.

For White's (1975) first experiment:

> Each of two new therapies requires special training and equipment, so that a physician can be trained and equipped for only one of them. Ten physicians are randomly divided into two groups of five, to be trained and equipped for the two therapies. Then each physician treats six of his patients and rates the

> six results. The data consists of 60 such results, for the purpose of comparing the two therapies.

The observational unit in this experiment is a patient and the factors are *Physicians*, *Patients* and *Therapies*. The unrandomized or first-tier factors (that is, those factors that index the units prior to randomization) are *Physicians* and *Patients*; the randomized factor (that is, that factor to be associated with the units by randomization) is *Therapies*. Further, let us suppose that *Therapies* is an expectation factor and that the others are variation factors. The structure sets and variation model for the study are then as given in table 6.3; the expectation model is just $\mathrm{E}[\boldsymbol{y}] = \boldsymbol{\mu}_{Therapies}$.

For the second experiment:

> At least 60 laboratory animals that respond to some stimulus are available for the testing of drugs that may alter the response to that stimulus. They are randomly divided among ten test days, six animals/day. The days are divided into two random groups of five and a drug assigned to each group. The six animals in a day-group are treated with the drug assigned to that day. The data consist of 60 animal responses, for the purpose of comparing the two drugs.

The observational unit in this experiment is an animal and the factors are *Animals*, *Days* and *Drugs*. The unrandomized or first-tier factor is *Animals*. The *Days* are associated randomly with the animals and so is a second-tier factor. The *Drugs* are randomly associated with the days and so is a third-tier factor. Let us assume *Drugs* to be the only expectation factor. The structure sets and variation model for the study are then as given in table 6.3; the expectation model is just $\mathrm{E}[\boldsymbol{y}] = \boldsymbol{\mu}_{Drugs}$.

For the third experiment:

> Sixty cars arriving at a car-wash emporium are randomly assigned to ten car-wash units, six cars/unit. The ten units are five of each of two types. The data consist of 60 "cleanliness scores", for the purpose of comparing the two types.

The observational unit in this experiment is a car and the factors are *Cars*, *Machines* and *Types*. The unrandomized factor is *Cars* and the randomized factors are *Machines* and *Types*. In this case, suppose *Types* is the only expectation factor. The structure sets and variation model for the study are then as given in table 6.3; the expectation model is just $\mathrm{E}[\boldsymbol{y}] = \boldsymbol{\mu}_{Types}$.

Table 6.3: Structure sets and models for the three experiments discussed by White (1975) and a multistage survey

STRUCTURE SETS

Tier	Experiment 1	2	3
1	*10 Physicians/6 Patients*	*60 Animals*	*60 Cars*
2	*2 Therapies*	*10 Days*	*2 Types/5 Machines*
3		*2Drugs*	
	Multistage		
1	*2 Sections/5 Trees/6 Leaves*		

VARIATION MODELS

Experiment	Model
1	$G + \textit{Physicians(P)} + \textit{Physicians.Patients(PI)}$
	$= \phi_G \mathbf{J}_{10} \otimes \mathbf{J}_6 + \phi_P \mathbf{I}_{10} \otimes \mathbf{J}_6 + \phi_{PI} \mathbf{I}_{10} \otimes \mathbf{I}_6$
2	$G + \textit{Days(D)} + \textit{Animals(A)}$
	$= \phi_G \mathbf{J}_{60} + \mathbf{U}_2(\phi_D \mathbf{I}_{10} \otimes \mathbf{J}_6)\mathbf{U}_2' + \phi_A \mathbf{I}_{60}$
3	$G + \textit{Types.Machines(TM)} + \textit{Cars(C)}$
	$= \phi_G \mathbf{J}_{60} + \mathbf{U}_2(\phi_{TM} \mathbf{I}_2 \otimes \mathbf{I}_5 \otimes \mathbf{J}_6)\mathbf{U}_2' + \phi_C \mathbf{I}_{60}$
multi-stage	$G + \textit{Sections.Trees(ST)} + \textit{Sections.Trees.Leaves(STL)}$
	$= \phi_G \mathbf{J}_2 \otimes \mathbf{J}_5 \otimes \mathbf{J}_6 + \phi_{ST} \mathbf{I}_2 \otimes \mathbf{I}_5 \otimes \mathbf{J}_6 + \phi_{STL} \mathbf{I}_2 \otimes \mathbf{I}_5 \otimes \mathbf{I}_6$

In addition, consider a multistage survey of leaf size of citrus trees in an orchard divided into two sections in each of which five trees are randomly sampled. Six leaves are randomly sampled from each tree. The data consist of 60 leaf area measurements. The observational unit for this survey is a leaf and the factors are *Sections*, *Trees* and *Leaves*. All three factors are unrandomized and so there is only one tier. *Sections* will be taken to be the only expectation factor. The structure set and variation model for the study are then as given in table 6.3; the expectation model is just $\mathrm{E}[\boldsymbol{y}] = \boldsymbol{\mu}_{Sections}$.

The structure sets obtained for the three experiments are the same as those described by White (1975) except for the second experiment, which is a multitiered experiment. The variation models differ only in that some include permutation matrices to account for the randomization employed in the studies.

The appropriate analysis of variance tables, obtained according to the rules given in section 2.2.5, are given in table 6.4. The tables are of the same form as those produced by GENSTAT 4 (Alvey *et al.*, 1977). The four tables are similar to the extent that the estimated effects and the sums of squares for each of the last three sources are computationally equivalent in all four cases. Also, the expected mean squares are shown in table 6.4. The expected mean squares are essentially the same for all of the studies, so that the 'eight degrees-of-freedom-source' will be used to test the 'one degree-of-freedom-source' in all cases.

As White says for the three experiments, traditionally the same linear model, and hence the same analysis of variance, would be applied to all four examples: the hierarchical analysis as exemplified by the analysis for the multistage survey in table 6.4.

Thus, the application of the method of chapter 2 leads to different models and analysis of variance tables for situations that have previously had the same models and tables applied to them. The basis of the difference between the traditional and the approach proposed herein is that the latter utilizes prerandomization, rather than postrandomization, factors. For example, in experiment 1, it is only postrandomization that one can group physicians on the basis of the therapy they are to administer, as is required for the hierarchical analysis; prior to randomization they are viewed as a single unpartitioned set.

Table 6.4: Analysis of variance tables for the three experiments described by White (1975) and a multistage survey

EXPERIMENT 1

SOURCE	DF	EXPECTED MEAN SQUARES
Physicians	9	
Therapies	1	$\phi_{PI}+6\phi_P+f_T(\boldsymbol{\mu})^\dagger$
Residual	8	$\phi_{PI}+6\phi_P$
Physicians.Patients	50	ϕ_{PI}

EXPERIMENT 2

SOURCE	DF	EXPECTED MEAN SQUARES
Animals	59	
Days	9	
Drugs	1	$\phi_A+6\phi_D+f_M(\boldsymbol{\mu})^\dagger$
Residual	8	$\phi_A+6\phi_D$
Residual	50	ϕ_A

EXPERIMENT 3

SOURCE	DF	EXPECTED MEAN SQUARES
Cars	59	
Types	1	$\phi_C+6\phi_{TM}+f_T(\boldsymbol{\mu})^\dagger$
Types.Machines	8	$\phi_C+6\phi_{TM}$
Residual	50	ϕ_C

MULTISTAGE SURVEY

SOURCE	DF	EXPECTED MEAN SQUARES
Sections	1	$\phi_{STL}+6\phi_{ST}+f_S(\boldsymbol{\mu})^\dagger$
Sections.Trees	8	$\phi_{STL}+6\phi_{ST}$
Sections.Trees.Leaves	50	ϕ_{STL}

$^\dagger f_X(\boldsymbol{\mu}) = 30\Sigma(\mu_i - \overline{\mu}_\cdot)^2$ where μ_i is the expectation of the ith level of factor X, and $\overline{\mu}_\cdot$ is the mean of the μ_is.

It is evident, upon examination of the analysis tables in table 6.4, that the studies are quite different in respect of the structures of their prerandomization populations (for example, we have *Patients* nested within *Physicians* in experiment 1, whereas we have an unpartitioned set of *Animals* in experiment 2). As a result the studies differ in the following respects:

1. Marginality relationships between sources in the analysis tables (for example, *Physicians* is marginal to *Physicians.Patients* in experiment 1, whereas *Animals* and *Days* are independent in experiment 2).
2. Population sampling procedures (for example, in experiment 1, physicians are randomly selected and patients of each physician randomly selected; in experiment 2, animals and days are independently and randomly selected). Consequently, the orders of equivalent factors differ (for example, *6 Patients* from each physician versus *60 Animals*).
3. Randomization procedures which are manifested in the different confounding arrangements evident in the analysis tables in table 6.4 (for example, in experiment 1, *Therapies* is confounded with *Physicians*; in experiment 2, *Drugs* is confounded with both *Animals* and *Days*). Consequently, equivalent terms from different experiments are protected from systematic differences between sets of terms which are not equivalent (for example, in experiment 1, *Therapies* is protected from systematic *Physicians* differences; in experiment 2, *Drugs* is protected from both systematic *Animals* and *Days* differences).
4. Differences in the form of assumptions (for example, in experiment 1, the *Patients* groups are assumed to be homogeneous in their covariance; in experiment 2, intertier additivity is assumed in that the effects of *Days* and *Animals* are assumed to be additive). That is, although essentially equivalent assumptions are required, the form in which they are expressed differs.

Thus, the structure of the prerandomization population and randomization procedures are exhibited in the table in the form of the set of sources included and their

and confounding relationships. The analysis of variance table provides a convenient representation of these aspects of a study.

However, it is not true that any difference in randomization will result in different analysis of variance tables. For example, consider the case of the two methods of superimposing, by separate randomization, a second set of treatments to a first set that had been assigned using a Latin square (section 5.3.3). In contrast to randomization-based analysis (Preece *et al.*, 1978 and Bailey, 1991), the analysis of variance table for a model-based analysis (table 5.14) is the same for both methods of randomization. This is because tables only reflect the sources produced by the allocation process in that they reflect the way in which the terms in one tier are assigned to those in a lower tier. That is, they reflect the terms to which they were assigned and the restrictions placed on the assignment. Hence, any method of allocating *Streats* in the superimposed experiment that assigns its levels to the combinations of *Rows* and *Columns* and keeps it orthogonal to *Rows*, *Columns* and *Ftreats* would have the same analysis of variance table as that presented in table 5.14; as pointed out in section 2.2.2 this includes systematic allocation.

6.6.2 Types of variability

The method of deriving analysis of variance tables given in sections 2.2.1–2.2.5 allows one to associate more than one source with a particular subspace of the sample space. A major advantage of this, as will be outlined in this section, is that it is possible to have several types of variability identified as contributing to the subspace.

Addelman (1970) recognizes a number of types of variability that may give rise to response variable differences associated with the sources in the analysis of variance table commonly designated 'experimental error'. These are:

> (a) variability that arises in the measuring or recording of responses of experimental units, (b) variability due to the inability to reproduce treatments exactly, (c) inherent variability in experimental units ..., (d) the interaction effect of treatments and experimental units, and (e) variability due to factors that are unknown to or beyond the control of the experimenter.

The most natural assumption to make about measurement error is that it is inde-

pendent between observations and that it has the same expectation and variance for all observations. Such an assumption implies that the measurement error will affect the whole sample space in a homogeneous manner and so cannot be separated from variability between individual observational units which, as indicated in section 2.2.6.2, is always incorporated in the variation model by virtue of the compulsory inclusion of the unit terms; hence, a specific term will not be included for measurement error. No allowance can be made in the structure set for (e) variability due to factors unknown to the experimenter.

