

RANDOMIZATION-BASED MODELS FOR MULTITIERED EXPERIMENTS: I. A CHAIN OF RANDOMIZATIONS

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We derive randomization-based models for experiments with a chain of randomizations. The estimation theory for these models leads to formulae for the estimators of treatment effects, their standard errors, and expected mean squares in the analysis of variance. We discuss the practicalities in fitting these models and outline the difficulties that can occur, many of which do not arise in two-tiered experiments.

1. Introduction. Bailey [2, 3], following Grundy and Healy [22], outlines a method of deriving randomization-based models for experiments. It provides mixed models that are randomization-based in the sense that it is the group of permutations for the randomization that defines the variance matrix on which the analysis is to be based. It applies to a general class of structures: those derived from a group of permutations. Although this approach is restricted to groups which are stratifiable, in the sense defined in Section 2, it includes all poset block structures and many other structures besides.

A restriction with this approach is that it only applies to a single randomization, as defined by Brien and Bailey [11], in that the randomization can be achieved using a single permutation of the set of observational units. Brien and Bailey [11] describe experiments with multiple randomizations, requiring multiple permutations, and show how to assess the properties of such experiments in [12, 13]. As for the analysis of such experiments, Curnow [20], in correcting the analysis of McIntyre [26], showed how to analyse the results of two-phase experiments by analysis of variance (anova). Wood, Williams and Speed [48] also discussed the analysis of two-phase experiments. Brien in [9] indicated how to use tiers to obtain the anova for multitiered experiments and in [10] derived expected mean squares under a mixed model. Brien and Payne [16] extended the sweep algorithm of Wilkinson [37, 46] to cover anova for multitiered experiments. Brien and Bailey [11] and Brien and Demétrio [14] describe how to analyse the data from such experiments by using mixed models. However, no one has so far given general formulae for the estimators of treatment effects and their standard errors for multitiered experiments, nor have formulae for the expected mean squares under randomization-based models been derived.

Section 2 formulates the randomization-based model for a two-tiered experiment and generalizes it to experiments with two randomizations in a chain. Section 3 describes families of expectation models that lead to a treatment decomposition; the assumption of structure balance is discussed. The properties of anovas corresponding to randomization-based models are outlined in Section 4. Section 5 contains

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a set of examples. Sections 6–9 address the estimation of treatment effects, first for two-tiered experiments and then for various cases of three-tiered experiments. Section 10 generalizes this to an arbitrary number of randomizations in a chain. Section 11 covers the use of software in estimating model parameters, including a discussion of randomization-based models in the class of all mixed models. Statistical inference is discussed in Section 12. Section 13 briefly touches on models other than those described in Section 2. See Section 3 of [12] for definitions of some terms and notation specific to the approach we take.

2. Randomization-based models.

2.1. *The randomization-based model for a two-tiered experiment.* As in [11–13], we randomize the set of objects Γ to another set of objects Υ , so we have a design function $h: \Upsilon \rightarrow \Gamma$. If the objects in Γ are treatments then $h(v)$ is the treatment assigned to unit v in Υ . We associate a structure with each of Υ and Γ . If V_Υ is the space of all real vectors indexed by Υ , then a *structure* on Υ is an orthogonal decomposition of V_Υ . This is specified by a set of symmetric, idempotent, mutually orthogonal matrices projecting onto the subspaces of V_Υ in the decomposition. Similarly, structure on Γ is an orthogonal decomposition of the space V_Γ .

The usual initial assumption for the response Y_v on unit v in Υ is additive:

$$(1) \quad Y_v = w_v + \tau_{h(v)}.$$

In some approaches, w_v is taken to be a constant, but here it is taken to be a random variable, as in [3, 22]. It depends only on the unit v which is providing the response. On the other hand, τ_i , for i in Γ , is a constant. It depends only on the treatment i which is applied to v . Permitting the w_v to be random allows for measurement error, without the assumption of any particular form for it, and any random sampling of units that may occur.

Let G be a group of permutations of Υ . We usually take G to be the largest group of permutations that preserve certain generalized factors on Υ , in the sense that if F is such a generalized factor and $g \in G$ and $F(v_1) = F(v_2)$ then we must have $F(g(v_1)) = F(g(v_2))$. In [2, 3] it is argued that if we randomize by choosing g from G at random then it is appropriate to replace w_v by W_v , which is the mixture of the $w_{g(v)}$ over g in G . Hence we get the randomization-based model

$$(2) \quad Y_v = W_v + \tau_{h(v)},$$

where the W_v are random variables which are exchangeable under G : in particular,

- (P.a) if there is any g in G for which $g(v_1) = v_2$ then W_{v_1} and W_{v_2} have the same distribution, in particular, the same expectation;
- (P.b) if there is any g in G for which $g(v_1) = v_2$ and $g(v_3) = v_4$ then the joint distribution of (W_{v_1}, W_{v_3}) is the same as the joint distribution of (W_{v_2}, W_{v_4}) , in particular, $\text{Cov}(W_{v_1}, W_{v_3}) = \text{Cov}(W_{v_2}, W_{v_4})$.

If the group G is transitive on Υ then property (P.a) is true for all choices of v_1 and v_2 , so we may incorporate the constant value of $E(W_v)$ into each τ_i and so assume that $E(W_v) = 0$ for all v in Υ . We restrict attention to cases where G is transitive, which implies that every unrandomized factor on Υ is equireplicate.

Let \mathbf{Y} and \mathbf{W} be the vectors of the random variables Y_v and W_v respectively. We often represent the design function h by a design matrix \mathbf{X}_h . This is an $\Upsilon \times \Gamma$ matrix with (v, i) -entry equal to 1 if $h(v) = i$ and to 0 otherwise. Then equation (2) can be rewritten in vector form as $\mathbf{Y} = \mathbf{W} + \mathbf{X}_h \boldsymbol{\tau}$, and $E(\mathbf{Y}) = \mathbf{X}_h \boldsymbol{\tau}$.

The pattern in the (co)variance matrix \mathbf{C} of \mathbf{W} is determined by property (P.b), which implies that \mathbf{C} is a patterned matrix with the same entries, including multiplicities, in every row; only their order differs. More specifically, there is a set \mathcal{B} of symmetric $\Upsilon \times \Upsilon$ adjacency matrices \mathbf{B} with entries 0 and 1, whose sum is the all-1 matrix \mathbf{J} , such that if the (v_1, v_2) -entry of \mathbf{B} is equal to 1 then the (v_3, v_4) -entry is equal to 1 if and only if there is some g in G for which either $g(v_1) = v_3$ and $g(v_2) = v_4$ or $g(v_1) = v_4$ and $g(v_2) = v_3$. Moreover, the product of any two adjacency matrices is a linear combination of matrices in \mathcal{B} . Property (P.b) implies that there are (co)variances $\zeta_{\mathbf{B}}$ such that $\mathbf{C} = \sum_{\mathbf{B} \in \mathcal{B}} \zeta_{\mathbf{B}} \mathbf{B}$. For simple orthogonal block structures, this form of \mathbf{C} is the same as the variance matrix for the null randomization distribution given by Nelder [29].

The group G is said to be *stratifiable* [1, 7] if the eigenvectors of the matrix \mathbf{C} do not depend on the values of the entries $\zeta_{\mathbf{B}}$ but depend only on their pattern. Then the common eigenspaces of \mathbf{C} , called *strata*, are the structure on Υ , and the collection of possible variance matrices is said to have *orthogonal variance structure* (OVS). OVS is called ‘orthogonal block structure’ by Houtman and Speed in [23]. Note that there is no linear dependence among the (co)variances $\zeta_{\mathbf{B}}$. Unless otherwise stated, we assume that G is stratifiable and so \mathbf{C} has OVS. Then the number of strata is equal to the number of adjacency matrices.

Let \mathcal{Q} be the collection of symmetric, mutually orthogonal, idempotent matrices projecting onto the strata. Then $\sum_{\mathbf{Q} \in \mathcal{Q}} \mathbf{Q}$ is the $\Upsilon \times \Upsilon$ identity matrix \mathbf{I}_{Υ} , and the variance matrix can be re-expressed as

$$(3) \quad \mathbf{C} = \sum_{\mathbf{Q} \in \mathcal{Q}} \eta_{\mathbf{Q}} \mathbf{Q},$$

with $\eta_{\mathbf{Q}} \geq 0$ for all \mathbf{Q} in \mathcal{Q} . The values $\eta_{\mathbf{Q}}$ are the eigenvalues of \mathbf{C} and are called *spectral components of variance*. The strata are subspaces within which all normalized contrasts have equal variance under randomization, this variance being the η for that stratum. Given \mathcal{Q} , any two matrices of the form (3) commute with each other. The matrices \mathbf{Q} are linear combinations of the matrices \mathbf{B} , and vice-versa, but in general there is no closed-form expression for the coefficients in these combinations.

2.2. Application to poset block structures. The majority of experiments conducted in practice, and all the subsequent examples in this paper, have poset block structures on their units. All poset block structures have stratifiable permutation groups, as shown in [6]. A poset block structure on Υ is defined by a set \mathcal{H} of generalized factors on Υ : see [11]. Following [45], we write $H < F$ if H and F are in \mathcal{H} and H is marginal to F . There are several ways in which to write \mathbf{C} , in terms of matrices and coefficients that depend on H in \mathcal{H} [43, 44]:

$$(4) \quad \mathbf{C} = \sum_{H \in \mathcal{H}} \zeta_H \mathbf{B}_H = \sum_{H \in \mathcal{H}} \psi_H \mathbf{S}_H = \sum_{H \in \mathcal{H}} \eta_H \mathbf{Q}_H.$$

Here ζ_H is the (co)variance under the randomization between elements of Υ with the same level of H but not the same level of any generalized factor F in \mathcal{H} to

which H is marginal; \mathbf{B}_H is the $\Upsilon \times \Upsilon$ adjacency matrix with entry 1 for such pairs and entry 0 otherwise; ψ_H is a canonical component; \mathbf{S}_H is the $\Upsilon \times \Upsilon$ relationship matrix [24] for H , with (v_1, v_2) -entry equal to 1 if v_1 and v_2 have the same level of H and to 0 otherwise. Thus $\mathbf{S}_H = \sum_{F \geq H} \mathbf{B}_F$. If k_H is the common replication of all levels of H , then $k_H^{-1} \mathbf{S}_H = \sum_{F < H} \mathbf{Q}_F$. When H is the generalized factor consisting of all factors on Υ , the subscript H will sometimes be replaced by Υ , while the subscript for the generalized factor corresponding to the overall mean is denoted 0. Expressions in [43, 44] show how to convert one set of coefficients in equation (4) to another. In particular,

$$(5) \quad \eta_H = \sum_{F \geq H} k_F \psi_F.$$

The natural interpretation of *canonical components* in this context is as components of excess covariance [32]. They are linear combinations of the covariances (ζ parameters) [29, 32, 44]. Except for ψ_Υ , which is the variance of each individual response, they measure the covariation, between the responses on the units in Υ , contributed by each particular generalized factor in excess of that of any generalized factor which is marginal to it. Thus ψ_H can be negative when $\zeta_H < \zeta_F$ and $F < H$, although $\psi_\Upsilon > 0$. This is in contrast to nonnegative variance components σ_H^2 , which occur in the usual formulations of mixed models that we discuss in Section 11. Estimates of standard errors of treatment effects require estimates of the spectral components. On the other hand, scientifically interesting hypotheses about the canonical components are often formulated and tested [19, 32] (see also Section 11.3) and so estimates of them may also be required.

2.3. *The randomization-based model for an experiment with two randomizations in a chain.* For a chain of two randomizations, there are three sets: Υ is randomized to Ω , and Γ is randomized to Υ . Let the corresponding design maps be $f: \Omega \rightarrow \Upsilon$ and $h: \Upsilon \rightarrow \Gamma$, as in Figure 1. The elements of Γ will be referred to as treatments and Υ and Ω as unrandomized sets.

