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Analysis of Variance Tables Based on Experimental Structure

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SUMMARY

A stepwise procedure for obtaining the experimental structure for a particular experiment is presented together with rules for deriving the analysis-of-variance table from that structure. The procedure involves the division of the factors into groups and is essentially a generalization of the method of Nelder (1965, *Proceedings of the Royal Society, Series A* **283**, 147–162; 1965, *Proceedings of the Royal Society, Series A* **283**, 163–178), to what are termed 'multi-tiered' experiments. The proposed method is illustrated for a wine-tasting experiment.

1. Introduction

Determining the analysis of variance table can be difficult, particularly for complex experiments; this is evidenced by the existence of papers such as those by Green and Tukey (1960), Millman and Glass (1967) and Federer (1975). As Millman and Glass comment, many complex experiments are under-analysed in that not all the sources of variation that can be isolated are in fact isolated.

To provide a formal basis for deriving the analysis of variance table appropriate for a particular experiment, several authors have used the relationships between the factors in the experiment to determine the lines that are to be included in the analysis (e.g. Bennett and Franklin, 1954; Schultz, 1955; Green and Tukey, 1960; Zyskind, 1962; Millman and Glass, 1967; Searle, 1971). A diagrammatic structural representation is given by Kempthorne and Folks (1971, §16.11).

Another approach to determining the analysis of complex experiments, that Wilk and Kempthorne (1956) assert is used intuitively by many experimenters, is to be found in the comments made by Fisher (1935) during the discussion of a paper by Yates. Fisher proposed two analyses, one the 'topographical' analysis corresponding to the 'blocks' and the other the factorial analysis corresponding to the 'treatments'. These were then combined to yield the final analysis. However, he did not explicitly determine the relationships between the factors in the experiment.

Nelder (1965a, b) and White (1975) have formalized this process by proposing that one should determine separately the structure for the 'treatment' factors or 'design-units' and that for the 'block' factors or 'experimental units'. This structure, together with the experimental layout, is then used to obtain the table; an algorithm for accomplishing this has been described by Wilkinson (1970) and Payne and Wilkinson (1977) and implemented in GENSTAT (Alvey *et al.*, 1977).

The technique presented here, a generalization of the procedure of Nelder (1965 a, b), is applicable to a wider range of experiments than either Nelder's or White's methods. A key premise of the technique is that the experimental structure should reflect the layout of the experiment, i.e. the innate physical structure and the randomization employed.

Key words: Analysis of variance; Experimental structure; Multi-phase experiments; Multi-tiered experiments; Randomized experiments; Tiers.

2. Determining the Experimental Structure and Analysis Table

In this section the steps to be followed in determining the experimental structure are given and illustrated. Firstly, a randomized complete block wine-evaluation experiment is presented to compare Nelder's and the proposed methods when they are equivalent. A two-phase wine-evaluation experiment (McIntyre, 1955) is then presented, establishing the need for the generalized method.

Consider an experiment to evaluate an unstructured set of wines. Suppose these wines are evaluated at a tasting in which several tasters are given the wines over a number of sittings. One wine is presented for scoring to each taster at a sitting and each wine is presented only once to a taster. The order of presentation of the wines is randomized for each taster.

To determine the structure of an experiment, the steps shown in Table 1 are followed. The first step is to identify the factors in the experiment and the observational unit. The factors are Tasters (t levels), Sittings (w levels) and Wines (w levels). The observational unit (of which there are wt) is the wine given to a taster at a particular sitting.

In the second step the factors in the experiment are divided into *tiers*. A tier is a *set of factors* characterized by all combinations of the levels of these factors being observable *in toto*, given the crossing and nesting relationships between the factors; the term is intended to be distinct from any terms previously used in the literature. For the example, the set of factors Tasters, Sittings and Wines do not form a single tier as their levels combinations are not observable *in toto* since only one wine can be evaluated by a taster at each sitting.

The factors in the first or bottom ('foundation') tier consist of those which would jointly identify the observational unit if no randomization had been performed. The particular *levels combination* of these factors which is associated with an observational unit is, in this sense, innate to that unit. For the example, the levels combinations of the factors Tasters and Sittings are observable *in toto* and these factors identify and are innate to the observational units. They form the bottom tier and are called 'block' factors by Nelder (1965a) and Alvey *et al.* (1977).

The factors in the second tier are those whose levels combinations have been directly associated with the levels combinations of factors in the first tier using some selection procedure, usually randomization. For the example, the factor Wines forms the second tier and is called a 'treatment' factor by Nelder (1965b) and Alvey *et al.* (1977).