In addition to the types of variability that might give rise to 'experimental error', one can envisage several other types of variability. For the purposes of this thesis, the types of variability that will be entertained include:

1. treatments;
2. treatment error;
3. experimental unit variability;
4. variability to be separated from experimental unit variability (often this is variability arising from blocking factors not having treatments applied to them);
5. sampling error; and
6. intertier interaction.

Of these types of variability, all but the last can be identified as arising from **intratier differences** or differences for a term which involves only factors from the same tier. The differences are between sets of observational units, a set being comprised of those units which have the same levels combination of the factors in the term.

For a particular term, and hence source, one can identify the one type of variability associated with that term. The type of variability associated with a term is the type that would generate the differences between the levels combinations for the term, if it was the only term contributing to the differences.

As an example, consider the randomized complete block design. The structure set and analysis of variance table, under the assumptions of intertier additivity and no

treatment error, are given in table 6.5A.

Presented, in table 6.5B, are the structure set and analysis table for the case in which the interaction of *Blocks* and *Treatments* is to be included in the analysis. The fact that the *Treatments* and the *Treatments.Blocks* are the only sources appearing under the *Blocks.Plots* source in the analysis table indicates that the subspace for the *Blocks.Plots* source orthogonal to that for the *Treatments* source is the same as the subspace for the *Treatments.Blocks* source. The first of these sources would be classified as deriving from experimental unit variability and the latter from intertier interaction.

Suppose that the treatments were in fact clones of a certain vine species and that the experimenter thought that the individual vines of a clone could vary, even when all other things are kept equal. As a result the experimenter randomly assigns individual vines of a clone to the replicates of the corresponding treatment. Now the factors in the experiment are *Blocks*, *Plots*, *Treatments* and *Vines*, with *Blocks* and *Plots* still being the unrandomized factors. The structure set, under the assumption of intertier additivity, and the corresponding analysis table, are shown in table 6.5C. The form of the analysis table indicates that the subspace for the *Treatments.Vines* source (treatment error) is a subspace of that for the *Blocks.Plots* source (experimental unit variability).

The structure set and analysis table with both of the above situations combined, that is when both intertier interaction and treatment error are thought to occur, are shown in table 6.6A. As the *Treatments.Blocks* term is totally aliased with Tier 2 terms that precede it, a source for it is not included in the table. If one wants to include such a source and the associated canonical covariance component in the table, then an extra structure for the intertier interactions will have to be given. The structure set, and associated analysis table, are also shown in table 6.6B. An examination of this table reveals that the subspace for the *Treatments.Blocks* source (intertier interaction) is the same as that for the *Treatments.Vines* source (treatment error) which is a subspace of that for the *Blocks.Plots* source (experimental unit variability).

The point to be made about the types of variability arising from intratier differences

Table 6.5: Structure sets and analysis of variance tables for the randomized complete block design assuming either a) intertier additivity, b) intertier interaction, or c) treatment error

A) INTERTIER ADDITIVITY

STRUCTURE SET

Tier	Structure
1	*b Blocks/t Plots*
2	*t Treatments*

ANALYSIS OF VARIANCE TABLE

SOURCE	DF	EXPECTED MEAN SQUARES
Blocks	$b-1$	$\phi_{BP}+t\phi_B$
Blocks.Plots	$b(t-1)$	
Treatments	$t-1$	$\phi_{BP}+f_T(\boldsymbol{\mu})$
Residual	$(b-1)(t-1)$	ϕ_{BP}

B) INTERTIER INTERACTION

STRUCTURE SET

Tier	Structure
1	*b Blocks/t Plots*
2	*t Treatments*Blocks*

ANALYSIS OF VARIANCE TABLE

SOURCE	DF	EXPECTED MEAN SQUARES
Blocks	$b-1$	$\phi_{BP}+\phi_{BT}+t\phi_B$
Blocks.Plots	$b(t-1)$	
Treatments	$t-1$	$\phi_{BP}+\phi_{BT}+f(_T\boldsymbol{\mu})$
Treatments.Blocks	$(b-1)(t-1)$	$\phi_{BP}+\phi_{BT}$

C) TREATMENT ERROR

STRUCTURE SET

Tier	Structure
1	*b Blocks/t Plots*
2	*t Treatments/b Vines*

ANALYSIS OF VARIANCE TABLE

SOURCE	DF	EXPECTED MEAN SQUARES
Blocks	$b-1$	$\phi_{BP}+\phi_{TV}+t\phi_B$
Blocks.Plots	$b(t-1)$	
Treatments	$t-1$	$\phi_{BP}+\phi_{TV}+f_T(\boldsymbol{\mu})$
Treatments.Vines	$(b-1)(t-1)$	$\phi_{BP}+\phi_{TV}$

Table 6.6: Structure sets and analysis of variance tables for the randomized complete block design assuming both intertier interaction and treatment error

A) SINGLE FORMULA

STRUCTURE SET

Tier	Structure
1	*b Blocks/t Plots*
2	*t Treatments/b Vines*
	+ *Treatments∗Blocks*

ANALYSIS OF VARIANCE TABLE

SOURCE	DF	EXPECTED MEAN SQUARES ϕ_{BP}	ϕ_{TV}	ϕ_B	$\boldsymbol{\mu}$
Blocks	$b-1$	1	1	t	
Blocks.Plots	$b(t-1)$				
Treatments	$t-1$	1	1		$f_T(\boldsymbol{\mu})$
Treatments.Vines	$(b-1)(t-1)$	1	1		

B) TWO FORMULÆ

STRUCTURE SET

Tier	Structure
1	*b Blocks/ t Plots*
2a	*t Treatments/b Vines*
2b	*Treatments∗Blocks*

ANALYSIS OF VARIANCE TABLE

SOURCE	DF	EXPECTED MEAN SQUARES ϕ_{BP}	ϕ_{TV}	ϕ_{BT}	ϕ_B	$\boldsymbol{\mu}$
Blocks	$b-1$	1	1	1	t	
Blocks.Plots	$b(t-1)$					
Treatments	$t-1$	1	1	1		$f_T(\boldsymbol{\mu})$
Treatments.Vines	$(b-1)(t-1)$	1	1	1		
Treatments.Blocks	$(b-1)(t-1)$	1	1	1		

Terms totally aliased:
Treatments.Blocks

is that their principal effect in the analysis is on the precision of conclusions drawn from the experiment. This is in contrast to intertier interactions which one would usually want to assume do not occur in the experiment since, if they do, they may limit the conclusions one is able to make about intratier terms marginal to the intertier interaction. For example, a significant *Area.Evaluator* interaction, an intertier interaction, in the two-tiered sensory experiment described in section 4.2.1 would have

meant overall conclusions about *Area* differences were not appropriate. For further discussion see section 6.7.

6.6.3 Highlighting inadequate replication

Inadequate replication is manifested as total and exhaustive confounding where an **exhaustively confounded term** is one for which all the sources for which it is a defining term have terms confounded with them. The occurrence of total and exhaustive confounding is a phenomenon that has previously worried statisticians (Addelman, 1970; Anderson, 1970) and which is illuminated by using the method of chapter 2. Consider an experiment intended to measure the effect of 3 light intensities on seedling growth. A batch of 60 seedlings is taken and seedlings are selected at random to be placed in one of three controlled environment growth cabinets. Suppose that the seedlings are kept in the same position in their respective growth cabinets and that the positions are equivalent across growth cabinets. The structure set and the analysis of variance, derived as prescribed in sections 2.2.1–2.2.5, are shown in table 6.7.

In this experiment, *Intensities* is totally confounded with *Cabinets* in that this is the only source with which *Intensities* is confounded. Further, the confounding between *Intensities* and *Cabinets* is such that there is no part of the subspace of the *Cabinets* source that is unconfounded with that for the *Intensities* source; that is, the *Cabinet* term is exhaustively confounded. Consequently we have no measure of *Cabinet* variability with which to test *Intensities* differences. This is also reflected in the expected mean squares. However, if we can 'neglect' the covariance within cabinets, then the *Cabinets.Positions* source can be used to test the *Intensities* source. That is, an assumption ($\phi_C = 0$) is required to make this test and this is revealed in the analysis of variance table.

The problems discussed by Addelman (1970) are also of the type just described. The structure sets and analysis tables for the original and revised experiments of his example 1, derived as prescribed in sections 2.2.1–2.2.5, are shown in table 6.8. Clearly, in the original experiment *Methods* is totally and exhaustively confounded

Table 6.7: Structure set and analysis of variance table for a growth cabinet experiment

STRUCTURE SET

Tier	Structure
1	*60 Seedlings*
2	*3 Cabinets*∗*20 Positions*
3	*3 Intensities*

ANALYSIS OF VARIANCE TABLE

SOURCE	DF	EXPECTED MEAN SQUARES
Seedlings	59	
Cabinets	2	
Intensities	2	$\phi_S + \phi_{CP} + 20\phi_C + f_I(\boldsymbol{\mu})^\dagger$
Positions	19	$\phi_S + \phi_{CP} + 3\phi_P$
Cabinets.Positions	38	$\phi_S + \phi_{CP}$

$^\dagger f_I(\boldsymbol{\mu}) = 20\Sigma(\mu_i - \overline{\mu}_.)^2/2$ where μ_i is the expectation for the ith *Intensity*, and $\overline{\mu}_.$ is the mean of the μ_is.

with *Teachers* while in the revised experiment it is not; this difference is immediately obvious from the analysis of variance table given here. For this type of experiment it is not likely that the differences between *Teachers* are negligible and so a test of *Methods* is not possible in the original experiment. The revised experiment is essentially the same as experiment 2 of table 6.4.

The valve-type experiment presented by Anderson (1970) is also of the type discussed in this section; the lack of replication of valve types parallels the lack of replication of *Cabinets* in the experiment discussed above. The revised animal experiment

Table 6.8: Structure sets and analysis of variance tables for Addelman's (1970) experiments

STRUCTURE SET

A) ORIGINAL EXPERIMENT

Tier	Structure
1	*ms Students*
2	*m Teachers*
3	*m Methods*

B) REVISED EXPERIMENT

Tier	Structure
1	*mgs Students*
2	*mg Teachers*
3	*m Methods*

ANALYSIS OF VARIANCE TABLE

SOURCE	DF	EXPECTED MEAN SQUARES
Students	$ms-1$	
Teachers	$m-1$	
Methods	$m-1$	$\phi_S+s\phi_T+f_M(\boldsymbol{\mu})^{\dagger}$
Residual	$m(s-1)$	ϕ_S

SOURCE	DF	EXPECTED MEAN SQUARES
Students	$mgs-1$	
Teachers	$mg-1$	
Methods	$m-1$	$\phi_S+s\phi_T+f_M(\boldsymbol{\mu})^{\ddagger}$
Residual	$m(g-1)$	$\phi_S+s\phi_T$
Residual	$mg(s-1)$	ϕ_S

$^{\dagger} f_M(\boldsymbol{\mu}) = s\Sigma(\mu_i - \overline{\mu}_.)^2/(m-1)$ where μ_i is the expectation for the ith *Method*, and $\overline{\mu}_.$ is the mean of the μ_is.
$^{\ddagger} f_M(\boldsymbol{\mu}) = gs\Sigma(\mu_i - \overline{\mu}_.)^2/(m-1)$ where μ_i is the expectation for the ith *Method*, and $\overline{\mu}_.$ is the mean of the μ_is.

discussed in section 5.4.2 also exhibits the same problem, as does the experiment reported by Hale and Brien (1978).

It has been my experience as a consultant that, in situations such as these but with no test possible, clients accept the explanation that the effects of two terms are inseparable or indistinguishable. The alternative explanation that there is a lack of replication in the experiment is commonly not appreciated by the client who usually responds 'But I have included several seedlings in each cabinet'.