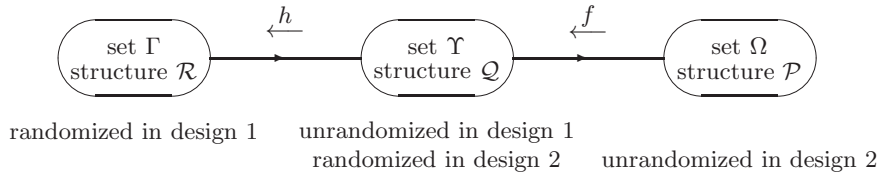


FIG 1. *Diagram of an experiment with two randomizations in a chain*

Suppose that f is randomized by choosing a random permutation from the group G_1 of permutations of Ω , and that G_1 is stratifiable with stratum projectors \mathbf{P} , for \mathbf{P} in \mathcal{P} . Like the matrices \mathbf{Q} in Section 2.1, the matrices \mathbf{P} are known orthogonal idempotents summing to the $\Omega \times \Omega$ identity matrix \mathbf{I}_Ω . In Section 2.1 the size of the idempotents is the size of Υ , while here it is the size of Ω .

Now let Y_ω be the response on observational unit ω in Ω . Applying the randomization argument from Section 2.1 to f gives $Y_\omega = Z_\omega + \tilde{Y}_{f(\omega)}$, where Z_ω is a random variable depending only on the unit ω and \tilde{Y}_v is a notional effect associated with unit v in Υ . Because G_1 is stratifiable, we can assume that the random variables

Z_ω are identically distributed with mean zero, and that $\text{Cov}(\mathbf{Z}) = \sum_{\mathbf{A} \in \mathcal{A}} \gamma_{\mathbf{A}} \mathbf{A}$, where \mathcal{A} is the set of adjacency matrices arising from G_1 and the $\gamma_{\mathbf{A}}$ are the associated (co)variances. Following Section 2.1, we can also write $\text{Cov}(\mathbf{Z}) = \sum_{\mathbf{P} \in \mathcal{P}} \xi_{\mathbf{P}} \mathbf{P}$ where, like the quantities $\eta_{\mathbf{Q}}$, the $\xi_{\mathbf{P}}$ are unknown nonnegative coefficients. Then $\text{Cov}(\mathbf{Z})$ has OVS because G_1 is stratifiable.

Similarly, h is randomized by choosing a random permutation from the group G_2 of permutations of Υ , and G_2 is stratifiable with $\Upsilon \times \Upsilon$ stratum projectors \mathbf{Q} , for \mathbf{Q} in \mathcal{Q} , as in Section 2.1. Rewriting equation (2) as $\tilde{Y}_v = W_v + \tau_{h(v)}$ gives

$$(6) \quad Y_\omega = Z_\omega + \tilde{Y}_{f(\omega)} = Z_\omega + W_{f(\omega)} + \tau_{h(f(\omega))}.$$

In turn, this randomization-based model can be rewritten in vector form as $\mathbf{Y} = \mathbf{Z} + \mathbf{X}_f \mathbf{W} + \mathbf{X}_f \mathbf{X}_h \boldsymbol{\tau}$, where \mathbf{X}_f is the $\Omega \times \Upsilon$ design matrix for f . Hence $\text{E}(\mathbf{Y}) = \mathbf{X}_f \mathbf{X}_h \boldsymbol{\tau}$, and the variance matrix \mathbf{V} of \mathbf{Y} is given by

$$\mathbf{V} = \text{Cov}(\mathbf{Z} + \mathbf{X}_f \mathbf{W}) = \sum_{\mathbf{A} \in \mathcal{A}} \gamma_{\mathbf{A}} \mathbf{A} + \sum_{\mathbf{B} \in \mathcal{B}} \zeta_{\mathbf{B}} \mathbf{X}_f \mathbf{B} \mathbf{X}'_f = \sum_{\mathbf{P} \in \mathcal{P}} \xi_{\mathbf{P}} \mathbf{P} + \sum_{\mathbf{Q} \in \mathcal{Q}} \eta_{\mathbf{Q}} \mathbf{X}_f \mathbf{Q} \mathbf{X}'_f,$$

because \mathbf{Z} and \mathbf{W} are independent. The two sets \mathcal{P} and \mathcal{Q} of idempotents correspond to the eigenspaces of the variance matrices of \mathbf{Z} and \mathbf{W} , respectively, but not necessarily to those of \mathbf{V} . Although the coefficients $\xi_{\mathbf{P}}$ and $\eta_{\mathbf{Q}}$ may not be eigenvalues of \mathbf{V} , we still call them spectral components of variance because they are the eigenvalues of $\text{Cov}(\mathbf{Z})$ and $\text{Cov}(\mathbf{W})$ respectively.

As noted in [12], the effect of the design function f is to embed a copy V_{Υ}^f of V_{Υ} inside the space V_{Ω} of real vectors indexed by Ω . Let \mathbf{D}_f be the $\Upsilon \times \Upsilon$ diagonal matrix whose (ν, ν) -entry is the replication of unit ν . Then $\mathbf{X}'_f \mathbf{X}_f = \mathbf{D}_f$, and the matrix of orthogonal projection onto V_{Υ}^f is $\mathbf{X}_f \mathbf{D}_f^{-1} \mathbf{X}'_f$.

To further simplify \mathbf{V} , the design f must be equireplicate. If \mathbf{Q}_1 and \mathbf{Q}_2 are in \mathcal{Q} then $(\mathbf{X}_f \mathbf{Q}_1 \mathbf{X}'_f)(\mathbf{X}_f \mathbf{Q}_2 \mathbf{X}'_f) = \mathbf{X}_f \mathbf{Q}_1 \mathbf{D}_f \mathbf{Q}_2 \mathbf{X}'_f$. If the common replication is r then $\mathbf{D}_f = r \mathbf{I}_{\Upsilon}$, so if we put $\mathbf{Q}^f = r^{-1} \mathbf{X}_f \mathbf{Q} \mathbf{X}'_f$ then the \mathbf{Q}^f are mutually orthogonal idempotents summing to $r^{-1} \mathbf{X}_f \mathbf{X}'_f$, which is the matrix of orthogonal projection onto the subspace V_{Υ}^f . To simplify notation, as in [12] we shall write \mathbf{Q}^f just as \mathbf{Q} , $\{\mathbf{Q}^f : \mathbf{Q} \in \mathcal{Q}\}$ as \mathcal{Q} , and $r^{-1} \mathbf{X}_f \mathbf{X}'_f$ as $\mathbf{I}_{\mathcal{Q}}$ in the three-tiered context. Thus we have

$$(7) \quad \mathbf{V} = \sum_{\mathbf{P} \in \mathcal{P}} \xi_{\mathbf{P}} \mathbf{P} + r \sum_{\mathbf{Q} \in \mathcal{Q}} \eta_{\mathbf{Q}} \mathbf{Q}.$$

The formula for \mathbf{V} in equation (7) appears very similar to that in equation (2) of [48]. There are three differences. Here, the two collections of idempotents sum to \mathbf{I} and $\mathbf{I}_{\mathcal{Q}}$ respectively, whereas those in [48] both sum to \mathbf{I} . Equation (7) is justified by the randomization; the formula in [48] is an assumed model. Moreover, [48] does not require f to be equireplicate, so the parametrization does not explicitly include the replication r .

2.4. *Pairs of poset block structures.* If the structure on Υ is a poset block structure with set \mathcal{H}_2 of generalized factors, then $r \sum_{H \in \mathcal{H}_2} \eta_H \mathbf{Q}_H^f = \sum_{H \in \mathcal{H}_2} \psi_H \mathbf{S}_H^f$, where $\mathbf{S}_H^f = \mathbf{X}_f \mathbf{S}_H \mathbf{X}'_f$ which is the $\Omega \times \Omega$ relationship matrix for H when it is regarded as a factor on Ω , in which case the common replication of its levels is $r k_H$. If we now write \mathbf{S}_H^f just as \mathbf{S}_H , we have $r \sum_{H \in \mathcal{H}_2} \eta_H \mathbf{Q}_H = \sum_{H \in \mathcal{H}_2} \psi_H \mathbf{S}_H$.

Suppose that the structure on Ω is also a poset block structure, with set \mathcal{H}_1 of generalized factors. For H in \mathcal{H}_1 , let the $\Omega \times \Omega$ relationship matrix for H be \mathbf{T}_H , with corresponding canonical component of variance ϕ_H and common replication k_H . Then

$$\sum_{H \in \mathcal{H}_1} \xi_H \mathbf{P}_H = \sum_{H \in \mathcal{H}_1} \phi_H \mathbf{T}_H \quad \text{and} \quad \xi_H = \sum_{F \in \mathcal{H}_1, F \geq H} k_F \phi_F.$$

Thus, when both structures are poset block structures, equation (7) becomes

$$(8) \quad \mathbf{V} = \sum_{H \in \mathcal{H}_1} \phi_H \mathbf{T}_H + \sum_{H \in \mathcal{H}_2} \psi_H \mathbf{S}_H.$$

As noted in Section 2.2, even for poset block structures the randomization-based model for variance differs from a variance-components model. In equation (7), it is the coefficients $\xi_{\mathbf{P}}$ and $\eta_{\mathbf{Q}}$ which must be nonnegative; the corresponding canonical components may well be negative, except for ϕ_{Ω} and ψ_{Υ} , which must be positive.

3. Treatment decomposition and structure balance.

3.1. *Families of expectation models in a two-tiered experiment.* Consider the two-tiered set-up in Section 2.1. The design function h embeds a copy V_{Γ}^h of V_{Γ} inside V_{Υ} . Let \mathbf{D}_h be the $\Gamma \times \Gamma$ diagonal matrix of replications of treatments. Then $\mathbf{X}'_h \mathbf{X}_h = \mathbf{D}_h$, and the matrix of orthogonal projection onto V_{Γ}^h is $\mathbf{X}_h \mathbf{D}_h^{-1} \mathbf{X}'_h$, which we write as $\mathbf{I}_{\mathcal{R}}$, because we always associate a structure \mathcal{R} with Γ . The elements of \mathcal{R} are derived from a family \mathcal{M} of expectation models on Γ , as we now show.

With treatment effects fixed, data analysis usually proceeds by selecting a model from \mathcal{M} and then estimating the parameters of the chosen model: see [4]. We assume that \mathcal{M} defines an orthogonal decomposition of V_{Γ} , in the following sense. There is a collection \mathcal{R} of $\Gamma \times \Gamma$ symmetric, mutually orthogonal, idempotent matrices whose sum is the $\Gamma \times \Gamma$ identity matrix \mathbf{I}_{Γ} ; each nonzero model in \mathcal{M} is the subspace of V_{Γ} corresponding to a sum of one or more of the idempotents in \mathcal{R} ; if M is such a model then there is at least one idempotent \mathbf{R} in \mathcal{R} such that $\text{Im}(\mathbf{R}) \leq M$ and $M \cap (\text{Im}(\mathbf{R}))^{\perp}$ is in \mathcal{M} ; each \mathbf{R} in \mathcal{R} occurs at least once in this way, so that it corresponds to the extra sum of squares for fitting a larger model compared to a smaller model.

For \mathbf{R} in \mathcal{R} , the subspace $\text{Im}(\mathbf{R})$ of V_{Γ} is translated by h into a subspace of V_{Γ}^h whose $\Upsilon \times \Upsilon$ matrix of orthogonal projection is $\mathbf{X}_h \mathbf{R} (\mathbf{R} \mathbf{D}_h \mathbf{R})^{-1} \mathbf{R} \mathbf{X}'_h$. We require that h have the property that all such matrices commute with each other. When \mathcal{M} is defined by a collection of orthogonal factors on Γ , this requirement is equivalent to the condition that the factors remain orthogonal when considered as factors on Υ . In the two-tiered context, we shall write \mathbf{R}^h and $\{\mathbf{R}^h : \mathbf{R} \in \mathcal{R}\}$ simply as \mathbf{R} and \mathcal{R} from now on, so that $\sum_{\mathbf{R} \in \mathcal{R}} \mathbf{R} = \mathbf{I}_{\mathcal{R}}$.