Once the factors have been divided into tiers the experimental structure is then formed as described in Steps 3 and 4 of Table 1. The experimental structure will be represented by structure formulae using the notation of Wilkinson and Rogers (1973). That is, the crossed relationship will be denoted by an asterisk ($*$), and the nested relationship by a slash (/).

Table 1
Steps for determining the experimental structure

Step 1: Identify the factors in the experiment and the observational unit.

Step 2: Divide the factors in the experiment into tiers so that the factors in the bottom tier are those innate to the observational units and those in each subsequent tier are those whose levels combinations were directly associated with the tier immediately preceding the current tier.

Step 3: Determine the relationships between the factors in the bottom tier, expressing them in Wilkinson–Rogers notation.

Step 4: For each of the remaining tiers determine the structure formula by specifying the relationships
(i) between all factors within a tier, and
(ii) between factors from a tier and from the tiers below it.

The experimental structure for the example is thus:

Tier	Structure formulae
1	Tasters/Sittings
2	Wines.

To obtain the analysis of variance table the experiment has to be combined with the experimental layout. The conventions for doing this are given in Table 2. Following Alvey *et al.* (1977, Part I, §6.2), the linear model for the experiment is obtained by combining additively the model for each tier, any repetitions of a term being deleted. The analysis of variance table for the example is given in Table 3. The form of this table is the same as the table produced by GENSTAT (Alvey *et al.*, 1977). The interpretation of the lines in the analysis is described by Wilkinson and Rogers (1973). Thus Tasters represents the overall Taster effects while Tasters.Sittings represents the differences between sittings within tasters as the line Sittings has been excluded. The indentation of the line Wines indicates that it is confounded with the first line above it that is not indented to the same extent, i.e. Wines is confounded with Tasters.Sittings. The Residual line corresponds to the unconfounded Tasters.Sittings contrasts. It provides the error mean square for Wines. The linear model for the experiment is

$$Y = \text{Tasters} + \text{Wines} + \text{Tasters.Sittings}.$$

Table 2

Rules for deriving the analysis of variance table from the experimental structure

Rule 1: Expand the structure formula for each tier, using the rules described in Wilkinson and Rogers (1973), to obtain a linear model for each tier.

Rule 2: All the terms in the model for the bottom tier will have a line in the table and these lines will all begin in the same column.

Rule 3: Terms from higher tiers will be included in the table under the term(s) from the tiers below, with which they are confounded. They will be indented so that terms from the same tier all start in the same column, there being a different starting column for each tier.

Rule 4: Terms that occur in the models of two consecutive tiers will not have a line entered for the higher of the tiers.

Rule 5: Terms totally aliased or confounded with terms occurring previously in the same tier will not be included in the table. A note of such terms will be made underneath the table.

Rule 6: For terms which have other terms from higher tiers confounded with them, residual lines are included if there is any information in excess of the confounded terms.

Table 3

Analysis of variance table for a randomized complete block wine-evaluation experiment

Source	Degrees of freedom
Tasters	$t-1$
Tasters.Sittings	$t(w-1)$
Wines	$w-1$
Residual	$(t-1)(w-1)$

Suppose that the wines of the previous section were not unstructured but that they were made from the produce of a field trial to test the effects of several viticultural treatments assigned to plots according to a randomized complete block design. This experiment is then a two-phase experiment (McIntyre, 1955). In the first phase the field trial is conducted, while in the second phase the wine made from the produce of each plot in the field trial is evaluated by several tasters.

Again, to determine the experimental structure the steps given in Table 1 are followed. The factors in the experiment are Blocks (b levels), Plots (p levels) and Treatments (p levels) from the field phase of the experiment, and Tasters (t levels) and Sittings (bp levels) from the tasting phase. An observational unit (of which there are pbt) is still the wine given to a taster at a particular sitting.

However, it is clear that two tiers will not be adequate to describe this experiment as the second tier of the previous example (Wines) now has a structure imposed on it by a field experiment which itself involves two tiers. In fact, three tiers are required and the experiment is said to be *multi-tiered.*

Tasters and Sittings are the factors that would index the observational unit if no randomization had been performed, 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. As the combinations of these factors were randomized to the sittings for each taster, they form the second tier. Treatments were randomized to the plots within each block and so it forms the third or top tier. The experimental structure, assuming no *inter-tier interaction* (a generalized term for block–treatment or unit–treatment interaction), is as follows:

Tier	Structure formulae
1	Tasters/Sittings
2	Blocks/Plots
3	Treatments.