6.7 Partition of the Total sum of squares

It has been argued in section 6.6.1 that if the proposed approach is employed, the randomization employed in the study will be incorporated in the analysis. However, in cases presented in that section, it had little bearing on the partition of the sample variance. One might think that this was generally the case and question the need for more than one structure formula, at least as far as partitioning the sample variance is concerned. Note that there can be no question as to the number of classes of factors or number of tiers that can be identified for a particular experiment; the issue is whether these are all needed to produce the analysis of variance.

However, the example presented in section 5.2.4 is one in which the correct decomposition cannot be obtained with less than the three tiers involved in the experiment. As outlined in section 5.2.4, the crucial aspects of this experiment are that it involves confounding of terms arising from the same structure with different terms from lower structures and that terms from both structures are nonorthogonal. Thus, it is clear that the strategy of transferring terms from the structure for a higher to that for lower tiers, as used above to analyse the randomized complete block design with a single formula, will not work here. Alternatively, for some designs it is possible to obtain a partial analysis using less than one structure for each tier: for example, the intra-block analysis of a balanced incomplete block design can be obtained with the single structure used in table 6.2A for the randomized complete block design. However, this also is impossible for our example, and three structures are required to achieve any valid analysis; thus, the least squares fit must be accomplished using a three-stage decomposition of the sample space as prescribed in section 3.3.1.1.

A final point about the example is that the field phase uses a two-tiered design that cannot be analysed with a single structure: suppose that data, such as the yields of the vines, had been collected from the field experiment; their analysis would require two structures and an algorithm for a two-stage decomposition of the sample space, like that of Wilkinson (1970) or Payne and Wilkinson (1977).

While the number of tiers of factors may be characteristic of a study and cannot be reduced in some experiments if the correct partition of the *Total* sum of squares is to

be obtained, the partition of the *Total* sum of squares for a study is not unique. The analysis will vary with the assumptions made about which terms need to be included; for example, as discussed below, one may or may not decide to include certain intertier interactions.

An important advantage, to the user, of basing analysis of variance tables on the structure for a study is that it removes the need to rely on a series of standard analysis tables (from a textbook on experimental design). Often, the randomization employed in an experiment is limited by practical considerations, leading to experiments not previously described in textbooks. The analysis of such experiments is commonly accomplished by using the table corresponding to the experiment that, of all the experiments described in a textbook, most closely resembles the experiment to be analysed. In contrast, the procedure described herein is based on the randomization procedures which are thereby incorporated into the analysis of variance table for the experiment. It is a well-defined procedure relying less on intuition than has previously been the case. As a result there should be more consistency in the formulation of an analysis for a particular experiment.

Further, it has been my experience that in many instances the structure set for many of the complex experiments presented in this thesis is misspecified, largely because the approach taken to the specification is to derive the structure set corresponding to an analysis determined as just described. Determination of the analysis for an experiment in this way (for example, by analogy with the split-plot experiment) can lead to its underanalysis (see a two-tiered sensory experiment (section 4.2.1), repetitions-in-time-and-space (section 4.3.2.2) compared to times-randomized-and-sites-unrandomized experiments (section 4.3.2.1) and the measurement-of-several-parts-of-a-pasture experiment (section 4.3.2.2)). The danger is that incorrect conclusions may be drawn if the wrong analysis is performed, as in the split-plot analysis of a two-tiered sensory experiment (section 4.2.1).

A particular issue that the use of the approach elucidates is the problem of whether to partition the 'Error (b)' source in the analysis of the standard split-plot experiment (see section 4.3.1) which has been shown to involve a decision about the occurrence of an intertier ('block-treatment') interaction (namely *D.Blocks*), rather than of intratier

differences. It is normal practice to assume that intertier interactions do not occur, particularly as their presence cannot usually be tested for (for example, as is clear from section 6.6.2, the presence of a *Block.Treatment* interaction cannot be tested for in a randomized complete block design). Further, the assumption of additivity is necessary if extensive inferences about the overall effects of randomized factors are to be made from the experiment. However, as Yates (1965), comments it may not always be advisable to pool intertier interactions (depending on experimental conditions) as they can be used as a partial check for nonadditivity in the experiment. For example, in sensory experiments, such as those discussed in sections 4.2.1 and 5.2.1, it is desirable to include intertier interactions as these are likely to arise in this area of experimentation. Thus, it is undesirable to give any strict rule, to be implemented rigidly, for the isolation of intertier interactions. For a detailed discussion of the pooling of these terms when they are not significant see Brien (1989).

On the other hand, intratier differences are usually isolated, initially at least. Thus, the *Blocks.Years* interaction in the repetitions-in-time experiment (see table 4.15), which is often thought to be analogous to the intertier interaction *D.Blocks* of the standard split-plot experiment, actually arises from intratier differences; it is variability to be separated from experimental unit variability. So that, whereas the isolation of the *D.Blocks* term is variable, the inclusion of the *Blocks.Years* term should be routine. Indeed, the analyses presented in section 4.3.2.2 indicate that, if this source is significant, incorrect conclusions will be drawn when the term is not included. Also, in this experiment, some of the terms of interest are shown to be intertier interactions (for example, *Clones.Years* from table 4.15), a hitherto unrecognized fact.

The method is of pedagogical interest as one has only to teach students the set of rules to be applied to all studies and then provide suitable experience in the use of the technique. This seems more satisfactory than teaching a series of analyses that cover only the range of studies discussed. Of course, for the structure set to be determined correctly, it is critical that one has identified all the (prerandomization) factors in the study and correctly specified the relationships between these factors.

Chapter 7

Conclusions

In this thesis, a paradigm is presented for factorial linear model analysis for experimental and observational studies. As outlined in Brien (1989), the overall analysis is a four-stage process in which the three stages of model identification, model fitting and model testing, jointly referred to as model selection, are repeated until the simplest model not contradicted by the data is selected. In the final stage the selected model is used for prediction. Model fitting fits proposed expectation and variation models, the terms to be included in the model having been derived from the structure sets formed from the randomization-based tiers in the model identification stage. The use of the paradigm is advocated on the grounds that, while the analysis of studies can be achieved with other methods, the present approach greatly facilitates the determination of the analysis. In particular, it ensures that the terms thought important in designing the study are included in the analysis. I have demonstrated that the conclusions from analyses derived using the proposed approach can differ from those that have been presented previously; when there is a difference, this is usually because previously presented methods omit important terms from the analysis or produce different expected mean squares. I suggest that the proposed approach clarifies the analyses of many studies and that the general employment of the approach should reduce the incidence of errors in the specification of linear models at the model identification stage.

In respect of the issues addressed in section 1.4, I believe the proposed approach deals with them satisfactorily. First, I have presented many examples illustrating the approach and so have demonstrated that it is applicable to a wide range of studies. These include multiple-error, change-over, two-phase, superimposed and nonorthogonal factorial experiments. While there is no restriction placed on the nonorthogonality between terms in the expectation model, the variation model may exhibit only some forms of nonorthogonal variation structure. The proposed approach is especially illuminating in analysis of multitiered experiments as is demonstrated in chapter 5.

I have chosen general linear models, rather than randomization models, as the primary basis for inference. This is because the randomization analysis cannot answer some scientifically interesting questions such as the significance of variation terms and intertier interactions. The major role of randomization in our linear model analysis is that it contains valuable information about how the investigator views the material under investigation; this information should, in turn, be taken into account at the model identification stage of the analysis. A secondary role for randomization is to provide insurance against bias in the allocation process and, hence, against the formulation of an inadequate model.

I contend that the relevant factor categorizations are the division of the factors into tiers and the classification of the factors as expectation or variation factors. An analysis based on the subdivision of the factors into tiers will result in a model that includes all the pertinent physical sources of differences in the study and so will reflect what was done in the study. The categorization of the factors as expectation or variation factors is based on the type of inference relevant to the study, not on whether or not the factor levels are a complete sample of the levels in the population of interest. It is demonstrated that difficulties in classifying factors, such as with the factor *Sex*, are resolved.

The form of the models used in the approach results in it being clear that the expected mean squares depend on the separation of the factors in a study into expectation and variation factors, this arising from differences between expectation and variation terms in respect of the treatment of terms marginal to significant terms.

The approach clarifies the appropriate comparisons of mean squares for model se-

lection. Thus it is clear that it is irrelevant, in model selection, to test any expectation effect that is marginal to a significant expectation effect. However, it can be necessary to test an effect marginal to a significant variation term so that this variation term will be in the denominator of the F-ratio; the significant variation term may be a randomized term.

The analysis of variance table summarizes the linear model employed. Its form when derived using the proposed approach has the advantage that it reflects the relevant physical features of the study. Consequences of this include: studies with different randomizations of the factors will have different analysis of variance tables; one obtains a more accurate portrayal of the types of variability that obtain; total and exhaustive confounding, when it occurs, is evident.

A further advantage of the proposed, and other similar, approaches is that the linear model for a particular study is derived from a set of basic principles rather than by analogy with a limited catalogue of standard analyses. This promotes the inclusion of all the appropriate sources in the analysis. Even so, it has been shown that similar approaches are easily misapplied to two-tiered experiments, particularly in the case of multiple-error experiments; examples have been presented in which this would lead to incorrect conclusions. The proposed approach uniquely allows for three or more tiers, these being required to describe the randomization employed in the study and hence to ensure the inclusion of all appropriate sources. It has been demonstrated that there are three-tiered experiments whose analysis cannot be achieved with less than three tiers and so are not satisfactorily analysable by the approaches of other authors. In other cases, such as superimposed and single-stage experiments, the recognition that they are three-tiered greatly elucidates their analyses.

Appendix A

Data for examples

A.1 Data for two-tiered sensory experiment of section 4.2.1

Table A.1: Scores for the two-tiered sensory experiment of section 4.2.1

Evaluator		1		2	
Occasion		1	2	1	2
Area	*Batch*				
1	1	15.5	14.0	12.0	12.0
	2	18.0	16.0	17.0	16.5
	3	16.0	17.0	11.0	14.0
2	1	18.0	16.0	16.5	16.5
	2	16.5	15.5	12.0	11.5
	3	17.5	17.5	15.5	16.0
3	1	14.5	13.5	11.5	12.0
	2	16.5	17.5	17.0	16.5
	3	17.5	16.5	15.0	14.0
4	1	14.5	13.5	10.0	11.0
	2	10.0	11.0	12.0	12.5
	3	15.5	16.0	16.0	16.0

A.2 Data for the sprayer experiment of section 4.2.3.2

Table A.2: Lightness readings (L) and assignment of *Pressure-Speed* combinations (PS)† for the sprayer experiment of section 4.2.3.2

	Blocks					
	1		2		3	
	PS	L	PS	L	PS	L
Plots						
1	3	18.2	10	20.2	12	20.9
2	12	20.2	7	19.9	8	19.4
3	8	19.2	1	19.4	10	19.8
4	7	18.6	2	19.5	4	20.1
5	11	19.3	4	19.8	2	18.8
6	2	19.4	3	19.6	7	18.8
7	5	20.2	11	20.6	3	19.5
8	9	20.3	6	20.6	11	19.9
9	6	19.5	9	20.3	9	21.0
10	10	18.9	8	20.5	5	20.2
11	4	18.9	12	20.4	6	20.6
12	1	18.0	5	20.7	1	18.7

†The *Pressure-Speed* combinations are numbered 1 – 12 across the three rows of the *Flow rates* section in table 4.7.