There is no requirement for the design h to be equireplicate. For example, suppose that Γ consists of the two levels of a treatment factor. If we parameterize the expectations as $\mu + \alpha$ and $\mu - \alpha$ then the estimators are not orthogonal unless the levels are equally replicated. Choice of parametrization should not affect model fitting, so we prefer to have one model M_1 in which we parameterize the expectations as α_1 and α_2 , with a submodel M_2 in which they are both μ , and a further submodel M_3 in which both expectations are zero. Then we do have orthogonality, with $\mathcal{R} = \{\mathbf{R}_1, \mathbf{R}_0\}$, where $\mathbf{R}_0 = |\Upsilon|^{-1} \mathbf{J}$, which is the projector for the grand mean, and $\mathbf{R}_1 = \mathbf{I}_{\mathcal{R}} - \mathbf{R}_0$.

3.2. *Structure balance in a two-tiered experiment.* Until Section 9 inclusive, we insist that h be such that \mathcal{R} is structure balanced in relation to \mathcal{Q} , in the sense defined in [12]. This means that there are scalars $\lambda_{\mathbf{QR}}$, for \mathbf{Q} in \mathcal{Q} and \mathbf{R} in \mathcal{R} , such that $\mathbf{RQI}_{\mathcal{R}} = \lambda_{\mathbf{QR}}\mathbf{R}$. This equation means that (i) $\mathbf{RQR} = \lambda_{\mathbf{QR}}\mathbf{R}$ and (ii) if $\mathbf{R}_1 \neq \mathbf{R}_2$ then $\mathbf{R}_1\mathbf{QR}_2 = \mathbf{0}$. The scalars $\lambda_{\mathbf{QR}}$ are called *efficiency factors*. It follows that each \mathbf{Q} is the sum of the following mutually orthogonal idempotents: (i) $\mathbf{Q} \triangleright \mathbf{R}$, for all \mathbf{R} in \mathcal{R} with $\lambda_{\mathbf{QR}} \neq 0$, and (ii) if it is nonzero, $\mathbf{Q} \vdash \mathcal{R}$. These idempotents are defined by $\mathbf{Q} \triangleright \mathbf{R} = \lambda_{\mathbf{QR}}^{-1}\mathbf{QRQ}$ and $\mathbf{Q} \vdash \mathcal{R} = \mathbf{Q} - \sum'_{\mathbf{R} \in \mathcal{R}} \mathbf{Q} \triangleright \mathbf{R}$, where the summation is over those \mathbf{R} for which $\lambda_{\mathbf{QR}} \neq 0$. This set of idempotents is denoted $\mathcal{Q} \triangleright \mathcal{R}$ in [12].

For each \mathbf{R} in \mathcal{R} , the efficiency factors $\lambda_{\mathbf{QR}}$ are nonnegative and sum to 1. If each \mathbf{R} has some \mathbf{Q} in \mathcal{Q} such that $\lambda_{\mathbf{QR}} = 1$ then the structure \mathcal{R} is said to be *orthogonal* in relation to the structure \mathcal{Q} .

Note that the matrices \mathbf{Q} are determined by the group of permutations used for randomizing, and hence ultimately by the relevant information about Υ , such as blocks or managerial constraints. On the other hand, the matrices \mathbf{R} depend on the family of expectation models chosen as appropriate. The former cannot be altered, but the latter may be refined, perhaps using pseudofactors, in order to achieve structure balance [27, 49]. This is achieved by judicious replacement of some matrices \mathbf{R} in \mathcal{R} by sub-idempotents so that there is a refinement of the decomposition given by \mathcal{R} into smaller subspaces: see [12], Section 4. Thus we have a larger collection \mathcal{R}^* of mutually orthogonal idempotents, such that each \mathbf{R} in \mathcal{R} is a sum of one or more of the idempotents in \mathcal{R}^* . For example, in a balanced lattice square design for k^2 treatments in $(k+1)/2$ squares, where k is odd, $\mathcal{R} = \{\mathbf{R}_0, \mathbf{R}_T\}$ where \mathbf{R}_0 and \mathbf{R}_T are the idempotents for the Mean and Treatments, respectively. However, \mathcal{R} is not structure balanced in relation to the structure \mathcal{Q} defined by $(k+1)/2$ squares, each formed by k rows crossed with k columns. We form \mathcal{R}^* by replacing \mathbf{R}_T by $\mathbf{R}_{T,R}$ and $\mathbf{R}_{T,C}$, where these are the idempotents corresponding to the treatment subspaces partly confounded with rows and columns, respectively: then \mathcal{R}^* is structure balanced in relation to \mathcal{Q} (see [12], Example 5).

3.3. *Treatment structure and structure balance in a three-tiered experiment with two randomizations in a chain.* Now consider the three-tiered set-up in Section 2.3. As in Section 3.1, the effects τ are taken to be fixed, and so we assume that the family of expectation models gives a set of mutually orthogonal idempotents \mathbf{R} in \mathcal{R} whose sum is the orthogonal projector onto V_{Γ}^h in V_{Υ} . Let \mathbf{M}^h be the $\Upsilon \times \Upsilon$ idempotent for one of these expectation models. The corresponding $\Omega \times \Omega$ idempotent $(\mathbf{M}^h)^f$ is given by $(\mathbf{M}^h)^f = \mathbf{X}_f \mathbf{M}^h (\mathbf{M}^h \mathbf{D}_f \mathbf{M}^h)^- \mathbf{M}^h \mathbf{X}'_f = r^{-1} \mathbf{X}_f \mathbf{M}^h \mathbf{X}'_f$ since $\mathbf{D}_f = r^{-1} \mathbf{I}_{\Upsilon}$. Therefore, putting $\mathbf{R}^f = r^{-1} \mathbf{X}_f \mathbf{R} \mathbf{X}'_f$ for \mathbf{R} in \mathcal{R} , we see that the mutually orthogonal idempotents \mathbf{R} in \mathcal{R} translate to mutually orthogonal idempotents \mathbf{R}^f on V_{Ω} . That is, because f is equireplicate, the same formula is used to convert both the expectation idempotents and the variance idempotents from $\Upsilon \times \Upsilon$ matrices to $\Omega \times \Omega$ matrices. There is still no need for h to be equireplicate. As in [12], we shall write \mathbf{R}^f as \mathbf{R} and $\{\mathbf{R}^f : \mathbf{R} \in \mathcal{R}\}$ as \mathcal{R} in the three-tiered context. We continue to write $\sum_{\mathbf{R} \in \mathcal{R}} \mathbf{R}$ as $\mathbf{I}_{\mathcal{R}}$, which is now an $\Omega \times \Omega$ matrix.

In addition to the condition that f be equireplicate, we assume until Section 9 inclusive that

- (i) \mathcal{Q} is structure balanced in relation to \mathcal{P} , or can be made so, in the sense

explained in Section 3.4;

(ii) \mathcal{R} is structure balanced in relation to \mathcal{Q} .

Then \mathcal{R} is structure balanced in relation to $\mathcal{P} \triangleright \mathcal{Q}$, $\mathcal{Q} \triangleright \mathcal{R}$ is structure balanced in relation to \mathcal{P} , and $(\mathcal{P} \triangleright \mathcal{Q}) \triangleright \mathcal{R} = \mathcal{P} \triangleright (\mathcal{Q} \triangleright \mathcal{R})$, as shown in [12].

Let \mathcal{Q}_1 be the set of \mathbf{Q} in \mathcal{Q} for which there is an idempotent \mathbf{P} in \mathcal{P} with $\lambda_{\mathbf{P}\mathbf{Q}} = 1$. Define the function c from \mathcal{Q}_1 to \mathcal{P} such that $c(\mathbf{Q}) = \mathbf{P}$ for $\lambda_{\mathbf{P}\mathbf{Q}} = 1$. If $\mathbf{Q} \in \mathcal{Q}_1$ then $\text{Im}(\mathbf{Q}) \leq \text{Im}(c(\mathbf{Q}))$, and $\mathbf{Q}\mathbf{P} = \mathbf{P}\mathbf{Q} = \mathbf{Q} = \mathbf{P} \triangleright \mathbf{Q}$ if $\mathbf{P} = c(\mathbf{Q})$, while $\mathbf{Q}\mathbf{P} = \mathbf{P}\mathbf{Q} = \mathbf{0}$ otherwise. Thus \mathcal{Q} is orthogonal in relation to \mathcal{P} when $\mathcal{Q}_1 = \mathcal{Q}$.

For $\mathbf{P} \in \mathcal{P}$, equation (7) shows that $\mathbf{V}(\mathbf{P} \vdash \mathcal{Q}) = \xi_{\mathbf{P}}(\mathbf{P} \vdash \mathcal{Q})$, because $(\mathbf{P} \vdash \mathcal{Q})\mathbf{Q} = \mathbf{0}$ for all \mathbf{Q} in \mathcal{Q} . Hence $\text{Im}(\mathbf{P} \vdash \mathcal{Q})$ is contained in an eigenspace of \mathbf{V} with eigenvalue $\xi_{\mathbf{P}}$. Moreover, if $\mathbf{Q} \in \mathcal{Q}$ and $\lambda_{\mathbf{P}\mathbf{Q}} \neq 0$, then

$$\mathbf{V}(\mathbf{P} \triangleright \mathbf{Q}) = \mathbf{V} \frac{\mathbf{P}\mathbf{Q}\mathbf{P}}{\lambda_{\mathbf{P}\mathbf{Q}}} = \frac{\xi_{\mathbf{P}}}{\lambda_{\mathbf{P}\mathbf{Q}}} \mathbf{P}\mathbf{Q}\mathbf{P} + r \sum_{\mathbf{Q}^*} \frac{\eta_{\mathbf{Q}^*}}{\lambda_{\mathbf{P}\mathbf{Q}}} \mathbf{Q}^* \mathbf{P}\mathbf{Q}\mathbf{P} = \xi_{\mathbf{P}}(\mathbf{P} \triangleright \mathbf{Q}) + r\eta_{\mathbf{Q}}\mathbf{Q}\mathbf{P}.$$

If $\mathbf{Q} \in \mathcal{Q}_1$ and $\mathbf{P} = c(\mathbf{Q})$ then $\text{Im}(\mathbf{P} \triangleright \mathbf{Q})$ is contained in an eigenspace of \mathbf{V} with eigenvalue $\xi_{\mathbf{P}} + r\eta_{\mathbf{Q}}$. Otherwise, $\text{Im}(\mathbf{P} \triangleright \mathbf{Q})$ is not contained in any eigenspace of \mathbf{V} .

If \mathcal{Q} is orthogonal in relation to \mathcal{P} then

$$(9) \quad \mathbf{V} = \sum_{\mathbf{Q} \in \mathcal{Q}} (\xi_{c(\mathbf{Q})} + r\eta_{\mathbf{Q}})\mathbf{Q} + \sum_{\mathbf{P} \in \mathcal{P}} \xi_{\mathbf{P}}(\mathbf{P} \vdash \mathcal{Q}).$$

The idempotents in this expression are those in $\mathcal{P} \triangleright \mathcal{Q}$, and the the image of each is contained in an eigenspace of \mathbf{V} . Thus the set of all positive semidefinite (p.s.d) matrices of the form (9) commute with each other, and have common eigenspaces: we call this *commutative variance structure* (CVS). If, in addition, there is no linear dependence among the coefficients in (9), we have OVS.

3.4. Choice of idempotents. The matrices \mathbf{P} are defined by the group G_1 of permutations used to randomize the design f . The matrices \mathbf{Q} are first defined as matrices on V_{Υ} by the group G_2 of permutations used to randomize the design h , and then translated by f to matrices on V_{Ω} . The matrices \mathbf{R} depend initially on the chosen family of expectation models, and are translated by h and then by f .