The analysis of variance table for the example is given in Table 4. The indentation of the Treatments line indicates that Treatments is confounded with Blocks.Plots. The Residual line immediately below the Treatments line corresponds to the unconfounded Blocks.Plots contrasts, i.e. the unconfounded differences between plots within a block. It provides the error variance for Treatments. Similarly, the Blocks and Blocks.Plots lines are confounded with the Tasters.Sittings line and the second Residual line provides the unconfounded Tasters.Sittings contrasts.

The linear model for the experiment is

$$Y = \text{Tasters} + \text{Blocks} + \text{Treatments} + \text{Blocks.Plots} + \text{Tasters.Sittings}.$$

It might be considered desirable to modify the experimental structure for the example to include inter-tier interactions likely to arise. For this purpose, factors from lower tiers have to be included in some tiers' structure formulae. An alternative structure for the example, involving such inter-tier interaction, is as follows:

Tier	Structure formulae
1	Tasters/Sittings
2	(Blocks/Plots)*Tasters
3	Treatments*Tasters.

When writing out the structure for a given tier, relationships between factors within a tier should usually be specified before the inter-tier relationships. This is because structure formulae are 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 may result in terms being incorrectly deleted.

Table 4
Analysis of variance table for a two-phase wine-evaluation experiment

Source	Degrees of freedom
Tasters	$t-1$
Tasters.Sittings	$t(bp-1)$
Blocks	$b-1$
Blocks.Plots	$b(p-1)$
Treatments	$(p-1)$
Residual	$(b-1)(p-1)$
Residual	$(bp-1)(t-1)$

3. Discussion

The method described above involves the division of the factors for an experiment into sets on the basis of the randomization employed in the experiment. These sets have been called 'tiers', this term reflecting the building up of the sets, one on another in an intrinsic order. On the other hand, Nelder's and White's methods allow only two sets of factors, (*unrandomized* and *randomized*), but where this approach is adequate, the resulting structures will represent the physical structure and randomization. Thus the proposed method and Nelder's method will produce the same analysis of variance for the many standard two-tiered designs such as randomized complete blocks, balanced and partially-balanced incomplete blocks, lattices, confounded factorials and split plots. The structures for many of these are discussed by Nelder (1965a, b) and Alvey *et al.* (1977).

While it might be argued that it is possible to obtain effectively the same analysis in fewer tiers than are required to represent the experimental structure, it has been accepted that this is undesirable for two-tiered experiments. Thus, rather than specify the structure of the randomized complete block experiment of §2 in one tier as

$$\text{Tasters} + \text{Wines},$$

it is considered preferable to use a two-tiered structure as described in the previous section. The single-tier structure (i) does not follow the approach suggested by Fisher and followed intuitively by many statisticians in determining the analysis table and error lines for the analysis; (ii) provides no clue to the randomization involved in the experiment; and (iii) does not reflect the experimental structure. In this paper, I have demonstrated that even a dichotomous structure is similarly inadequate in some instances.

Another shortcut sometimes employed in the specification of experiments is to replace a factor in a tier by factors from higher tiers; e.g. for the first example, the structure could be specified as follows:

Tier	Structure formulae
1	Tasters/Wines
2	Wines.

While this may be more efficient from the viewpoint of computer storage, the structure formulae no longer adequately reflect the experimental structure and this can be confusing in more complicated experiments. The same effect is produced by a rule followed in GENSTAT, namely that terms included in both block and treatment models will be deleted from the block model. This also contradicts Rule 4 of Table 2.

A vital step in the procedure is the specification of the crossing and nesting relationships. These relationships are usually thought of as being innate to the experimental material (Nelder, 1965a, b; Millman and Glass, 1967; White, 1975). However, it is evident that the particular relationships which are finally used in the experimental structure depend on the randomization procedures 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 experimental material), 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 experimental structure for a particular experiment depends on the innate physical structure and the randomization employed. It is clear that a structure so based has incorporated the experimental procedures. A further influence on the experimental structure is the subjective assumptions made about the occurrence (or not) of terms. For example, as above, we may or may not decide to assume that there is inter-tier additivity. Thus, the analysis decided upon in a particular instance is not unique to the experimental arrangement.

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Résumé

Une procédure pas à pas pour obtenir la structure expérimentale d'une expérience particulière est présentée avec des règles d'obtention du tableau d'analyse de variance pour cette strucutre. La procédure implique la division des facteurs en grupes, c'est une généralisation de la méthode de Nelder (1965, *Proceedings of the Royal Society, Series A* **283**, 147–162; 1965, *Proceedings of the Royal Society, Series A* **283**, 163–178) à ce que l'on appelle des expériences à plusieurs étages. La méthode proposée est illustrée pour une expérience de dégustation de vin.

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