A.3 Data for repetitions in time experiment of section 4.3.2.2

Table A.3: Yields and assignment of *Clones* for the repetitions in time experiment of section 4.3.2.2

		Plots					
		1		2		3	
		Clone	Yield	*Clone*	Yield	*Clone*	Yield
Blocks	*Years*						
1	1	1	148.8	2	152.7	3	159.9
	2		142.4		142.3		150.6
	3		146.9		141.9		157.7
	4		155.4		142.9		152.2
2	1	3	159.0	1	152.5	2	151.4
	2		158.0		154.4		145.7
	3		166.5		162.7		151.6
	4		164.0		162.3		147.5
3	1	3	153.2	2	148.5	1	152.1
	2		149.1		144.4		158.4
	3		157.4		153.6		168.3
	4		151.7		144.7		168.2
4	1	1	152.3	3	158.6	2	151.2
	2		156.6		157.5		145.1
	3		145.6		145.6		135.7
	4		165.3		163.1		154.6
5	1	1	160.5	3	160.5	2	156.2
	2		162.0		152.1		150.9
	3		148.1		136.7		135.0
	4		164.4		151.9		149.8

A.4 Data for the three-tiered sensory experiment of section 5.2.4

Table A.4: Scores and assignment of factors for *Occasion* 1, *Judges* 1–3 from the experiment of section 5.2.4

(R = *Rows*; C = *Columns*; T = *Trellis*; M = *Method*)

Occasion 1

		Sittings	1					2					3					4				
			R	*C*	*T*	*M*	Score	*R*	*C*	*T*	*M*	Score	*R*	*C*	*T*	*M*	Score	*R*	*C*	*T*	*M*	Score
Judges	*Intervals*	*Positions*																				
1	1	1	3	3	2	1	14.5	3	1	3	1	16.0	3	2	1	2	15.5	3	4	4	2	15.5
		2	3	3	2	2	13.5	3	1	3	2	16.0	3	2	1	1	14.5	3	4	4	2	16.0
		3	3	3	2	1	14.5	3	1	3	2	15.5	3	2	1	1	16.5	3	4	4	1	15.5
		4	3	3	2	2	15.0	3	1	3	1	14.5	3	2	1	2	14.5	3	4	4	1	16.0
	2	1	1	3	1	1	14.0	1	4	3	1	15.5	1	2	4	1	15.0	1	1	2	2	15.0
		2	1	3	1	1	15.0	1	4	3	1	14.0	1	2	4	2	15.0	1	1	2	1	14.0
		3	1	3	1	2	14.5	1	4	3	2	13.5	1	2	4	2	15.0	1	1	2	1	15.0
		4	1	3	1	2	15.0	1	4	3	2	15.0	1	2	4	1	14.5	1	1	2	2	15.0
	3	1	2	1	4	2	16.0	2	2	2	1	15.0	2	4	1	2	16.5	2	3	3	1	15.5
		2	2	1	4	1	15.0	2	2	2	2	14.5	2	4	1	2	16.0	2	3	3	2	15.0
		3	2	1	4	2	15.0	2	2	2	1	15.0	2	4	1	1	15.5	2	3	3	1	15.5
		4	2	1	4	1	16.0	2	2	2	2	15.0	2	4	1	1	15.0	2	3	3	2	16.5
2	1	1	2	1	4	2	15.5	2	3	3	1	16.0	2	4	1	1	16.5	2	2	2	1	15.5
		2	2	1	4	1	16.0	2	3	3	1	16.0	2	4	1	2	15.0	2	2	2	1	17.0
		3	2	1	4	2	16.5	2	3	3	2	16.5	2	4	1	2	15.0	2	2	2	2	16.5
		4	2	1	4	1	16.5	2	3	3	2	15.0	2	4	1	1	15.5	2	2	2	2	16.0
	2	1	3	2	1	1	16.0	3	1	3	2	16.0	3	3	2	1	16.0	3	4	4	2	15.5
		2	3	2	1	1	14.0	3	1	3	1	15.5	3	3	2	2	15.5	3	4	4	1	15.5
		3	3	2	1	2	15.5	3	1	3	2	16.0	3	3	2	2	14.0	3	4	4	2	15.5
		4	3	2	1	2	16.0	3	1	3	1	16.5	3	3	2	1	15.0	3	4	4	1	16.0
	3	1	1	2	4	1	16.5	1	1	2	1	16.0	1	3	1	1	16.0	1	4	3	1	16.5
		2	1	2	4	2	15.5	1	1	2	1	15.0	1	3	1	2	17.0	1	4	3	1	17.0
		3	1	2	4	1	16.0	1	1	2	2	16.0	1	3	1	2	16.5	1	4	3	2	16.5
		4	1	2	4	2	16.0	1	1	2	2	15.5	1	3	1	1	15.5	1	4	3	2	16.0
3	1	1	1	1	2	2	14.5	1	3	1	2	15.0	1	4	3	2	16.0	1	2	4	2	16.0
		2	1	1	2	1	15.0	1	3	1	2	14.5	1	4	3	2	15.5	1	2	4	1	16.0
		3	1	1	2	1	16.5	1	3	1	1	15.0	1	4	3	1	15.0	1	2	4	2	15.0
		4	1	1	2	2	16.5	1	3	1	1	16.5	1	4	3	1	15.5	1	2	4	1	14.0
	2	1	2	2	2	1	16.5	2	1	4	2	15.5	2	3	3	2	16.0	2	4	1	2	16.5
		2	2	2	2	2	14.5	2	1	4	2	15.5	2	3	3	1	16.5	2	4	1	1	15.0
		3	2	2	2	1	16.0	2	1	4	1	16.0	2	3	3	2	17.0	2	4	1	2	17.0
		4	2	2	2	2	15.5	2	1	4	1	15.5	2	3	3	1	17.0	2	4	1	1	17.5
	3	1	3	2	1	2	15.5	3	1	3	2	16.0	3	3	2	2	14.5	3	4	4	2	15.5
		2	3	2	1	2	16.5	3	1	3	1	15.5	3	3	2	1	15.5	3	4	4	1	15.5
		3	3	2	1	1	15.0	3	1	3	2	14.5	3	3	2	1	16.0	3	4	4	2	15.5
		4	3	2	1	1	15.0	3	1	3	1	16.0	3	3	2	2	15.5	3	4	4	1	16.0

Table A.5: Scores and assignment of factors for *Occasion* 1, *Judges* 4–6 from the experiment of section 5.2.4

(R = *Rows*; C = *Columns*; T = *Trellis*; M = *Method*)

Occasion 1

		Sittings	1					2					3					4				
			R	*C*	*T*	*M*	Score	*R*	*C*	*T*	*M*	Score	*R*	*C*	*T*	*M*	Score	*R*	*C*	*T*	*M*	Score
Judges	*Intervals*	*Positions*																				
4	1	1	3	1	3	2	14.5	3	3	2	1	14.5	3	4	4	2	13.0	3	2	1	2	14.0
		2	3	1	3	2	14.0	3	3	2	1	12.5	3	4	4	1	13.5	3	2	1	2	14.0
		3	3	1	3	1	14.0	3	3	2	2	12.5	3	4	4	1	13.0	3	2	1	1	13.5
		4	3	1	3	1	15.0	3	3	2	2	14.5	3	4	4	2	13.5	3	2	1	1	13.0
	2	1	1	2	4	1	14.5	1	1	2	1	15.0	1	3	1	2	14.0	1	4	3	1	14.5
		2	1	2	4	2	14.5	1	1	2	2	14.0	1	3	1	1	15.0	1	4	3	2	15.5
		3	1	2	4	1	15.0	1	1	2	2	15.0	1	3	1	2	14.5	1	4	3	2	15.0
		4	1	2	4	2	15.5	1	1	2	1	14.5	1	3	1	1	14.5	1	4	3	1	15.0
	3	1	2	2	2	2	15.0	2	1	4	1	15.5	2	3	3	1	15.5	2	4	1	2	15.5
		2	2	2	2	1	15.0	2	1	4	1	14.5	2	3	3	2	15.0	2	4	1	1	16.5
		3	2	2	2	1	14.5	2	1	4	2	15.0	2	3	3	1	15.5	2	4	1	2	15.0
		4	2	2	2	2	14.5	2	1	4	2	14.5	2	3	3	2	16.0	2	4	1	1	15.5
5	1	1	2	3	3	1	15.5	2	1	4	2	16.0	2	2	2	2	14.5	2	4	1	2	15.5
		2	2	3	3	2	16.0	2	1	4	1	15.5	2	2	2	1	16.0	2	4	1	1	14.0
		3	2	3	3	1	15.5	2	1	4	1	15.5	2	2	2	2	15.5	2	4	1	2	16.0
		4	2	3	3	2	16.0	2	1	4	2	15.5	2	2	2	1	14.5	2	4	1	1	16.5
	2	1	3	3	2	2	13.5	3	4	4	1	14.5	3	2	1	2	14.5	3	1	3	2	15.0
		2	3	3	2	1	13.5	3	4	4	2	14.0	3	2	1	1	14.5	3	1	3	2	15.0
		3	3	3	2	1	14.5	3	4	4	2	14.0	3	2	1	1	13.5	3	1	3	1	15.0
		4	3	3	2	2	15.0	3	4	4	1	14.5	3	2	1	2	15.5	3	1	3	1	13.5
	3	1	1	1	2	1	14.0	1	2	4	2	15.5	1	4	3	2	15.0	1	3	1	1	15.0
		2	1	1	2	1	14.0	1	2	4	2	14.5	1	4	3	1	15.0	1	3	1	2	15.5
		3	1	1	2	2	14.5	1	2	4	1	14.5	1	4	3	2	14.5	1	3	1	2	16.0
		4	1	1	2	2	14.0	1	2	4	1	16.0	1	4	3	1	15.0	1	3	1	1	15.5
6	1	1	1	3	1	2	14.5	1	1	2	1	14.5	1	2	4	1	15.0	1	4	3	1	15.0
		2	1	3	1	1	15.0	1	1	2	2	14.0	1	2	4	1	14.0	1	4	3	2	14.5
		3	1	3	1	2	15.0	1	1	2	1	14.5	1	2	4	2	14.5	1	4	3	1	15.0
		4	1	3	1	1	15.5	1	1	2	2	13.5	1	2	4	2	13.0	1	4	3	2	14.0
	2	1	2	3	3	2	15.0	2	4	1	2	15.0	2	2	2	2	13.5	2	1	4	1	14.0
		2	2	3	3	1	15.0	2	4	1	2	14.5	2	2	2	1	15.5	2	1	4	1	13.5
		3	2	3	3	2	15.5	2	4	1	1	15.5	2	2	2	1	14.5	2	1	4	2	15.5
		4	2	3	3	1	15.5	2	4	1	1	13.5	2	2	2	2	15.5	2	1	4	2	16.0
	3	1	3	1	3	2	15.0	3	2	1	2	14.5	3	4	4	2	14.5	3	3	2	2	14.0
		2	3	1	3	1	14.0	3	2	1	2	15.0	3	4	4	1	15.0	3	3	2	1	14.5
		3	3	1	3	1	14.5	3	2	1	1	15.0	3	4	4	1	14.5	3	3	2	2	13.0
		4	3	1	3	2	15.0	3	2	1	1	14.0	3	4	4	2	15.0	3	3	2	1	14.5

Table A.6: Scores and assignment of factors for *Occasion* 2, *Judges* 1–3 from the experiment of section 5.2.4

(R = *Rows*; C = *Columns*; T = *Trellis*; M = *Method*)