Strictly speaking, there is no freedom of choice over the \mathbf{Q} matrices. However, as already outlined for design h in Section 3.2, it is sometimes possible to turn a design f without structure balance into one with structure balance by judicious replacement of some matrices \mathbf{Q} in \mathcal{Q} by sub-idempotents, yielding \mathcal{Q}^* . The variance matrix in equation (7) is defined by the original \mathcal{Q} : when it is rewritten in terms of \mathcal{Q}^* it has the constraint that if \mathbf{Q} in \mathcal{Q} is the sum $\mathbf{Q}_1^* + \dots + \mathbf{Q}_n^*$ with \mathbf{Q}_i^* in \mathcal{Q}^* then each of $\mathbf{Q}_1^*, \dots, \mathbf{Q}_n^*$ has the *same* spectral component $\eta_{\mathbf{Q}}$.

There are two types of multiple randomization that form a chain as shown in Figure 1: see [11, 12]. For *composed* randomizations, the randomizations may be done in either order, because neither needs knowledge of the outcome of the other. In contrast, *randomized-inclusive* randomizations have the complication that knowledge of the outcome of the randomization of Γ to Υ is needed before Υ can be randomized to Ω .

As explained in [11], Section 5.1 and [12], Section 6, this knowledge is needed in the second case partly because the structure \mathcal{Q} on Υ defined by the randomization of design h is not structure balanced in relation to \mathcal{P} . Thus \mathcal{Q} needs to be refined

into sub-idempotents or pseudosources, as described above. The second necessary ingredient for randomized-inclusive randomizations is that there is at least one source on Γ that is confounded or partly confounded with one of the sources on Υ that needs to be split up. In order to work out the partial confounding of sources on Γ with those on Ω , it is necessary to keep track of the partial confounding of the former with the pseudosources on Υ . This may require pseudosources on Γ . Most importantly, the unrandomized version of f is constrained to ensure the correct partial confounding of (pseudo)sources on Γ with those on Ω .

Although this makes the procedure more complicated than that for composed randomizations, the randomization-based model is virtually the same. As above, we have to keep track of pseudosources. For the pseudosources on Υ , it is important to remember that pseudosources of the same source have the *same* spectral component η . This complication can occur for experiments with two composed randomizations when the second randomization is not consonant: see Example 2. It always occurs for experiments with two randomized-inclusive randomizations: see Example 4.

4. Analysis of variance.

4.1. *A two-tiered experiment.* Consider the two-tiered experiment in Sections 2.1 and 3.2. In [12] decomposition tables were used to display the decomposition of V_Υ appropriate for such an experiment. Such a table is a precursor to an anova table and consists of rows and columns. There is a set of columns for each tier: one column containing sources, one column containing degrees of freedom, and, if the design is structure balanced but not orthogonal, a further column showing efficiency factors. The sources and pseudosources correspond to idempotents in \mathcal{Q} or \mathcal{R} which, when they are based on generalized (pseudo)factors, are labelled as described in Section 3 of [12]. Each row of the decomposition table corresponds to a subspace in the decomposition specified by $\mathcal{Q} \triangleright \mathcal{R}$. In this paper, we add a column for expected mean squares to decomposition tables in order to form skeleton anova tables.

The anova table for the analysis of a response variable when the variance matrix has the form (3), the τ_i are fixed effects and \mathcal{R} is structure balanced in relation to \mathcal{Q} is given in [2, 23, 30]. The data vector \mathbf{y} is projected onto each stratum in turn and then $\mathbf{Q}\mathbf{y}$, which is the projection into stratum $\text{Im}(\mathbf{Q})$, is further decomposed according to the elements of $\mathcal{Q} \triangleright \mathcal{R}$ involving \mathbf{Q} . The following hold.

- (A.a) The projections onto different strata are uncorrelated.
- (A.b) Any orthonormal basis for $\text{Im}(\mathbf{Q})$ gives uncorrelated random variables all with variance $\eta_{\mathbf{Q}}$.
- (A.c) If $\lambda_{\mathbf{QR}} \neq 0$, then the expected mean square for $\mathbf{Q} \triangleright \mathbf{R}$ is equal to

$$\eta_{\mathbf{Q}} + \frac{\lambda_{\mathbf{QR}} \boldsymbol{\tau}' \mathbf{X}'_h \mathbf{R} \mathbf{X}_h \boldsymbol{\tau}}{\text{rank}(\mathbf{R})}.$$

- (A.d) If $\mathbf{Q} \vdash \mathcal{R}$ is nonzero, then the expected mean square for $\mathbf{Q} \vdash \mathcal{R}$ is equal to $\eta_{\mathbf{Q}}$.

For poset block structures, the spectral component $\eta_{\mathbf{Q}}$ can be expanded using equation (5) to provide expressions for the expected mean squares in terms of the canonical components.

The expression $\boldsymbol{\tau}' \mathbf{X}'_h \mathbf{R} \mathbf{X}_h \boldsymbol{\tau} / \text{rank}(\mathbf{R})$ in (A.c) is a p.s.d. quadratic form in the parameters τ_i . If \mathcal{R} is defined by a poset block structure on Γ then $\mathbf{R} = \mathbf{R}_F$ for a

generalized factor F on Γ , just as $\mathbf{Q} = \mathbf{Q}_H$ in equation (4). In anova tables, this expression is written as $q(F)$. In particular, $q_0 = \boldsymbol{\tau}'\mathbf{X}'_h\mathbf{R}_0\mathbf{X}_h\boldsymbol{\tau}$, where $\mathbf{R}_0 = |\Upsilon|^{-1}\mathbf{J}$.

4.2. *An experiment with two randomizations in a chain.* First consider expectations. If $\mathbf{P} \in \mathcal{P}$ then $(\mathbf{P} \vdash \mathbf{Q})\mathbf{I}_\mathcal{Q} = \mathbf{0}$. If, further, $\mathbf{Q} \in \mathcal{Q}$ and $\lambda_{\mathbf{PQ}} \neq 0$, then $((\mathbf{P} \triangleright \mathbf{Q}) \vdash \mathcal{R})\mathbf{I}_\mathcal{Q}\mathbf{I}_\mathcal{R} = \mathbf{0}$. Since $\mathbf{E}(\mathbf{Y}) = \mathbf{X}_f\mathbf{X}_h\boldsymbol{\tau} = \mathbf{I}_\mathcal{Q}\mathbf{I}_\mathcal{R}\mathbf{X}_f\mathbf{X}_h\boldsymbol{\tau}$, it follows that $\mathbf{E}((\mathbf{P} \triangleright \mathbf{Q})\mathbf{Y}) = \mathbf{E}(((\mathbf{P} \triangleright \mathbf{Q}) \vdash \mathcal{R})\mathbf{Y}) = \mathbf{0}$. If, moreover, $\mathbf{R} \in \mathcal{R}$ and $\lambda_{\mathbf{QR}} \neq 0$, Section 5 of [12] shows that $(\mathbf{P} \triangleright \mathbf{Q}) \triangleright \mathbf{R} = \lambda_{\mathbf{PQ}}^{-1}\lambda_{\mathbf{QR}}^{-1}\mathbf{PQRQP}$. Therefore

$$\mathbf{E}(((\mathbf{P} \triangleright \mathbf{Q}) \triangleright \mathbf{R})\mathbf{Y}) = \frac{1}{\lambda_{\mathbf{PQ}}\lambda_{\mathbf{QR}}}\mathbf{PQRQP}\mathbf{I}_\mathcal{Q}\mathbf{I}_\mathcal{R}\mathbf{X}_f\mathbf{X}_h\boldsymbol{\tau} = \mathbf{PQRX}_f\mathbf{X}_h\boldsymbol{\tau}.$$

Hence

$$\begin{aligned} (\mathbf{E}(((\mathbf{P} \triangleright \mathbf{Q}) \triangleright \mathbf{R})\mathbf{Y}))'\mathbf{E}(((\mathbf{P} \triangleright \mathbf{Q}) \triangleright \mathbf{R})\mathbf{Y}) &= \boldsymbol{\tau}'\mathbf{X}'_h\mathbf{X}'_f\mathbf{RQPPQRX}_f\mathbf{X}_h\boldsymbol{\tau} \\ &= \lambda_{\mathbf{PQ}}\lambda_{\mathbf{QR}}\boldsymbol{\tau}'\mathbf{X}'_h\mathbf{X}'_f\mathbf{R}\mathbf{X}_f\mathbf{X}_h\boldsymbol{\tau}. \end{aligned}$$

Consider a fixed \mathbf{P} in \mathcal{P} . Equation (7) shows that

$$\begin{aligned} \text{Cov}(\mathbf{PY}) &= \mathbf{PVP} = \xi_{\mathbf{P}}\mathbf{P} + r \sum_{\mathbf{Q} \in \mathcal{Q}} \eta_{\mathbf{Q}}\mathbf{PQP} = \xi_{\mathbf{P}}\mathbf{P} + r \sum_{\mathbf{Q} \in \mathcal{Q}} \eta_{\mathbf{Q}}\lambda_{\mathbf{PQ}}\mathbf{P} \triangleright \mathbf{Q} \\ (10) \quad &= \sum_{\mathbf{Q} \in \mathcal{Q}}' (\xi_{\mathbf{P}} + r\lambda_{\mathbf{PQ}}\eta_{\mathbf{Q}})(\mathbf{P} \triangleright \mathbf{Q}) + \xi_{\mathbf{P}}(\mathbf{P} \vdash \mathcal{Q}). \end{aligned}$$

Here $\sum'_{\mathbf{Q} \in \mathcal{Q}}$ denotes summation over $\mathbf{Q} \in \mathcal{Q}$ with $\lambda_{\mathbf{PQ}} \neq 0$. The matrices in equation (10) are mutually orthogonal idempotents which sum to \mathbf{P} and have linearly independent coefficients. Hence they are the projectors onto the eigenspaces of $\text{Cov}(\mathbf{PY})$ with nonzero eigenvalues. Therefore the results for \mathbf{Y} in Section 4.1 carry over to \mathbf{PY} as follows.

- (A.e) The projections onto any two different subspaces of the form $\text{Im}(\mathbf{P} \triangleright \mathbf{Q})$ or $\text{Im}(\mathbf{P} \vdash \mathcal{Q})$ are uncorrelated.
- (A.f) If $\lambda_{\mathbf{PQ}} \neq 0$, any orthonormal basis for $\text{Im}(\mathbf{P} \triangleright \mathbf{Q})$ gives uncorrelated random variables all with variance $\xi_{\mathbf{P}} + r\lambda_{\mathbf{PQ}}\eta_{\mathbf{Q}}$.
- (A.g) Any orthonormal basis for $\text{Im}(\mathbf{P} \vdash \mathcal{Q})$ gives uncorrelated random variables all with variance $\xi_{\mathbf{P}}$.
- (A.h) If $\lambda_{\mathbf{PQ}}\lambda_{\mathbf{QR}} \neq 0$, then the expected mean square for $(\mathbf{P} \triangleright \mathbf{Q}) \triangleright \mathbf{R}$ is

$$\xi_{\mathbf{P}} + r\lambda_{\mathbf{PQ}}\eta_{\mathbf{Q}} + \frac{\lambda_{\mathbf{PQ}}\lambda_{\mathbf{QR}}\boldsymbol{\tau}'\mathbf{X}'_h\mathbf{X}'_f\mathbf{R}\mathbf{X}_f\mathbf{X}_h\boldsymbol{\tau}}{\text{rank}(\mathbf{R})}.$$

- (A.i) If $\lambda_{\mathbf{PQ}} \neq 0$ and $(\mathbf{P} \triangleright \mathbf{Q}) \vdash \mathcal{R}$ is nonzero, then the expected mean square for $(\mathbf{P} \triangleright \mathbf{Q}) \vdash \mathcal{R}$ is $\xi_{\mathbf{P}} + r\lambda_{\mathbf{PQ}}\eta_{\mathbf{Q}}$.
- (A.j) If $\mathbf{P} \vdash \mathcal{Q}$ is nonzero, then the expected mean square for $\mathbf{P} \vdash \mathcal{Q}$ is $\xi_{\mathbf{P}}$.