Occasion 2

		Sittings	1					2					3					4				
			R	*C*	*T*	*M*	Score	*R*	*C*	*T*	*M*	Score	*R*	*C*	*T*	*M*	Score	*R*	*C*	*T*	*M*	Score
Judges	*Intervals*	*Positions*																				
1	1	1	3	4	2	2	15.0	3	1	1	2	14.0	3	2	4	1	14.5	3	3	3	1	16.0
		2	3	4	2	2	13.5	3	1	1	2	15.5	3	2	4	2	15.0	3	3	3	2	14.0
		3	3	4	2	1	13.5	3	1	1	1	14.5	3	2	4	1	15.5	3	3	3	2	15.0
		4	3	4	2	1	14.0	3	1	1	1	14.0	3	2	4	2	15.0	3	3	3	1	15.0
	2	1	2	4	3	1	15.5	2	1	2	1	15.5	2	3	4	2	15.5	2	2	1	2	16.0
		2	2	4	3	2	14.5	2	1	2	2	16.0	2	3	4	2	15.0	2	2	1	1	15.0
		3	2	4	3	1	16.5	2	1	2	2	15.0	2	3	4	1	16.0	2	2	1	2	16.0
		4	2	4	3	2	17.5	2	1	2	1	16.0	2	3	4	1	16.0	2	2	1	1	15.5
	3	1	1	3	2	2	15.0	1	2	3	1	16.0	1	1	4	2	14.5	1	4	1	2	15.5
		2	1	3	2	1	15.5	1	2	3	2	15.0	1	1	4	1	14.5	1	4	1	1	14.5
		3	1	3	2	1	15.5	1	2	3	2	14.0	1	1	4	1	14.5	1	4	1	2	15.5
		4	1	3	2	2	15.0	1	2	3	1	15.0	1	1	4	2	16.0	1	4	1	1	14.5
2	1	1	1	3	2	1	15.0	1	2	3	2	15.0	1	1	4	2	15.0	1	4	1	1	14.5
		2	1	3	2	2	15.0	1	2	3	1	15.0	1	1	4	1	14.5	1	4	1	2	15.0
		3	1	3	2	1	14.0	1	2	3	1	16.5	1	1	4	1	15.5	1	4	1	1	14.5
		4	1	3	2	2	16.0	1	2	3	2	16.0	1	1	4	2	15.5	1	4	1	2	15.0
	2	1	3	1	1	1	15.0	3	4	2	2	14.5	3	2	4	2	14.0	3	3	3	1	15.0
		2	3	1	1	2	15.0	3	4	2	2	14.0	3	2	4	1	14.5	3	3	3	2	14.0
		3	3	1	1	1	14.5	3	4	2	1	14.5	3	2	4	2	15.5	3	3	3	1	15.5
		4	3	1	1	2	14.5	3	4	2	1	14.0	3	2	4	1	15.0	3	3	3	2	14.5
	3	1	2	1	2	2	14.5	2	4	3	1	15.5	2	3	4	2	15.0	2	2	1	1	14.5
		2	2	1	2	1	14.0	2	4	3	2	15.5	2	3	4	1	15.0	2	2	1	2	15.5
		3	2	1	2	2	15.5	2	4	3	1	14.0	2	3	4	1	14.0	2	2	1	2	15.0
		4	2	1	2	1	15.0	2	4	3	2	14.5	2	3	4	2	15.5	2	2	1	1	14.0
3	1	1	2	3	4	2	14.5	2	2	1	2	15.0	2	1	2	2	14.5	2	4	3	2	16.5
		2	2	3	4	2	16.0	2	2	1	1	14.5	2	1	2	1	14.5	2	4	3	1	14.5
		3	2	3	4	1	15.0	2	2	1	1	15.0	2	1	2	1	15.5	2	4	3	2	15.5
		4	2	3	4	1	14.5	2	2	1	2	15.0	2	1	2	2	14.5	2	4	3	1	15.0
	2	1	1	1	4	2	15.5	1	4	1	1	14.5	1	2	3	1	15.0	1	3	2	1	14.0
		2	1	1	4	2	15.0	1	4	1	2	15.5	1	2	3	2	14.5	1	3	2	2	14.0
		3	1	1	4	1	15.5	1	4	1	2	15.0	1	2	3	2	15.0	1	3	2	2	15.0
		4	1	1	4	1	14.5	1	4	1	1	15.0	1	2	3	1	15.0	1	3	2	1	15.5
	3	1	3	1	1	1	14.5	3	4	2	1	15.5	3	3	3	1	16.0	3	2	4	1	15.0
		2	3	1	1	2	14.0	3	4	2	2	14.5	3	3	3	2	15.0	3	2	4	2	15.0
		3	3	1	1	2	14.5	3	4	2	2	15.0	3	3	3	1	14.5	3	2	4	2	14.5
		4	3	1	1	1	14.0	3	4	2	1	14.0	3	3	3	2	14.5	3	2	4	1	14.0

Table A.7: Scores and assignment of factors for *Occasion* 2, *Judges* 4–6 from the experiment of section 5.2.4

(R = *Rows*; C = *Columns*; T = *Trellis*; M = *Method*)

Occasion 2

		Sittings	1					2					3					4				
			R	*C*	*T*	*M*	Score	*R*	*C*	*T*	*M*	Score	*R*	*C*	*T*	*M*	Score	*R*	*C*	*T*	*M*	Score
Judges	*Intervals*	*Positions*																				
4	1	1	3	3	3	2	16.0	3	2	4	1	15.0	3	1	1	1	16.0	3	4	2	1	16.0
		2	3	3	3	1	16.0	3	2	4	2	15.5	3	1	1	2	15.0	3	4	2	2	14.0
		3	3	3	3	1	14.5	3	2	4	2	15.5	3	1	1	2	15.0	3	4	2	1	15.5
		4	3	3	3	2	14.5	3	2	4	1	16.0	3	1	1	1	15.0	3	4	2	2	14.5
	2	1	2	1	2	1	15.0	2	4	3	2	17.5	2	2	1	2	16.5	2	3	4	2	15.5
		2	2	1	2	1	16.0	2	4	3	1	16.0	2	2	1	1	15.5	2	3	4	2	15.0
		3	2	1	2	2	16.0	2	4	3	1	16.5	2	2	1	2	15.5	2	3	4	1	15.5
		4	2	1	2	2	15.5	2	4	3	2	17.0	2	2	1	1	15.5	2	3	4	1	15.5
	3	1	1	1	4	2	14.5	1	4	1	2	15.5	1	3	2	2	13.5	1	2	3	2	14.0
		2	1	1	4	1	14.0	1	4	1	1	14.5	1	3	2	1	14.5	1	2	3	1	14.5
		3	1	1	4	2	15.0	1	4	1	2	15.0	1	3	2	1	15.5	1	2	3	1	15.0
		4	1	1	4	1	14.5	1	4	1	1	13.5	1	3	2	2	13.0	1	2	3	2	14.5
5	1	1	1	4	1	1	14.0	1	1	4	2	15.0	1	2	3	1	15.0	1	3	2	2	14.5
		2	1	4	1	2	15.5	1	1	4	1	15.5	1	2	3	2	15.5	1	3	2	1	13.5
		3	1	4	1	1	14.0	1	1	4	2	15.0	1	2	3	1	15.5	1	3	2	1	16.0
		4	1	4	1	2	16.0	1	1	4	1	16.5	1	2	3	2	16.0	1	3	2	2	14.5
	2	1	3	4	2	2	15.5	3	1	1	2	15.0	3	3	3	2	15.0	3	2	4	2	15.0
		2	3	4	2	2	14.5	3	1	1	1	16.0	3	3	3	1	15.0	3	2	4	1	15.0
		3	3	4	2	1	16.5	3	1	1	2	15.5	3	3	3	2	15.5	3	2	4	2	16.0
		4	3	4	2	1	16.0	3	1	1	1	15.0	3	3	3	1	15.5	3	2	4	1	16.0
	3	1	2	3	4	1	15.5	2	2	1	2	15.0	2	1	2	2	14.5	2	4	3	1	16.0
		2	2	3	4	2	15.5	2	2	1	2	15.5	2	1	2	1	15.5	2	4	3	1	14.0
		3	2	3	4	1	14.0	2	2	1	1	15.0	2	1	2	1	14.0	2	4	3	2	15.0
		4	2	3	4	2	15.5	2	2	1	1	14.5	2	1	2	2	14.5	2	4	3	2	16.0
6	1	1	2	4	3	2	15.5	2	1	2	1	16.0	2	2	1	1	15.5	2	3	4	1	15.5
		2	2	4	3	1	15.0	2	1	2	2	14.5	2	2	1	2	16.0	2	3	4	1	15.0
		3	2	4	3	2	14.0	2	1	2	1	15.0	2	2	1	1	15.5	2	3	4	2	15.5
		4	2	4	3	1	15.5	2	1	2	2	16.0	2	2	1	2	16.5	2	3	4	2	16.0
	2	1	1	4	1	1	15.0	1	1	4	1	15.0	1	3	2	2	13.5	1	2	3	1	16.0
		2	1	4	1	2	16.0	1	1	4	1	15.5	1	3	2	2	15.0	1	2	3	1	15.0
		3	1	4	1	2	14.0	1	1	4	2	15.0	1	3	2	1	14.0	1	2	3	2	15.0
		4	1	4	1	1	15.0	1	1	4	2	15.5	1	3	2	1	13.5	1	2	3	2	15.5
	3	1	3	3	3	2	15.5	3	2	4	1	14.5	3	1	1	1	14.5	3	4	2	1	15.5
		2	3	3	3	1	14.0	3	2	4	2	14.5	3	1	1	1	14.5	3	4	2	1	15.5
		3	3	3	3	2	15.0	3	2	4	2	15.0	3	1	1	2	14.0	3	4	2	2	14.5
		4	3	3	3	1	14.0	3	2	4	1	14.5	3	1	1	2	14.5	3	4	2	2	13.5

Appendix B

Reprint of Brien (1983). Analysis of variance tables based on experimental structure. *Biometrics*, 39:53–59.

Appendix C

Reprint of Brien (1989). A model comparison approach to linear models. *Utilitas Mathematica*, 36:225–254.

Glossary

Aliased source. A source that is neither orthogonal nor marginal to sources whose defining terms arise from the same structure as its own. Aliasing arises when it is decided to replicate disproportionately the levels combinations of factors, possibly excluding some levels combinations altogether. Thus, aliasing occurs in connection with the fractional and nonorthogonal factorial designs but not the balanced incomplete block designs. (cf. **partial aliasing**, **total aliasing**, and **confounded** and **marginal sources**)

Aliased term. A term which is the defining term for a source that is not orthogonal to sources whose defining terms arise from the same structure as it but which is not marginal to their defining terms. (cf. **aliased sources**, **partial aliasing**, **total aliasing**, and **confounded** and **marginal terms**)

Analysis of variance table. An analysis of variance table provides a convenient representation of the structure of the prerandomization population and the randomization procedures employed in a study. These are exhibited in the table in the form of the set of sources included and their marginality and confounding relationships. The table may contain some or all of the following columns:

1) SOURCE — (see **Source**)
2) DF — Degrees of Freedom
3) SSq — Sums of Squares
4) MSq — Mean Squares
5) EMS — Expected Mean Squares
6) F — F-ratios each being the ratio of two (linear combinations of) mean squares.

Backsweep. A sweep for previously fitted terms required to adjust for nonorthogonality between the current term and previously fitted terms (Wilkinson, 1970).

Canonical covariance components. ($\phi_{T_{iw}}$) The components measuring the covariation, between the observational units, contributed by a particular term in excess of that of marginal terms (Nelder, 1965a and 1977).

Change-over design. A design in which measurements on experimental units are repeated and the treatments are changed between measurements in such a way that the carry-over effects of treatments can be estimated (Cochran and Cox, 1957, section 4.6a; John and Quenouille, 1977, section 11.4).

Confounded source. A source is said to be confounded with another if the defining term for the first source is in a higher structure than that of the second and the subspaces for the two sources are not orthogonal. (see also **Confounded term**)

Confounded term. A term is said to be confounded with another if the first term is in a higher structure and the two terms are the defining terms for two sources whose subspaces are not orthogonal. Confounding arises because of the need to associate one and only one levels combination of factors with a levels combination of factors from a lower tier, it being impossible to observe more than one levels combination from the first set with a levels combination from the second set. (cf. **aliased** and **marginal sources**)

Note that this definition of confounding represents an extension of the traditional restricted usage of the expression to situations where terms from a particular structure are confounded with more than one term from lower structures, for example, in a blocked experiment, where some treatment terms are confounded with *Blocks* and others are not (Kendall and Buckland, 1960; Bailey, 1982b).