For poset block structures, the spectral components $\xi_{\mathbf{P}}$ and $\eta_{\mathbf{Q}}$ can be expanded to express the expected mean squares in terms of the canonical components.

We write the expression $\boldsymbol{\tau}'\mathbf{X}'_h\mathbf{X}'_f\mathbf{R}\mathbf{X}_f\mathbf{X}_h\boldsymbol{\tau}/\text{rank}(\mathbf{R})$ as $q(F)$ if \mathcal{R} is defined by a poset block structure on Γ and $\mathbf{R} = \mathbf{R}_F$ for some generalized factor F on Γ .

Finally, consider the whole of \mathcal{P} . If \mathcal{Q} is orthogonal in relation to \mathcal{P} then we have CVS and so the projected data corresponding to any two different rows of the

anova table are uncorrelated. Otherwise, we have the situation, such as the one in [33], where some subspaces corresponding to idempotents of the form $\mathbf{P} \triangleright \mathbf{Q}$ do not consist of eigenvectors of \mathbf{V} . Then it is still possible to do anova in the sense of decomposing the sum of squares of the responses according to the subspaces, and equating the observed values of the mean squares to their expectations, but this may not have all the properties of classical anova.

In particular, let \mathbf{Q} be an idempotent in \mathcal{Q} for which there are distinct \mathbf{P}_1 and \mathbf{P}_2 in \mathcal{P} with $\lambda_{\mathbf{P}_1\mathbf{Q}}$ and $\lambda_{\mathbf{P}_2\mathbf{Q}}$ both nonzero. Then the projections of the data onto $\text{Im}(\mathbf{P}_1)$ and $\text{Im}(\mathbf{P}_2)$ are not independent, because

$$\begin{aligned} \text{Cov}((\mathbf{P}_1 \triangleright \mathbf{Q})\mathbf{Y}, (\mathbf{P}_2 \triangleright \mathbf{Q})\mathbf{Y}) &= (\mathbf{P}_1 \triangleright \mathbf{Q})' \left(\sum_{\mathbf{P} \in \mathcal{P}} \xi_{\mathbf{P}} \mathbf{P} + r \sum_{\mathbf{Q}^* \in \mathcal{Q}} \eta_{\mathbf{Q}^*} \mathbf{Q}^* \right) (\mathbf{P}_2 \triangleright \mathbf{Q}) \\ &= \frac{\mathbf{P}_1 \mathbf{Q} \mathbf{P}_1}{\lambda_{\mathbf{P}_1 \mathbf{Q}}} \left(\sum_{\mathbf{P} \in \mathcal{P}} \xi_{\mathbf{P}} \mathbf{P} + r \sum_{\mathbf{Q}^* \in \mathcal{Q}} \eta_{\mathbf{Q}^*} \mathbf{Q}^* \right) \frac{\mathbf{P}_2 \mathbf{Q} \mathbf{P}_2}{\lambda_{\mathbf{P}_2 \mathbf{Q}}} \\ &= \frac{r \eta_{\mathbf{Q}}}{\lambda_{\mathbf{P}_1 \mathbf{Q}} \lambda_{\mathbf{P}_2 \mathbf{Q}}} \mathbf{P}_1 \mathbf{Q} \mathbf{P}_1 \mathbf{Q} \mathbf{P}_2 \mathbf{Q} \mathbf{P}_2 = r \eta_{\mathbf{Q}} \mathbf{P}_1 \mathbf{Q} \mathbf{P}_2, \end{aligned}$$

which has the same rank as \mathbf{Q} . A similar calculation shows that $(\mathbf{P}_1 \triangleright \mathbf{Q}_1)\mathbf{Y}$ is not correlated with $(\mathbf{P}_2 \triangleright \mathbf{Q}_2)\mathbf{Y}$ if $\mathbf{Q}_1 \neq \mathbf{Q}_2$.

5. Examples. Our first two examples show how straightforward the anova table is when both designs are orthogonal, in the sense defined in Section 3.2. Subsequent examples illustrate the application of our results to other structure-balanced experiments. Further examples are available in [15].

EXAMPLE 1 (Meat loaves). The two-phase sensory experiment in Figure 2 is from [11], Section 4.1; the design in the second phase consists of a pair of 6×6 Latin squares in each session.

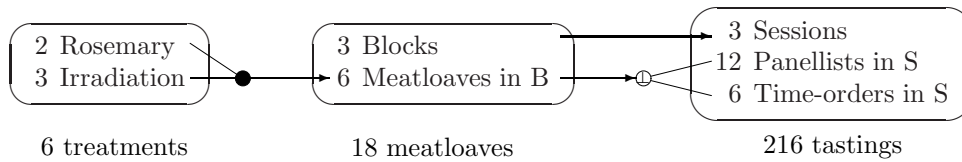


FIG 2. Randomization diagram for Example 1: treatments are randomized to meatloaves, which are in turn randomized to tastings; B denotes Blocks, S denotes Sessions.

Table 1 expands Table 2 of [12] to give the skeleton anova that includes the expected mean squares under randomization; there is no need to show efficiency factors because both designs are orthogonal.

One consequence of this simple orthogonality, and the lack of pseudosources, is that each η -coefficient appears in the final column in conjunction with exactly one ξ -coefficient. Under randomization all of these coefficients must be nonnegative. However, canonical components such as ϕ_{SP} and ϕ_{ST} can be negative, allowing for correlations within panellists (ϕ_{SP}), or within time-orders (ϕ_{ST}), to be negative.

The appropriate ‘Residual’ for each of the three treatments sources is the one with 10 degrees of freedom, which is $((\mathbf{P} \# \mathbf{T} [\mathbf{S}]) \triangleright (\text{Meatloaves} [\mathbf{B}])) \vdash \mathcal{R}$, where \mathcal{R} is the structure on the treatments tier.

TABLE 1
Skeleton analysis of variance for Example 1

tastings tier		meatloaves tier		treatments tier		E.M.S.
source	d.f.	source	d.f.	source	d.f.	
Mean	1	Mean	1	Mean	1	$\xi_0 + 12\eta_0 + q_0$
Sessions	2	Blocks	2			$\xi_S + 12\eta_B$
Panellists [S]	33					ξ_{SP}
Time-orders [S]	15					ξ_{ST}
P # T [S]	165	Meatloaves [B]	15	Rosemary	1	$\xi_{STP} + 12\eta_{BM} + q(R)$
				Irradiation	2	$\xi_{STP} + 12\eta_{BM} + q(I)$
				R # I	2	$\xi_{STP} + 12\eta_{BM} + q(RI)$
				Residual	10	$\xi_{STP} + 12\eta_{BM}$
		Residual	150			ξ_{STP}

EXAMPLE 2 (Cotton fibres). Example 4 of [11] describes a two-phase experiment that consists of a field phase in which cotton is produced in a field trial and a testing phase in which the cotton is tested for strength. In this example, the use of both the spectral and canonical components will be illustrated.

The randomization diagram for Plan B is in Figure 3. As discussed in [11], there is a lack of consonance between the randomization of fibres to tests and the nesting of the associated factors: nested Fibres is randomized to nesting Operatives and nesting Block \wedge Plots is randomized to nested Tests. This forces us to introduce a two-level pseudofactor F_1 that indexes the two groups of 15 fibres; it neither is nested in nor nests anything.

The middle panel in Figure 3 indicates that the proper randomization for the first phase is to randomly permute blocks, randomly permute plots independently within each block, and then randomly permute fibres within each plot. As noted in [11], the two fibres taken from each plot must be independently randomized to the two levels of the pseudofactor F_1 , so that its levels do not correspond to any inherent property such as strength or length.

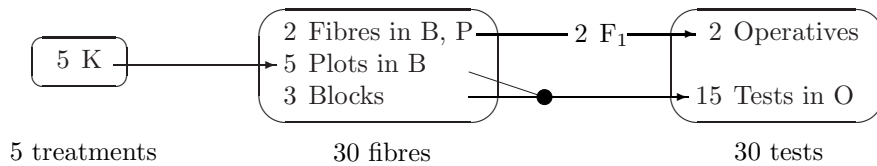


FIG 3. *Composed randomizations in Example 2: treatments are randomized to fibres, which are in turn randomized to tests; K denotes Potash treatments; B denotes Blocks, P denotes Plots; O denotes Operatives; F_1 is a pseudofactor for Fibres.*

The variance matrix under the randomizations is

$$\begin{aligned} \mathbf{V} &= \xi_0 \mathbf{P}_0 + \xi_O \mathbf{P}_O + \xi_{OT} \mathbf{P}_{OT} + \eta_0 \mathbf{Q}_0 + \eta_B \mathbf{Q}_B + \eta_{BP} \mathbf{Q}_{BP} + \eta_{BPF} \mathbf{Q}_{BPF} \\ &= \phi_0 \mathbf{T}_0 + \phi_O \mathbf{T}_O + \phi_{OT} \mathbf{T}_{OT} + \psi_0 \mathbf{S}_0 + \psi_B \mathbf{S}_B + \psi_{BP} \mathbf{S}_{BP} + \psi_{BPF} \mathbf{S}_{BPF}, \end{aligned}$$

where \mathbf{T}_H and \mathbf{S}_H are the relationship matrices and ϕ_H and ψ_H are the canonical

components for a generalized factor H from the tests or fibres tiers, respectively.

There is no \mathbf{Q} -matrix for the pseudofactor: it is irrelevant to the randomization of treatments to fibres and is not one of the unrandomized factors, that gives rise to covariance, in the other randomization. However, we can rewrite \mathbf{Q}_{BPF} as the sum of two \mathbf{Q}^* matrices, one for each of F_1 and Fibres $[\text{Plots} \wedge \text{Blocks}] \vdash F_1$; the coefficient of both is η_{BPF} .

The following expressions show how the canonical components in this example measure excess covariance:

$$\begin{aligned} \phi_{\text{OT}} &= \gamma_{\text{OT}} - \gamma_{\text{O}}, \quad \phi_{\text{O}} = \gamma_{\text{O}} - \gamma_{\text{O}}, \quad \phi_{\text{O}} = \gamma_{\text{O}}, \\ \psi_{\text{BPF}} &= \zeta_{\text{BPF}} - \zeta_{\text{BP}}, \quad \psi_{\text{BP}} = \zeta_{\text{BP}} - \zeta_{\text{B}}, \quad \psi_{\text{B}} = \zeta_{\text{B}} - \zeta_{\text{O}}, \quad \psi_{\text{O}} = \zeta_{\text{O}}. \end{aligned}$$

Thus, ϕ_{O} , ϕ_{O} and ϕ_{OT} measure, respectively, the basic covariance of ‘unrelated’ tests, the excess of the covariance of different tests by the same operator over that of ‘unrelated’ tests, and the excess of the (co)variance of the same tests over that of different tests by the same operator. The ψ -parameters from the fibres tier can be similarly interpreted using the ζ -parameters.

The skeleton anova is in Table 2; again, there is no need to show efficiency factors because both designs are orthogonal. Now the coefficient η_{BPF} occurs with two different ξ -coefficients. This is because the source Fibres $[\text{Plots} \wedge \text{Blocks}]$ has been split into two by the pseudofactor.

EXAMPLE 3 (Two-phase sensory experiment). Section 3 of [16] describes a two-phase sensory experiment. The first, or field, phase is a viticultural experiment and the second, or evaluation, phase involves the assessment of wine made from the produce of the first-phase plots. The randomization diagram for it, given in [11], is in Figure 4 and the decomposition table for it is derived in [12], Example 1. Here the skeleton anova is in Table 3. Although there are pseudofactors for the Judges factor in the evaluations tier, they are ignored in doing the randomization as the six judges are permuted with no distinction. These pseudofactors are used only to obtain the systematic layout; they do not give rise to pseudosources.