Covariance components. ($\gamma_{T_{iw}}$) Contribution from the ith structure to the covariance between a pair of observations. A particular covariance component will contribute if the pair of observations:

- have the same levels combinations of the factors in the component's term; and
- do not have the same levels combination of the factors from any term marginal to the component's term.

The covariance components will be actual covariances when variation terms arise from the first structure only and the set of variation terms is closed under the formation of both minima and maxima of terms.

Crossed factors in a structure. Two factors are said to be crossed if having the same level of one factor endows the observational units with a special relationship, even if they have different levels of the other factor. (cf. **nested factors in a structure**)

Data vector. The vector containing the original observations for a single response variable.

Decomposition tree. A diagram depicting the confounding relationships between sources and so illustrating the analysis of variance decomposition. Its root is the sample space or uncorrected *Total* source. Connected directly to the root are the sources arising from the first structure. The sources arising from the second structure are connected to the sources in the first structure with which they are confounded; sources in the third structure, if any, are similarly connected to sources in the second and so on.

Defining term for a source. The term from which the source takes its name or, for a residual source, the term from the highest nonresidual source with which it is confounded, highest meaning from the highest structure.

Effective mean. A mean divided by an efficiency factor. The efficiency factor adjusts for nonorthogonality between the term to which the mean corresponds and terms previously fitted (Wilkinson, 1970).

Effects vector. The vector for a particular term which is a linear form in the means vectors for terms marginal to that term.

Efficiency factor. The proportion of information available to estimate a term from a source with which it is confounded and, in general, taking into account sources with which it is aliased (Payne *et al.*, 1987). Note, however, that experiments involving partially aliased terms do not fulfil the conditions required of experiments to be covered by the approach put forward in this thesis. For orthogonal terms, the efficiency factor equals one. For nonorthogonal terms, they can be obtained from a catalogue of plans (if it contains the experiment), by an eigenanalysis of the model spaces for the two terms, or using an adaptive analysis such as described by Wilkinson (1970) and Payne and Wilkinson (1977).

Exhaustively confounded term. A term is said to be exhaustively confounded if all the sources for which it is a defining term have terms confounded with them.

Expectation factor. A factor for which it is considered most appropriate or desirable to make inferences about the relative performance of individual levels. Hence, inference would be based on location summary measures ('means'). Also called systematic factors. (cf. **variation factor**)

Experiment. A study that involves the manipulation of conditions between different observational units by the experimenter, the particular conditions assigned to a unit being chosen by randomization.

Experimental error. Variability between observational units which may arise from experimental unit variability, treatment error, measurement error and intertier interaction (Addelman, 1970).

Experimental unit. An identifiable physical entity in the experiment corresponding to a term which has had other terms confounded with it. Thus it may be possible to identify more than one experimental unit such as in the standard split-plot experiment where the experimental units are *Plots* and *Subplots*. This definition is consistent with that given by Cochran and Cox (1957) and Federer (1975); it differs from that employed by other authors (for example, Tjur, 1984) where their usage corresponds to what I have termed the observational unit.

Experimental unit variability. Variability between observational units arising from experimental units (Addelman, 1970).

Factor. A factor is a variable observed for each observational unit and so is indexed by the observational units. It corresponds to a possible source of differences in the response variable between observational units (Kendall and Buckland, 1960). A factor's values are called its levels. Factors determined prior to the conduct of a study are to be included in the structure set for the study. Unlike a term, it may be that a single factor does not represent a meaningful partition of the observational units. (see also **crossed factor**, **nested factor**, **term**)

First-order balance in experiments. An experiment is said to exhibit first-order balance when all aliased and confounded terms have a single efficiency factor for each source with which they are aliased or confounded (James and Wilkinson, 1971). Note that a statement on whether or not a study is first-order balanced must be qualified by the set of terms in respect of which the study is being assessed. Further, this definition is independent of the expectation and variation models for the study. (cf. **structure balance**)

First-order balanced terms. Two terms are said to be first-order balanced if, in the context of the analysis being performed, they have a single efficiency factor (James and Wilkinson, 1971).

Fixed factor. A factor whose levels are chosen arbitrarily and systematically and are regarded as a complete sample of the levels of interest to the researcher (see section 1.2.2). (cf. **random factor**)

General balance. (see **first-order balance**; **structure balance**)

Hasse diagram. A diagrammatic representation of a poset. An element is placed above another if it is 'less than' the other and the two elements are linked by a line.

Hasse diagram of term marginalities. This diagram represents the marginality relationships between terms by linking, with descending lines, terms that are immediately marginal; the marginal term is placed above the term to which it

is marginal. This diagram is called the Hasse diagram for ancestral subsets by Bailey (1982a, 1984) and the factor structure diagram by Tjur (1984).

Hasse diagram of expectation model marginalities. This diagram represents the marginality relationships between expectation models by linking, with descending lines, models that are immediately marginal; the marginal model is placed above the model to which it is marginal.

Hasse diagram of variation model subsets. This diagram represents the subset relationships between variation models by linking, with descending lines, models that are immediately marginal; the marginal model is placed above the model to which it is marginal.

Idempotent operator. (**E**) A member of the set of operators that projects orthogonally onto the minimal, orthogonal and invariant subspaces of terms from a Tjur structure (James, 1982; Tjur, 1984).

Immediately marginal model. One model is immediately marginal to another if it is in the minimal set of marginal models of the other.

Immediately marginal term. One term (A) is said to be immediately marginal to another (B) if A is marginal to B but not marginal to any other term marginal to B.

Incidence matrix. (**W**) A symmetric matrix for a set of factors making up a term. Its order is equal to the number of observational units. The rows and columns of the matrix are ordered lexicographically on the factors in the structure for the first tier. The elements are ones and zeros with an element equal to one if the observation corresponding to the row of the matrix has the same levels combinations of the factors in the term as the observation corresponding to the column, but no levels combinations in common for terms marginal to the term. These matrices correspond to the **W** matrices of Nelder (1965a) and the association matrices of Speed (1986).

Index set for study. The set of observational units, I. This index set indexes the observed values of the response variable.

Intertier interaction. Interaction for a term which involves factors from different tiers. In two-tiered experiments, this has been referred to previously as block-treatment interaction (Addelman, 1970).

Intratier differences. Differences for a term which involves only factors from the same tier. The differences are between sets of observational units, a set being comprised of those units which have the same levels combination of the factors in the term.

Lattice. A set L of elements $a, b, c, \ldots$ with two binary operations $\vee$ ('join') and $\wedge$ ('meet') which satisfy the following properties:

$$\begin{array}{lrcll}
\text{i)} & a \vee a & = & a \wedge a = a, & \text{(Idempotent)} \\
\text{ii)} & a \vee b & = & b \vee a, & \\
 & a \wedge b & = & b \wedge a, & \text{(Commutative)} \\
\text{iii)} & a \vee (b \vee c) & = & (a \vee b) \vee c, & \\
 & a \wedge (b \wedge c) & = & (a \wedge b) \wedge c, & \text{(Associative)} \\
\text{iv)} & a \vee (a \wedge b) & = & a \wedge (a \vee b) = a & \text{(Absorption)}
\end{array}$$

(Grätzer, 1971). For further information see definition 3.1 in section 3.2.

Levels combination of a set of factors. The combination of one level from each of the factors in the set; that is, an element from the set of observed combinations of the levels of the factors in a set.

Levels of a factor. The values a factor takes. Alternatively, they can be thought of as the labels of the classes corresponding to the values of the factor (for example, $1, 2, \ldots, n_{t_{ih}}$ where $n_{t_{ih}}$ is the order of the factor)

Marginal model. One model is marginal to another if the terms in the first model are either contained in, or marginal to, those in the second model.

Marginal source. A source is said to be marginal to another if its defining term is marginal to that for the other source.

Marginal term. One term (T_{iu}) is said to be marginal to another (T_{iw}) from the same structure if the model space of T_{iu} is a subspace of the model space of T_{iw}, this being the case because of the innate relationship between the levels combinations of the two terms and being independent of the replication of the

levels combination of the two terms (Nelder, 1977). This will occur if the factors included in T_{iu} are a subset of those included in T_{iw}. The marginality relation between terms or, more precisely, between the models spaces of terms, can be viewed as a partial order relation between terms so that $T_{iu} \leq T_{iw}$ means that T_{iu} is marginal to T_{iw} and the set of terms forms a poset. (cf. **aliased** and **confounded sources**)

Maximal expectation model. The sum of terms in the minimal set of marginal terms for the full set of expectation terms. The maximal expectation model represents the most saturated model for the mechanism by which the expectation factors might affect the response variable.

Maximal term. The term in a structure to which every other term in that structure is marginal.

Maximal variation model. The model for the variance matrix of the observations that is the sum of several variance matrices, one for each structure in the study. Each of these matrices is the linear combination of the summation matrices for the variation terms from the structure; the coefficient of a summation matrix in the linear combination is the canonical covariance components for the corresponding variation term.

Maximum of terms. The term that is the union of the factors from the terms for which it is the maximum.

Means vector. The observational-unit-length vector for a particular term obtained by computing the mean for each unit from all observations with the same levels combination of the factors in the term as the unit for which the mean is being calculated.

Measurement error. Variability in the observations arising from inaccuracy in the taking of measurements *per se* (Addelman, 1970).

Minimal set of marginal models for a model. This set is obtained by listing all models marginal to the model and deleting those models marginal to another model in the list.

Minimal set of marginal terms for a model. The smallest set of terms whose model space is the same as that of the full set of terms marginal to those in the model; that is, the set obtained after all marginal terms have been deleted.

Minimum of terms. The term corresponding to the intersection of the model spaces of the set of terms. (cf. Tjur's (1984) minimum of factors)

Model comparison approach. An approach to linear model analysis in which a series of models is fitted and the simplest model not contradicted by the data is selected (Burdick and Herr, 1980). (cf. **parametric interpretation approach**)

Model space of a term. The subspace of the observation space, $\mathbf{R}^n$, which is the range of the summation matrix for the term.

Multiple-error experiments. Experiments in which there is more than one source with which terms are confounded.

Multitiered experiments. Experiments that involve more than two tiers of factors.

Nested factors in a structure. A factor is said to be nested within another if there is no special relationship between the levels of the first factor associated with observational units that have different levels of the second factor (Bailey, 1985). Particular levels of the nested factor can be identified as 'belonging' to one and only one level of a nesting term. (cf. **crossed factors in a structure**)

Nesting term for a nested factor. A nesting term for a nested factor is a term that does not contain the nested factor but which is immediately marginal to a term that does.

Null analysis of variance. In two-tiered experiments, the analysis of variance derived from unrandomized factors (Nelder, 1965a).

Null randomization distribution. In two-tiered experiments it is the population of vectors produced by applying to the sample vector all permissible randomizations of the unrandomized factors (Nelder, 1965a).

Observational unit. The unit on which individual measurements are taken (Federer, 1975). The set of observational units can be thought of as a finite index set, I, indexing the observed values of the response variable and the factors in the study.

Observational-unit subset for a term. A subset consisting of all those observational units that have the same levels combination of the factors in the term.

Order of a factor. The order of a factor, that is not nested within another factor, is its number of levels; the order of a nested factor is the maximum number of different levels of the factor that occurs in the observational-unit subsets of the nesting term(s) from the structure for the tier to which the factor belongs.