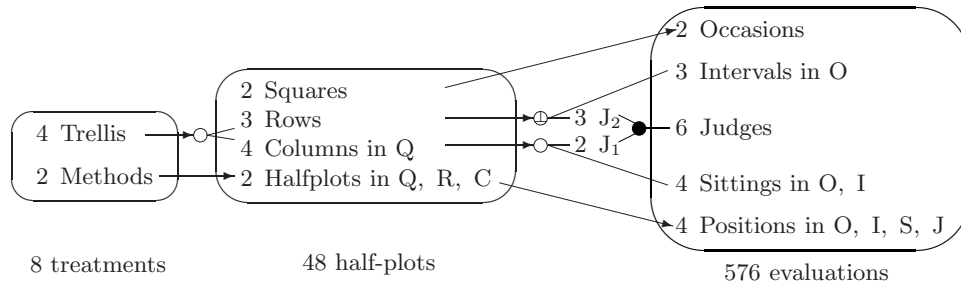


FIG 4. Randomization diagram for Example 3: treatments are randomized to half-plots, which are, in turn, randomized to evaluations; Q, R, C, O, I, S, J denote Squares, Rows, Columns, Occasions, Intervals, Sitzings and Judges, respectively; J_1 and J_2 are pseudofactors for Judges.

In this example, neither design is orthogonal, and so efficiency factors need to be shown in the anova table. The only source in the halfplots tier which is not orthogonal to the sources in the evaluations tier is Columns [Squares]: the corresponding coefficient η_{QC} occurs in conjunction with two different ξ -coefficients. Similarly, the treatment source Trellis is nonorthogonal to three idempotents in $\mathcal{P} \triangleright \mathcal{Q}$, and

TABLE 2. *Skeleton analysis of variance for Example 2 with expected mean squares in terms of spectral components and canonical components*

tests tier		fibres tier		treatments tier		E.M.S.	
source	d.f.	source	d.f.	source	d.f.	spectral components	canonical components
Mean	1	Mean	1	Mean	1	$\xi_0 + \eta_0 + q_0$	$\phi_{OT} + 15\phi_O + 30\phi_0$ $+ \psi_{BPF} + 2\psi_{BP} + 10\psi_B$ $+ 30\psi_0 + q_0$
Operatives	1	F_1	1			$\xi_O + \eta_{BPF}$	$\phi_{OT} + 15\phi_O + \psi_{BPF}$
Tests [O]	28	Blocks	2			$\xi_{OT} + \eta_B$	ϕ_{OT} $+ \psi_{BPF} + 2\psi_{BP} + 10\psi_B$
		Plots [B]	12	K	4	$\xi_{OT} + \eta_{BP} + q(K)$	ϕ_{OT} $+ \psi_{BPF} + 2\psi_{BP} + q(K)$
				Residual	8	$\xi_{OT} + \eta_{BP}$	ϕ_{OT} $+ \psi_{BPF} + 2\psi_{BP}$
		Fibres $[P \wedge B] \vdash F_1$	14			$\xi_{OT} + \eta_{BPF}$	ϕ_{OT} $+ \psi_{BPF}$

TABLE 3

Skeleton analysis of variance table for Example 3 ($O = Occasions$, $I = Intervals$, $S = Sittings$, $J = Judges$, $P = Positions$, $Q = Squares$, $C = Columns$, $R = Rows$, $H = Halfplots$, $T = Trellis$, $M = Methods$)

evaluations tier		halfplots tier		treatments tier			E.M.S.	
source	d.f.	eff.	source	d.f.	eff.	source		d.f.
Mean	1	1	Mean	1	1	Mean	1	$\xi_0 + 12\eta_0 + q_0$
O	1	1	Q	1				$\xi_O + 12\eta_Q$
I [O]	4							ξ_{OI}
S [O \wedge I]	18	$\frac{1}{3}$	C [Q]	6	$\frac{1}{27}$	T	3	$\xi_{OIS} + \frac{1}{3}12\eta_{QC} + \frac{1}{27}q(T)$
			Residual	12		Residual	3	$\xi_{OIS} + \frac{1}{3}12\eta_{QC}$
J	5							ξ_J
O # J	5							ξ_{OJ}
I # J [O]	20	1	R	2				$\xi_{OIJ} + 12\eta_R$
		1	R # Q	2				$\xi_{OIJ} + 12\eta_{QR}$
			Residual	16				
S # J [O \wedge I]	90	$\frac{2}{3}$	C [Q]	6	$\frac{2}{27}$	T	3	$\xi_{OISJ} + \frac{2}{3}12\eta_{QC} + \frac{2}{27}q(T)$
			Residual	12		Residual	3	$\xi_{OISJ} + \frac{2}{3}12\eta_{QC}$
		1	R # C [Q]	12	$\frac{8}{9}$	T	3	$\xi_{OISJ} + 12\eta_{QRC} + \frac{8}{9}q(T)$
			Residual	72		Residual	9	$\xi_{OISJ} + 12\eta_{QRC}$
P [O \wedge I \wedge S \wedge J]	432	1	H [Q \wedge R \wedge C]	24	1	M	1	$\xi_{OISJP} + 12\eta_{QRCH} + q(M)$
				Residual	20	1	T # M	3
			Residual	408		Residual	20	$\xi_{OISJP} + 12\eta_{QRCH}$
			Residual	408				ξ_{OISJP}

so information about Trellis differences is available in three different subspaces, as shown by the three occurrences of $q(T)$ in the table.

EXAMPLE 4 (Duplicated wheat measurements). Example 9 of [11] is an experiment with a field phase and a laboratory phase. In the field phase 49 lines of wheat are investigated using a randomized complete-block design with four blocks. Here the laboratory phase is modified by supposing that the procedure described in [11] is repeated on a second occasion. That is, two samples are obtained from each plot, one to be processed on each occasion. Figure 5 gives the randomization diagram for the modified experiment. Recall that a 7×7 balanced lattice square design with four replicates is used to assign the blocks, plots and lines to four intervals in each occasion. In each interval on each occasion there are seven runs at which samples are processed at seven consecutive times. Pseudofactors are introduced for lines and plots in order to define the design of the second phase.

The variance matrix under the randomizations is

$$\begin{aligned} \mathbf{V} = & \xi_0 \mathbf{P}_0 + \xi_O \mathbf{P}_O + \xi_{OI} \mathbf{P}_{OI} + \xi_{OIR} \mathbf{P}_{OIR} + \xi_{OIT} \mathbf{P}_{OIT} + \xi_{OIRT} \mathbf{P}_{OIRT} \\ & + \eta_0 \mathbf{Q}_0 + \eta_B \mathbf{Q}_B + \eta_{BP} \mathbf{Q}_{BP} + \eta_{BPS} \mathbf{Q}_{BPS}. \end{aligned}$$

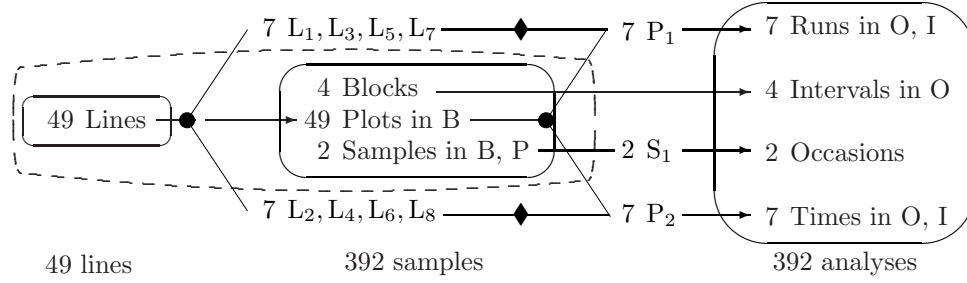


FIG 5. *Randomized-inclusive randomizations in Example 4: lines are randomized to samples, which are in turn randomized to analyses; B, P, O, I denote Blocks, Plots, Occasions, Intervals, respectively; L_1, \dots, L_8 are mutually orthogonal pseudofactors for Lines; P_1 and P_2 are pseudofactors for Plots, determined from different Lines pseudofactors in different blocks; S_1 is a pseudofactor for Samples.*

TABLE 4
Skeleton analysis of variance for Example 4

analyses tier		samples tier		lines tier			E.M.S.
source	d.f.	source	d.f.	eff.	source	d.f.	
Mean	1	Mean	1		Mean	1	$\xi_0 + \eta_0 + q_0$
Occasions	1	S_1	1				$\xi_O + \eta_{BPS}$
Intervals [O]	6	Blocks	3				$\xi_{OI} + \eta_B$
		$S_1 \# B$	3				$\xi_{OI} + \eta_{BPS}$
Runs [O \wedge I]	48	$P_1 [B]$	24	$\frac{1}{4}$	Lines _R	24	$\xi_{OIR} + \eta_{BP} + \frac{1}{4}q(L_R)$
		$S_1 \# P_1 [B]$	24				$\xi_{OIR} + \eta_{BPS}$
Times [O \wedge I]	48	$P_2 [B]$	24	$\frac{1}{4}$	Lines _T	24	$\xi_{OIT} + \eta_{BP} + \frac{1}{4}q(L_T)$
		$S_1 \# P_2 [B]$	24				$\xi_{OIT} + \eta_{BPS}$
R # T [O \wedge I]	288	Plots [B] _⊥	144	$\frac{3}{4}$	Lines _R	24	$\xi_{OIRT} + \eta_{BP} + \frac{3}{4}q(L_R)$
				$\frac{3}{4}$	Lines _T	24	$\xi_{OIRT} + \eta_{BP} + \frac{3}{4}q(L_T)$
					Residual	96	$\xi_{OIRT} + \eta_{BP}$
		Samples [B \wedge P] _⊥	144				$\xi_{OIRT} + \eta_{BPS}$

Randomized-inclusive randomizations are used in this experiment, as the outcome of the randomization of lines to samples must be known before the samples can be randomized to analyses. The Plots pseudofactors P_1 and P_2 are used to ensure appropriate partial confounding of sources from the lines tier with sources in the analyses tier. These pseudofactors do not give idempotents in \mathbf{V} , because they do not contribute to the variance matrix; they are irrelevant to the randomization of lines to samples, and are not among the unrandomized factors, that give rise to covariance, in the randomization of samples to analyses. However, as in Example 2, \mathbf{Q}_{BP} can be rewritten as the sum of three \mathbf{Q}^* -matrices each with coefficient η_{BP} . This results in the coefficient η_{BP} occurring with three different ξ -coefficients in the skeleton anova in Table 4, which is an extended version of the decomposition table given for Example 5 in [12]. To obtain structure balance, $\text{Im}(\mathbf{Q}_{BPS})$ is decomposed as the sum of five subspaces involving the pseudofactor S_1 so that \mathbf{Q}_{BPS} can be rewritten as the sum of five \mathbf{Q}^* -matrices each with coefficient η_{BPS} . As a conse-

quence, the coefficient η_{BPS} occurs with five different ξ -coefficients in Table 4.

EXAMPLE 5 (Small example). Figure 6 is the randomization diagram for the first example in [48]. The levels of pseudofactor U_1 give the treatments allocated to units in the first phase. The small open circle indicates the nonorthogonal block design (group-divisible for U_1) for the second phase. As the design allocating units to plots in the second phase depends on the outcome of the randomization of treatments to units in the first phase, the randomizations are randomized-inclusive.

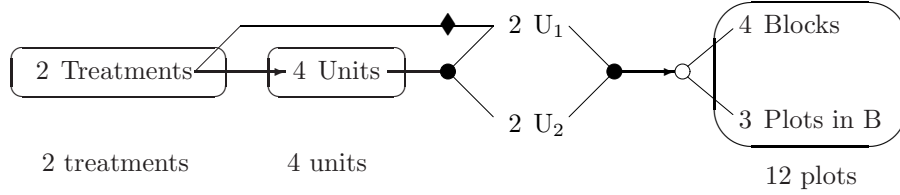


FIG 6. Randomization diagram for Example 5: treatments are randomized to units, which are in turn randomized to plots; B denotes Blocks; U_1 and U_2 are pseudofactors for Units, forming groups of units determined by the treatments.