Orthogonal terms. Two terms are orthogonal if, in their model spaces, the orthogonal complements of their intersection subspace are orthogonal (Wilkinson, 1970; Tjur, 1984, section 3.2). Thus, two subspaces, L_1 and L_2, of $\mathbf{R}^n$ are orthogonal if

$$L_1 \cap (L_1 \cup L_2)^{\perp} \perp L_2 \cap (L_1 \cup L_2)^{\perp}$$

Orthogonal variation structure. (OVS) The hypothesized variance matrix $\mathbf{V}$ for the study can be written as a linear combination of a complete set of known mutually orthogonal idempotent matrices where the coefficients of the linear combination are positive.

Parametric interpretation approach. An approach to linear model analysis in which a single maximal model is fitted and the pattern in the data is investigated by testing hypotheses specified in terms of linear parametric functions (Burdick and Herr, 1980). (cf. **model comparison approach**)

Partial aliasing. A source, or term that is the defining term for a source, is partially aliased if it is aliased and only part of the information is estimable; that is, the efficiency factor for the partially aliased source, given the sources with which it is aliased have been fitted before it, is strictly between zero and one. (see **aliased sources** and **total aliasing**)

Partial confounding. Confounding in which only part of the information about a confounded term is estimable from a single source; that is, the efficiency factor for the confounded term is strictly between zero and one. (see **confounded source** and **total confounding**

Partially ordered set. A set P of elements $a, b, c, \ldots$ with a binary relation, denoted by '$\leq$', which satisfy the following properties:

i)	$a \leq a$,	(Reflexive)
ii)	If $a \leq b$ and $b \leq c$, then $a \leq c$,	(Transitive)
iii)	If $a \leq b$ and $b \leq a$, then $a = b$	(Antisymmetric)

(Grätzer, 1971). A commonly occurring poset in this thesis is the set of terms from a structure, the order relation being the marginality relation between terms. For further information see definition 3.1 in section 3.2.

Permutation matrix for a structure. (**U**) A matrix that specifies the association between the observed levels combinations of the factors in the structure and the observational units.

Pivotal projection operator. An operator that produces the effects for fitting a term to a source. In general, this will involve: a sequence of pivotal and residual projection operators for fitting the source; the adjusted effects operator for the term; and a repetition of the same sequence of pivotal and residual operators to adjust for previously fitted sources to which the model space of term is nonorthogonal.

Pivotal sweep. A sweep in which the vector of (effective) means from that sweep is to be the input for the next sweep (Wilkinson, 1970).

Poset. (see **Partially ordered set**)

Previous-structure projection operator. A projection operator that has the same range and defining term as a projection operator from a previous structure.

Projection operator. (**P**) An operator that projects onto the orthogonal subspace corresponding to a source in the analysis of variance. Three basic types of

projection operators, all of which are orthogonal projection operators, occur in this thesis:

(i) previous-structure projection operator;

(ii) pivotal projection operator; and

(iii) residual projection operator.

Note that, except for those of type (i), any projection operator is said to correspond to a source in that it is the projection operator for the source associated with the structure from which the source arises.

Pseudofactors. Factors included in a structure for the study which have no scientific meaning but which aid in the analysis (Wilkinson and Rogers, 1973). The name derives from their application to the analysis of the pseudofactorial experiments introduced by Yates (1936).

Pseudoterms. Terms whose factors include at least one pseudofactor. Such terms have no scientific meaning and are included only as an aid to performing the analysis; for example, their inclusion may result in a structure-balanced study.

Random factor. A factor whose levels are randomly sampled and represent an incomplete sample of the levels of the factor of interest to the researcher (see section 1.2.2). (cf. **fixed factor**)

Random sampling. The selection of a fraction from a population, the whole of which is observable, such that each sample has a fixed and determinate probability of selection (Kendall and Buckland, 1960).

Randomization. (*verb*) The allocation, at random, of the levels combinations of the factors in one tier to those of the factors in a previous, usually the immediately preceding, tier.

Randomization. (*noun*) A random permutation of the levels combinations of the factors in a tier, the permutation respecting the structure derived from that tier (Bailey, 1981).

Randomized factor. A factor whose levels are associated with a particular observational unit by randomizing. (cf. **unrandomized factor**)

Regular term. A term in a structure for which there is the same number of elements in the observational-unit subsets for the term. Thus regular terms correspond to Tjur's (1984) balanced factors and Bailey's (1984) regular factors.

Regular structure. A structure in which all terms are regular.

Relationship matrices. (**S**) (see **Summation matrices**)

Repeated measurements experiment. An experiment in which observations are repeated over several times, *Times* representing an unrandomized factor. This definition is not consistent with that of Koch, Elashoff and Amara (1988), but is consistent with the traditional definition (Winer, 1971).

Replication factors. Factors whose primary function is to provide different conditions, resulting from uncontrolled variation, under which the treatments are observed. The classes of replication factors that commonly occur include factors indexing plots, animals, subjects, time periods and production runs.

Replication of a levels combination. The number of observational units with that levels combinations of the factors in a term or, equivalently, the size of the observational-unit subset for that levels combination of the factors in a term.

Residual projection operator. An operator that produces the residuals after fitting a term to a source. In general, this will involve: a sequence of pivotal and residual projection operators for fitting the source; the identity operator minus the adjusted effects operator for the term; and a repetition of the same sequence of pivotal and residual operators to adjust for previously fitted sources to which the model space of a term is nonorthogonal. (Wilkinson, 1970).

Residual source. A source in the analysis table for the remainder after all terms confounded with a particular source, whose defining term is in a lower structure than theirs, have been removed.

Residual sweep. A sweep in which the residual vector of that sweep is to be the input for the next sweep.

Series-of-experiments experiment. Experiment involving repetition, usually in time and/or space, and which involves a different set of experimental units at each repetition (Cochran and Cox, 1957, chapter 14).

Simple factor. A factor that is not nested in any other factor or a nested factor for which the same number of different levels of the factor occurs in the observational-unit subsets of its nesting term(s); this number is the order of the factor.

Simple orthogonal structure. A structure for which:

1. all the factors are simple;
2. the only relationships between the factors are crossing and nesting; and
3. either the product of the order of the factors in the structure equals the number of observational units or that the replication of the levels combinations of the factors in the structure is equal.

(Nelder, 1965a). (cf. **Tjur structure**)

Single-stage experiment. An experiment which cannot be subdivided into one or more completely self-contained subexperiments from the point of view of both the design and conduct of the experiment.

Source. A subspace of the sample space, the whole of which is identified as arising from a particular set of terms. A source will either correspond to a term (called the **defining term**) or be a residual source, the latter being the remainder for a source once terms confounded with it have been removed. Each source is labelled by its defining term and, if confounded, the source(s) with which it is confounded. A residual source takes its defining term from the highest non-residual source with which it is confounded, highest meaning from the highest structure. The sources with which a source is confounded are not cited specifically if no ambiguity will result. The analysis of variance gives a measure of the differences arising from the terms associated with each subspace.

Spectral component. ($\lambda_{T_{iw}}$) The contribution to the variance associated with a term in the ith structure by the variation terms in that structure.

Split-plot principle. The principle of randomizing two or more factors so that the randomized factors differ in the experimental unit to which they are randomized (Kendall and Buckland, 1960).

Standard split-plot experiment. An experiment involving two randomized factors. One of these factors is applied to main plots according to a randomized complete block design. The other factor is randomized to the subplots in each main plot, the number of subplots in each main plot equalling the order of the factor randomized to it (Federer, 1975).

Stratum. A source in an analysis of variance table whose expected mean square includes canonical covariance components but not functions of the expectation vector. That is, a source whose defining term is a variation term. This usage differs from that of Nelder (1965a,b) who uses it to mean a source in the null analysis of variance and hence one whose defining term consists of unrandomized factors only.

Stratum component. (ξ_{sk}) The covariance associated with a stratum which is expressible as the linear combination of canonical covariance components corresponding to the expected mean square for the stratum.

Structure. A structure summarizes the relationships between the factors in a tier and, perhaps, between the factors in a tier and those from lower tiers; it may include pseudofactors. It is labelled according to the tier from which it is primarily derived in that it is the relationships between all the factors in that tier that are specified in the structure. However, the set of factors in a structure may not be the same as the set of factors in a tier as the set of factors in a structure may include factors from more than one tier. The relationships between the factors are given in Wilkinson and Rogers (1973) notation. That is, the crossed relationship is denoted by an asterisk ($*$), the nested relationship by a slash ($/$), the additive operator by a plus ($+$) and the compound operator by a dot ($.$); the pseudofactor operator is denoted by two slashes ($//$) (Alvey *et al.*, 1977). In addition, the order of each factor will precede the factor's name in the lowest structure in which it appears. When writing out the structure,

relationships between factors within a tier should usually be specified before the intertier relationships. Each structure has associated with it a set of terms.

Structure balance in experiments. An experiment is said to exhibit structure balance when all terms from the same structure are orthogonal and there is a single efficiency factor between any term and the term(s) with which it is confounded (Nelder, 1965b, 1968). Note that a statement on whether or not a study is structure balanced must be qualified by the set of terms in respect of which the study is being assessed. Further, this definition is independent of the expectation and variation models for the study. (cf. **first-order balance**)

Structure set for a study. A set of structures summarizing the relationships between the factors in a study, these factors having been determined prior to the conduct of the study. There is usually one structure for each tier of factors which is labelled with that tier's number and ordered in the same way as the tiers; each structure will involve the factors in the tier from which it is derived and, perhaps, factors in lower tiers.

Summation matrices. (**S**) A symmetric matrix for a set of factors making up a term. Its order is equal to the number of observational units. The rows and columns of the matrix are ordered lexicographically on the factors in the structure for the first tier. The elements are ones and zeros with an element equal to one if the observation corresponding to the row of the matrix has the same levels combinations of the factors in the term as the observation corresponding to the column (James, 1957, 1982; Speed, 1986).

Superimposed experiment. An experiment in which an initial experiment is to be extended to include one or more extra randomized factors (Preece *et al.*, 1978).

Sweep for a term. The means for each levels combination of the factors in the term are calculated from the input vector to the sweep. The resulting (effective) means, divided by an efficiency factor if appropriate, are placed in an observational-unit-length vector such that the mean for a particular unit is the one with the same levels combination as the unit. This vector is subtracted

from the input vector to form a residual vector (Wilkinson, 1970).

Term. A set of factors, obtained by expanding a structure, which might contribute, in combination, to differences between observational units. It usually represents a meaningful partition of the observational units into subsets formed by placing in a subset those observational units that have the same levels combination of the factors in the term. The subsets formed in this way will be referred to as the term's observational-unit subsets.

A term is, in some ways, equivalent to a factor as defined by Tjur (1984) and Bailey (1984). It obviously is when the term consists of only one of the factors from the original set of factors making up the tiers; when a term involves more than one factor from the original set, it can be thought of as defining a new factor whose levels correspond to the levels combinations of the original factors. However, I reserve the name factor for those in the original set. A term is written as a list of factors or letters, separated by full stops. The list of letters for a term is formed by taking one letter, usually the first, from each factor's name; on occasion, to economize on space, the full stops will be omitted from the list of letters.

Tier. A set of factors having the same randomization status; a particular factor can occur in one and only one tier. The first tier will consist of unrandomized factors, or, in other words factors innate to the observational unit; these factors will uniquely index the observational units. The second tier consists of the factors whose levels combinations are randomized to those of the factors in the first tier, and subsequent tiers the factors whose levels combinations are randomized to those of the factors in a previous, in the great majority of cases the immediately preceding, tier.

The factors in different tiers are further characterized by the property that it is physically impossible to assign simultaneously more than one of the levels combinations of the factors in one tier to one of the levels combinations of the factors in a lower tier.

Tjur structure. A structure for which:

1. there is a term derived from the structure that is equivalent to the term derived by combining all the factors in the structure, or there is a maximal term derived from the structure to which all other terms derived from the structure are marginal;
2. any two terms from the structure are orthogonal; and
3. the set of terms in the structure is closed under the formation of minima.

(Tjur, 1984, section 4.1; Bailey, 1984)

Total aliasing. A source, or term that is the defining term for a source, is totally aliased with a set of sources if it is aliased and there is no information available for it, given the sources with which it is aliased have been fitted before it; that is, the efficiency factor for the totally aliased source is zero. A source is totally aliased if it is a subspace of the subspaces of sources arising from the same structure. (see **aliased source** and **partial aliasing**)

Total confounding. Confounding in which the only information about a confounded term is estimable from a single term. Cochran and Cox (1957) refer to this as complete confounding.

Treatment error. Variability arising from an inability to reproduce exactly for each unit the conditions specified for a particular level of a factor (Addelman, 1970).

Two-phase experiments. Experiments that involve an initial subexperiment that produces material which is incorporated into a second subexperiment (McIntyre, 1955).

Unit term. A term for which each of its levels combinations is associated with one and only one observational unit.

Unrandomized factors. The factors in the first or bottom ('foundation') tier which are those that would jointly identify the observational unit if no randomization had been performed. (cf. **randomized factor**)

Variation factor. A factor for which the performance of the set of levels as a whole is potentially informative; in such cases, the performance of a particular level is inferentially uninformative. Hence, inference would be based on dispersion summary measures ('variances' and 'covariances'). (cf. **expectation factor**)

Notation

Here we detail the notation used throughout the thesis.

Factors are given names which are shortened when necessary, most often to just the first letter and on other occasions to the first three letters. In general, t_{ih} denotes a factor from the ith structure.

Scalars

Scalars are denoted by lower-case letters. The following are commonly occurring scalars:

$a_{T_{iu}}$ The coefficient, usually ± 1, in a linear form of means vectors which make up an effects vector.

$e^{q}_{T_{iu}}$ The efficiency factor corresponding to term T_{iu} from the ith structure when it is estimated from the qth source of the $(i-1)$th structure; for orthogonal terms the efficiency factor is 1.

f_i The number of factors in the ith structure.

n The number of observations in the study.

$n_{t_{ih}}$ Order of the factor t_{ih}.

$n_{T_{iu}}$ The number of levels combinations of the factors in term T_{iu} that were actually observed in the study.

p_i The number of projection operators to effect the decomposition up to the ith structure.

q_{ik} The sum of squares for a source in the analysis table.

r_i The replication of the levels combinations of the factors in the ith structure, provided the structure is simple orthogonal; that is, the number of observational units that have the same levels combination of the factors in the ith structure.

$r_{T_{iu}}$ The replication for regular term T_{iu}; that is, the number of observational units that have the same levels combination of the factors in regular term T_{iu}.

s The number of structures in the study.

t_i The number of terms in the ith structure.

δ_{ij} The Kronecker delta where $\delta_{ij} = \begin{cases} 1 & \text{for } i = j \\ 0 & \text{for } i \neq j \end{cases}$.

$\gamma_{T_{iu}}$ The covariance component for the term T_{iu}.

$\phi_{T_{iu}}$ The canonical covariance component for the term T_{iu}.

$\lambda_{T_{iu}}$ The spectral component for the term T_{iu}, being the contribution, by the terms in the ith structure, to the expected mean square for the term T_{iu}.

ν_{ik} The degrees of freedom of a source in the analysis table.

$\nu_{T_{iu}}$ The degrees of freedom of the term T_{iu}.

ξ_{ik} The contribution of the variation to the expected mean square for a particular source in the analysis.

Vectors

Vectors are denoted by bold lower-case letters. The following are commonly occurring vectors:

$\mathbf{1}$ The vector of ones.

$\boldsymbol{c}_i$ The t_i-vector of coefficients of the linear combination of the incidence matrices for the ith structure.

$\boldsymbol{d}_{T_{iu}}$ The effects n-vector for term T_{iu} which is a linear combination of means n-vectors for terms marginal to T_{iu}.

$\boldsymbol{e}_i$ The symbolic t_i-vector of the elements of E_i.

$\boldsymbol{f}_i$ The t_i-vector of coefficients of the linear combination of the summation matrices for the ith structure.

$\boldsymbol{l}_i$ The t_i-vector of coefficients of the linear combination of the mutually orthogonal idempotent matrices for the ith structure.

$\boldsymbol{s}_i$ The symbolic t_i-vector of the elements of S_i.

$\boldsymbol{w}_i$ The symbolic t_i-vector of the elements of W_i.

$\boldsymbol{y}$ The n-vector of observations for a single response variable which we assume is arranged in lexicographical order with respect to the factors indexing the first tier.

$\overline{\boldsymbol{y}}_{T_{iu}}$ The means n-vector containing, for each observational unit, the mean of the elements of $\boldsymbol{y}$ corresponding to that unit's levels combination of the factors in term T_{iu}.

$\boldsymbol{\gamma}_i$ The t_i-vector of covariance component parameters for the terms in the ith structure.

$\boldsymbol{\phi}_i$ The t_i-vector of canonical covariance component parameters for the terms in the ith structure (zeroes are included for expectation terms).

$\boldsymbol{\lambda}_i$ The t_i-vector of spectral component parameters for the terms in the ith structure.

$\boldsymbol{\mu}$ The expectation n-vector containing the expectation parameters of the observations.

$\boldsymbol{\mu}_i$ The n-vector of parameters corresponding to the terms from the ith structure that have been included in the maximal expectation model; the maximal expectation model is derived as described in section 2.2.6.1. The parameters are arranged in the vector in a manner consistent with the ordering of the summation matrices for the structure. The vector contains only zeroes

if there is no expectation factor in the structure, or if a structure contains the same set of expectation factors as a previous structure.

$\boldsymbol{\mu}_{T_{iu}}$ The n-vector of expectation parameters for an expectation term T_{iu}. A particular element of the vector corresponds to a particular observational unit and will be the parameter for the levels combination of the term T_{iu} observed for that observational unit; there will be $n_{T_{iu}}$ unique elements in the vector.

Matrices

Matrices are denoted by bold upper-case letters. The direct product of two matrices, $\mathbf{A}$ and $\mathbf{B}$ say, is frequently required. It is denoted by $\mathbf{A} \otimes \mathbf{B} = \{a_{ij}\mathbf{B}\}$. The following are commonly occurring matrices:

$\mathbf{A}_{T_{iu}}$ The averaging operator of order n for term T_{iu} $(= \mathbf{R}_{T_{iu}}^{-1}\mathbf{S}_{T_{iu}})$.

$\mathbf{E}_{T_{iu}}$ The orthogonal idempotent matrix of order n for term T_{iu}.

$\mathbf{E}_{T_{iu}}^{k}$ The adjusted idempotent operator of order n for term T_{iu} when term T_{iu} is estimated from the kth source in the $(i-1)$th structure.

$\mathbf{G}$ The Grand mean operator $(= \mathbf{J}/m$ where m is the order of $\mathbf{J})$.

$\mathbf{I}$ The identity matrix.

$\mathbf{J}$ The matrix of ones.

$\mathbf{K}$ The matrix of ones everywhere except the diagonal $(= \mathbf{J} - \mathbf{I})$.

$\mathbf{M}$ The projection operator onto the subspace of the sample space corresponding to the expectation model.

$\mathbf{P}_{ik}$ The kth projection operator of order n from the ith structure. Note that, in this thesis, the term projection operator will be taken to mean orthogonal projection operator.

$\mathbf{R}_{T_{iu}}$ The diagonal replications matrix of order n. A particular diagonal element is the replication of the levels combination of the factors in term T_{iu} for the

observational unit corresponding to that element. For a regular term, all diagonal elements are equal to $r_{T_{iu}}$.

$\mathbf{S}_{T_{iu}}$ The summation matrix of order n for term T_{iu}.

$\mathbf{T}_{\boldsymbol{e}_i\boldsymbol{s}_i}$ The matrix of order t_i that transforms the set of matrices in $\boldsymbol{s}_i$ to the set of matrices in $\boldsymbol{e}_i$.

$\mathbf{T}_{\boldsymbol{e}_i\boldsymbol{w}_i}$ The matrix of order t_i that transforms the set of matrices in $\boldsymbol{w}_i$ to the set of matrices in $\boldsymbol{e}_i$.

$\mathbf{T}_{\boldsymbol{s}_i\boldsymbol{e}_i}$ The matrix of order t_i that transforms the set of matrices in $\boldsymbol{e}_i$ to the set of matrices in $\boldsymbol{s}_i$.

$\mathbf{T}_{\boldsymbol{s}_i\boldsymbol{w}_i}$ The matrix of order t_i that transforms the set of matrices in $\boldsymbol{w}_i$ to the set of matrices in $\boldsymbol{s}_i$.

$\mathbf{T}_{\boldsymbol{w}_i\boldsymbol{e}_i}$ The matrix of order t_i that transforms the set of matrices in $\boldsymbol{e}_i$ to the set of matrices in $\boldsymbol{w}_i$.

$\mathbf{T}_{\boldsymbol{w}_i\boldsymbol{s}_i}$ The matrix of order t_i that transforms the set of matrices in $\boldsymbol{s}_i$ to the set of matrices in $\boldsymbol{w}_i$.

$\mathbf{U}_i$ The permutation matrix of order n for the ith structure that specifies the association between the observed levels combinations of the factors in that structure and the observational units. If the number of observed levels combinations for the factors in the structure is not equal to the number of observational units, include a dummy factor nested within all the other factors in the structure.

$\mathbf{V}$ The variance matrix of order n for the observations.

$\mathbf{V}_i$ The variation matrix of order n arising from variation terms in the ith structure.

$\mathbf{W}_{T_{iu}}$ The incidence matrix of order n for term T_{iu}.

$\mathbf{X}$ The independent-variables matrix of order n; it specifies the linear combination of the expectation parameters of a linear model associated with a particular observational unit.

Sets

Sets are denoted by upper-case letters. The following are commonly occurring sets:

$D_{T_{iu}}$ The terms in the ith structure that are the minima of terms immediately marginal to the term T_{iu}.

E_i The orthogonal idempotent matrices for the ith structure.

F_i The factors in the ith structure.

I The index set, the elements of which are the observational units, and which indexes the observed values of the response variable and the factors in the study.

$N_{T_{iu}}$ The factors in T_{iu} that nest other factors in T_{iu}.

P_i The orthogonal projection operators for the ith structure.

S_i The summation matrices for the ith structure.

T_i The terms derived from the ith structure.

T_{iu} A term in the ith structure, consisting of one or more factors in F_i; it is written as a list of factors, or the list of first letters of the factors' names, separated by full stops; on occasion, to economize on space, the full stops will be omitted from the list of letters.

$T_{\mathbf{V}_i}$ The terms from the ith structure that have been included in the maximal variation model.

$T_{\boldsymbol{\mu}_i}$ The terms from the ith structure that have been included in the maximal expectation model.

U_{jq}^{gi} The set of indices specifying the projection operators that correspond to the sources in the gth structure which:

- are confounded with the source corresponding to the qth projection operator from the jth structure; and
- have no terms from structure $(j+1)$ through to the ith structure confounded with them.

That is, the projection operators in the gth structure such that, for $u \in U_{jq}^{gi}$,

$$\begin{aligned} \mathbf{P}_{jq}\mathbf{P}_{gu} &= \mathbf{P}_{gu}, \text{ and} \\ \mathbf{E}_{T_{hz}}\mathbf{P}_{gu} &= 0, \quad \text{for all } T_{hz} \in T_h, \quad g < h \leq i. \end{aligned}$$

W_i The incidence matrices for the ith structure.

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