The skeleton anova in Table 5 agrees with the conclusions reported in [48]. However, it is more informative. For example, using Section 7, the variance of the within-blocks estimator of the treatment difference is equal to $(2/6) \times (\xi_{\text{BP}} + (8/3)\eta_U)/(8/9)$. Table 5 shows that an estimator of $\xi_{\text{BP}} + (8/3)\eta_U$ is twice the mean square for Plots [B] $\triangleright (U \vdash U_1)$ minus the Residual mean square.

TABLE 5
Skeleton analysis of variance for Example 5

plots tier		units tier			treatments tier			E.M.S.
source	d.f.	eff.	source	d.f.	eff.	source	d.f.	
Mean	1		Mean	1		Mean	1	$\xi_0 + 3\eta_0 + q_0$
Blocks	3	$\frac{1}{9}$	U_1	1	$\frac{1}{9}$	Treatments	1	$\xi_B + \frac{1}{9}3\eta_U + \frac{1}{9}q(T)$
		$\frac{5}{9}$	$U \vdash U_1$	2	$\xi_B + \frac{5}{9}3\eta_U$			
Plots [B]	8	$\frac{8}{9}$	U_1	1	$\frac{8}{9}$	Treatments	1	$\xi_{\text{BP}} + \frac{8}{9}3\eta_U + \frac{8}{9}q(T)$
		$\frac{4}{9}$	$U \vdash U_1$	2	$\xi_{\text{BP}} + \frac{4}{9}3\eta_U$			
			Residual	5	ξ_{BP}			

6. Estimation in a two-tiered experiment. Estimation of treatment effects and variances is straightforward in a two-tiered experiment with structure balance.

6.1. *Estimating treatment effects and variances in one stratum.* For data satisfying the conditions in Section 4.1, the following are also shown in [2, 23, 30].

- (E.a) The best linear unbiased estimator of the treatment effects $\mathbf{R}\mathbf{X}_h\boldsymbol{\tau}$, using only the projected data $\mathbf{Q}\mathbf{Y}$, is $\mathbf{R}(\mathbf{Q} \triangleright \mathbf{R})\mathbf{Y}/\lambda_{\mathbf{QR}}$, which is equal to $\mathbf{R}\mathbf{Q}\mathbf{Y}/\lambda_{\mathbf{QR}}$.
- (E.b) The variance matrix of the above estimator is $(\eta_{\mathbf{Q}}/\lambda_{\mathbf{QR}})\mathbf{R}$.
- (E.c) From (A.d) in Section 4.1, an unbiased estimate of $\eta_{\mathbf{Q}}$ is given by the mean square for $\mathbf{Q} \vdash \mathcal{R}$, if $\mathbf{Q} \vdash \mathcal{R}$ is nonzero.

6.2. *Treatment structure orthogonal to variance structure.* If \mathcal{R} is orthogonal in relation to \mathcal{Q} then each \mathbf{R} in \mathcal{R} has some \mathbf{Q} in \mathcal{Q} such that $\lambda_{\mathbf{QR}} = 1$. Then all the information on $\mathbf{R}\mathbf{X}_h\boldsymbol{\tau}$ is in stratum $\text{Im}(\mathbf{Q})$. Hence result (E.a) in Section 6.1 gives $\mathbf{R}\mathbf{Q}\mathbf{Y}$ as the overall best linear unbiased estimator of $\mathbf{R}\mathbf{X}_h\boldsymbol{\tau}$. Result (E.b) shows that the variance matrix of this estimator is $\eta_{\mathbf{Q}}\mathbf{R}$, and result (E.c) that the mean square for $\mathbf{Q} \vdash \mathcal{R}$ is an unbiased estimator for $\eta_{\mathbf{Q}}$, if $\mathbf{Q} \vdash \mathcal{R}$ is nonzero.

6.3. *Estimating treatment effects from multiple strata when variances are known.* Suppose that \mathcal{R} is not orthogonal in relation to \mathcal{Q} . As shown in [23, 31], if the coefficients $\eta_{\mathbf{Q}}$ are known then we can combine information on $\mathbf{R}\mathbf{X}_h\boldsymbol{\tau}$ from all strata for which $\lambda_{\mathbf{QR}} \neq 0$ to obtain its generalized least squares (GLS) estimator, which is the best linear unbiased estimator. In our notation, it is given by

$$(11) \quad \mathbf{R}\mathbf{X}_h\hat{\boldsymbol{\tau}} = \theta_{\mathbf{R}}^{-1} \sum_{\mathbf{Q} \in \mathcal{Q}} \eta_{\mathbf{Q}}^{-1} \mathbf{R}\mathbf{Q}\mathbf{Y},$$

where $\theta_{\mathbf{R}} = \sum_{\mathbf{Q} \in \mathcal{Q}} \lambda_{\mathbf{QR}} \eta_{\mathbf{Q}}^{-1}$. The variance matrix of this estimator is $\theta_{\mathbf{R}}^{-1} \mathbf{R}$.

6.4. *Estimating treatment effects and variances from multiple strata.* However, usually the coefficients $\eta_{\mathbf{Q}}$ are unknown and must be estimated. One method for this is to use the mean square for $\mathbf{Q} \vdash \mathcal{R}$ to estimate $\eta_{\mathbf{Q}}$. Nelder [31] argued that, especially for designs in which some strata have few Residual degrees of freedom, estimates should instead be obtained by equating the expected and observed values of the mean squares for what Houtman and Speed [23] called ‘actual residuals’. Even though normality is not assumed, these estimates are the same as those obtained by REML [34] because, as is shown in [23], Section 4.5, and [35], the same set of equations has to be solved for both. As will be discussed in Section 11.2, the constraints on the variance parameters being estimated here are different from those for a variance-components model.

As noted in [23, 31], the estimation of the coefficients $\eta_{\mathbf{Q}}$ requires an iterative procedure, because their estimation needs the estimated value of $\boldsymbol{\tau}$ and vice versa. Given working estimates $\hat{\eta}_{\mathbf{Q}}^*$ of $\eta_{\mathbf{Q}}$, a working estimate $\hat{\boldsymbol{\tau}}^*$ of $\boldsymbol{\tau}$ can be obtained from equation (11): thus a revised estimate of each $\eta_{\mathbf{Q}}$ can be computed as

$$(12) \quad \frac{\mathbf{y}'(\mathbf{Q} \vdash \mathcal{R})\mathbf{y} + (\sum'_{\mathbf{R} \in \mathcal{R}} \{ \mathbf{y}'(\mathbf{Q} \triangleright \mathbf{R})\mathbf{y} - \lambda_{\mathbf{QR}} \hat{\boldsymbol{\tau}}^{*\prime} \mathbf{X}'_h \mathbf{R}\mathbf{X}_h \hat{\boldsymbol{\tau}}^* \})}{d'_{\mathbf{Q}}},$$

where $\sum'_{\mathbf{R} \in \mathcal{R}}$ means summation over $\mathbf{R} \in \mathcal{R}$ for which $\lambda_{\mathbf{QR}} \neq 0$, and $d'_{\mathbf{Q}}$ are the *effective* degrees of freedom for this estimator, which are given by

$$d'_{\mathbf{Q}} = \text{trace}(\mathbf{Q} \vdash \mathcal{R}) + \sum'_{\mathbf{R} \in \mathcal{R}} [1 - \theta_{\mathbf{R}}^{-1} (\hat{\eta}_{\mathbf{Q}}^*)^{-1} \lambda_{\mathbf{QR}}] \text{trace} \mathbf{R}.$$

Since $\mathbf{Q} \vdash \mathcal{R}$ and \mathbf{R} are both idempotent, their traces are equal to their ranks.

The numerator of expression (12) is the sum of two parts. The first is the Residual sum of squares in this stratum from the anova; the second is the difference between the sum of squares of the treatment estimates from just the data projected onto $\text{Im}(\mathbf{Q})$ and the sum of squares of the combined estimates, summed over all \mathbf{R} for which $\lambda_{\mathbf{QR}} \neq 0$. The former does not depend on $\eta_{\mathbf{Q}}$, but the latter does. The

effective degrees of freedom make it clear that, even when $\mathbf{Q} \vdash \mathcal{R} = \mathbf{0}$, there can be information to estimate $\eta_{\mathbf{Q}}$.

If estimates of the canonical components are required these can be obtained from the estimates of the spectral components.

7. Estimating treatment effects and variances in a single part of $\mathcal{P} \triangleright \mathcal{Q}$.

Suppose that $\lambda_{\mathbf{PQ}} \neq 0$, so that there is an idempotent $\mathbf{P} \triangleright \mathbf{Q}$. Consider an idempotent \mathbf{R} in \mathcal{R} for which $\lambda_{\mathbf{P} \triangleright \mathbf{Q}, \mathbf{R}} \neq 0$. Theorem 5.1 of [12] shows that $\lambda_{\mathbf{P} \triangleright \mathbf{Q}, \mathbf{R}} = \lambda_{\mathbf{PQ}} \lambda_{\mathbf{QR}}$. Applying the results of Section 6.1 with \mathbf{Y} and \mathbf{Q} replaced by \mathbf{PY} and $\mathbf{P} \triangleright \mathbf{Q}$ respectively, and using equation (10) for $\text{Cov}(\mathbf{PY})$, we find that the best linear unbiased estimator of the treatment effect $\mathbf{R}\mathbf{X}_f\mathbf{X}_h\boldsymbol{\tau}$, using only the projected data $(\mathbf{P} \triangleright \mathbf{Q})\mathbf{Y}$, is $\mathbf{R}((\mathbf{P} \triangleright \mathbf{Q}) \triangleright \mathbf{R})\mathbf{Y} / \lambda_{\mathbf{PQ}} \lambda_{\mathbf{QR}}$, which is equal to $\mathbf{RQP}\mathbf{Y} / \lambda_{\mathbf{PQ}} \lambda_{\mathbf{QR}}$. Moreover, the variance matrix of this estimator is equal to $\mathbf{R}(\xi_{\mathbf{P}} + r\lambda_{\mathbf{PQ}}\eta_{\mathbf{Q}}) / \lambda_{\mathbf{PQ}} \lambda_{\mathbf{QR}}$. Result (A.i) in Section 4.2 shows that the mean square for $(\mathbf{P} \triangleright \mathbf{Q}) \vdash \mathcal{R}$ is an unbiased estimator for $\xi_{\mathbf{P}} + r\lambda_{\mathbf{PQ}}\eta_{\mathbf{Q}}$, if $(\mathbf{P} \triangleright \mathbf{Q}) \vdash \mathcal{R}$ is nonzero.

In Example 3, the effects for M and T#M are estimated in just the source $\mathbf{P} [O \wedge I \wedge S \wedge J] \triangleright \mathbf{H} [Q \wedge R \wedge C]$ and the Residual mean square for $\mathbf{H} [Q \wedge R \wedge C]$ is an unbiased estimator of $\xi_{\text{OISJP}} + 12\eta_{\text{QRCH}}$.

8. Full estimation in a three-tiered experiment which is anova-applicable.

8.1. *Full or partial anova.* Call the triple $(\mathcal{P}, \mathcal{Q}, \mathcal{R})$ *anova-applicable* if it satisfies the following condition:

$$(13) \quad \text{for every } \mathbf{Q} \text{ in } \mathcal{Q}, \text{ if } \mathbf{QI}_{\mathcal{R}} \neq \mathbf{0} \text{ then } \mathbf{Q} \in \mathcal{Q}_1.$$

That is, if the source for an \mathbf{R} in \mathcal{R} is (partially) confounded with a source for some \mathbf{Q} , then the latter source must be confounded with the source corresponding to a single \mathbf{P} . Section 4.2 shows that when this condition is satisfied then the idempotents in $\mathcal{P} \triangleright \mathcal{Q}$ whose subspaces are contained in eigenspaces of \mathbf{V} include all those which have any part of \mathcal{R} partially or totally confounded with them.

Condition (13) is satisfied when \mathcal{Q} is orthogonal in relation to \mathcal{P} , so that $\mathcal{Q}_1 = \mathcal{Q}$. Then \mathbf{V} is given by equation (9), possibly with OVS. Estimation of treatment effects and their variances proceeds as in Section 6. Examples 1, 2 and 4 are like this. We call this *full anova*.

Under full anova, if no $(\mathbf{P} \triangleright \mathbf{Q}) \vdash \mathcal{R} = \mathbf{0}$, we estimate linear combinations of spectral components from the anova, even if they are not needed for standard errors of treatment effects. Otherwise, formula (12) can be used, but with $\mathbf{P} \triangleright \mathbf{Q}$ replacing \mathbf{Q} . In Example 1, all the information about each treatment source in $\mathcal{R} \setminus \mathbf{R}_0$ is contained in $(\mathbf{P} \# \mathbf{T} [\mathbf{S}]) \triangleright \mathbf{M} [\mathbf{B}]$. Also, the difference between the mean squares for $((\mathbf{P} \# \mathbf{T} [\mathbf{S}]) \triangleright (\mathbf{M} [\mathbf{B}])) \vdash \mathcal{R}$ and $(\mathbf{P} \# \mathbf{T} [\mathbf{S}]) \vdash \mathcal{Q}$ estimates $12\eta_{\text{BM}}$.

In general, put $\mathcal{P} * \mathcal{Q} = \mathcal{Q}_1 \cup \{\mathbf{P} \vdash \mathcal{Q} : \mathbf{P} \in \mathcal{P}\}$. Then the images of all the idempotents in $\mathcal{P} * \mathcal{Q}$ are contained in eigenspaces of \mathbf{V} . If $(\mathcal{P}, \mathcal{Q}, \mathcal{R})$ is anova-applicable but \mathcal{Q} is not orthogonal in relation to \mathcal{P} then we have *partial anova*, using only the information in $\mathcal{P} * \mathcal{Q}$. A treatment idempotent \mathbf{R} in \mathcal{R} may be nonorthogonal to more than one part of $\mathcal{P} \triangleright \mathcal{Q}$, but these are all in $\mathcal{P} * \mathcal{Q}$. Section 4.2 shows that estimators of variances of treatment effects which are in different parts of $\mathcal{P} * \mathcal{Q}$ are uncorrelated, and so information can be combined as in Section 6.4.

However, the linear combinations of spectral components in the expected mean square for parts of $\mathcal{P} \triangleright \mathcal{Q}$ outside $\mathcal{P} * \mathcal{Q}$ are not involved in this process, and their

anova-estimators may not have good properties. A similar situation arises in two-tiered experiments if the group is not stratifiable but all treatment subspaces are contained in known eigenspaces of the variance matrix (see Example 16 in [3]).

In the special case that \mathcal{R} is orthogonal in relation to $\mathcal{P} \triangleright \mathcal{Q}$, each \mathbf{R} in \mathcal{R} has unique idempotents \mathbf{Q} in \mathcal{Q} and \mathbf{P} in \mathcal{P} such that $\lambda_{\mathbf{PQ}}\lambda_{\mathbf{QR}} = 1$, so that $\lambda_{\mathbf{PQ}} = \lambda_{\mathbf{QR}} = 1$. Hence, Condition (13) is satisfied. Then $\mathbf{P} \triangleright \mathbf{Q} = \mathbf{Q}$, $\mathbf{RQP} = \mathbf{R}$ and the effect $\mathbf{RX}_f\mathbf{X}_h\boldsymbol{\tau}$ is estimated in just the one part $\mathbf{P} \triangleright \mathbf{Q}$ of $\mathcal{P} * \mathcal{Q}$. The anova may be either full or partial. The full anova tables obtained by putting data into each of Tables 1 and 2 are like this. The estimator for $\mathbf{RX}_f\mathbf{X}_h\boldsymbol{\tau}$, and its variance matrix, obtained by simplifying the expressions given in Section 7, are \mathbf{RY} and $(\xi_{\mathbf{P}} + r\eta_{\mathbf{Q}})\mathbf{R}$, respectively. If $\xi_{\mathbf{P}}$ and $\eta_{\mathbf{Q}}$ are not known, the mean square for $(\mathbf{P} \triangleright \mathbf{Q}) \vdash \mathcal{R}$ provides an unbiased estimate of $\xi_{\mathbf{P}} + r\eta_{\mathbf{Q}}$, unless $(\mathbf{P} \triangleright \mathbf{Q}) \vdash \mathcal{R} = \mathbf{0}$. Estimation of treatment effects and their standard errors proceeds exactly as in Section 6.2.

8.2. *Difficulties that do not arise in two-tiered experiments.* Even when $(\mathcal{P}, \mathcal{Q}, \mathcal{R})$ is anova-applicable, some phenomena can occur that are not possible in two-tiered experiments, even for the straightforward special case where \mathcal{P} and \mathcal{Q} are both poset block structures, \mathcal{Q} is orthogonal in relation to \mathcal{P} , and \mathcal{R} is orthogonal in relation to \mathcal{Q} .

8.2.1. *Inestimability of some spectral and canonical components.* For a two-tiered experiment with OVS and \mathcal{R} orthogonal in relation to \mathcal{Q} , the estimability of spectral components of variance is easily determined. If $\mathbf{Q} \vdash \mathcal{R}$ is nonzero then its mean square provides the best unbiased quadratic estimator of $\eta_{\mathbf{Q}}$; otherwise, there is no estimator for $\eta_{\mathbf{Q}}$. In particular, η_0 is never estimable.

In a three-tiered experiment, the expected mean square for each Residual source is a linear combination of a ξ -parameter and an η parameter. It may not be possible to estimate ξ and η separately. This affects the estimability of canonical components, although it appears that often more individual canonical, than spectral, components are estimable. The parameters ξ_0 , η_0 , ϕ_0 and ψ_0 are never estimable.

Otherwise, the simplest way in which two spectral components cannot be estimated separately occurs when a generalized factor F on Υ is randomly assigned to a generalized factor H on Ω with the same number of levels. Then only a linear combination of ξ_H and η_F can be estimated, and hence only a linear combination of ϕ_H and ψ_F . In Example 1, Blocks are assigned to Sessions, both of which have three levels. As a result, only $\xi_S + 12\eta_B$ is estimable, as is shown in Table 1, where these two components only occur together. Correspondingly, only $\phi_S + \psi_B$ is estimable.

In the special case that $|\Upsilon| = |\Omega|$, Lemma 4.2 of [12] shows that $\mathcal{P} \triangleright \mathcal{Q} = \mathcal{Q}$ and so there are no idempotents of the form $\mathbf{P} \vdash \mathcal{Q}$. Thus every expected mean square contains one $\eta_{\mathbf{Q}}$ and one $\xi_{\mathbf{P}}$. If κ is any constant smaller in modulus than all the $\eta_{\mathbf{Q}}$ and all the $\xi_{\mathbf{P}}$, then $\kappa\mathbf{I}_{\Omega}$ can be added to $\sum \xi_{\mathbf{P}}\mathbf{P}$ and subtracted from $\sum \eta_{\mathbf{Q}}\mathbf{Q}$ without changing the variance matrix \mathbf{V} in equation (7). Thus none of the spectral components of variance can be estimated, although sums of the form $\xi_{c(\mathbf{Q})} + \eta_{\mathbf{Q}}$ can be. For estimates of standard errors, these sums are all that is needed, and so there is no problem. However, for comparing sources of variation, estimates of canonical components are required. Except for ϕ_{Ω} and ψ_{Υ} , each canonical component is a multiple of a difference between spectral components. This may well be estimable, even though the corresponding spectral component is not.

In Example 2, none of the spectral components is estimable. If relative magnitudes of sources of variation are to be investigated, then the canonical components are needed: all of these are estimable except for ϕ_{OT} and ψ_{BPF} , whose sum is estimable, and ϕ_0 and ψ_0 . Thus the only real restriction in estimating canonical components in this experiment is that it is not possible to separate variability arising from Tests and Fibres. Plan A for Example 4 of [11] is an alternative design for this experiment. It has no pseudosources, but exhibits the same inestimability.

8.2.2. *Negative estimates of spectral components.* As noted in Section 2.3, all spectral components of variance must be nonnegative and hence so must any linear combination with positive coefficients. However, if one mean square involving both a ξ and an η is less than that involving just the same ξ , then the anova-estimate of η is negative. This is analogous to a negative estimate of a nonnegative variance component; the component should be set to zero.

In Example 1, Table 1 shows that the appropriate Residual source for all three treatment sources is the one with expected mean square equal to $\xi_{\text{STP}} + 12\eta_{\text{BM}}$. Suppose that this mean square turns out to be smaller than the one whose expectation is ξ_{STP} . Then we set η_{BM} to zero and combine the two Residual mean squares to obtain a better estimate of ξ_{STP} . See Section 11.3 for further discussion.

8.2.3. *The effect of pseudosources.* If there are pseudosources for \mathcal{Q} then some η -coefficients occur with more than one ξ -coefficient, even if \mathcal{Q} is orthogonal in relation to \mathcal{P} . This can lead to what we call *linearly dependent commutative variance structure* (LDCVS), in which the eigenspaces of \mathbf{V} are known but the eigenvalues satisfy some linear equations. This gives a set of sources whose expected mean squares are linearly dependent: simply equating them all to their data mean squares may give inconsistent results. Suppose that for i, j in $\{1, 2\}$ the idempotent \mathbf{Q}_{ij}^* corresponds to a pseudosource for \mathbf{Q}_j and is totally confounded with \mathbf{P}_i . Then the expected mean squares for the four idempotents $(\mathbf{P}_i \triangleright \mathbf{Q}_{ij}^*) \vdash \mathcal{R}$ are $\xi_1 + r\eta_1$, $\xi_1 + r\eta_2$, $\xi_2 + r\eta_1$ and $\xi_2 + r\eta_2$. To estimate either the spectral or canonical components by equating expected and observed mean squares requires that the sum of the middle two observed mean squares is equal to the sum of the outer two. This situation is similar to the case, discussed by Bailey et al. [5], of a mixed model with LDCVS that is orthogonal to the treatment structure. They show that all four combinations of the following can occur: all variance components can be estimable, or not; and each estimable component may, or may not, have a unique estimator using the mean squares in the anova.

9. Estimation in a three-tiered experiment which is not anova-applicable.

If \mathbf{V} is known then we can estimate treatment effects by GLS, which gives different results from ordinary least squares if \mathcal{R} is not orthogonal in relation to $\mathcal{P} \triangleright \mathcal{Q}$.

Equation (7) gives

$$\mathbf{V} = \mathbf{IVI} = \sum_{\mathbf{P} \in \mathcal{P}} \xi_{\mathbf{P}} \mathbf{P} + r \sum_{\mathbf{P} \in \mathcal{P}} \sum_{\mathbf{Q} \in \mathcal{Q}} \sum_{\mathbf{P}^* \in \mathcal{P}} \eta_{\mathbf{Q}} \mathbf{PQP}^*.$$

Put $\alpha_{\mathbf{Q}} = \sum_{\mathbf{P}} (\lambda_{\mathbf{PQ}} / \xi_{\mathbf{P}})$. Then direct calculation shows that

$$\mathbf{V}^{-1} = \sum_{\mathbf{P} \in \mathcal{P}} \frac{1}{\xi_{\mathbf{P}}} \mathbf{P} - \sum_{\mathbf{P} \in \mathcal{P}} \sum_{\mathbf{Q} \in \mathcal{Q}} \sum_{\mathbf{P}^* \in \mathcal{P}} \left(\frac{r\eta_{\mathbf{Q}}}{1 + r\eta_{\mathbf{Q}}\alpha_{\mathbf{Q}}} \right) \frac{1}{\xi_{\mathbf{P}}\xi_{\mathbf{P}^*}} \mathbf{PQP}^*.$$

Consider \mathbf{R} in \mathcal{R} . When the $\xi_{\mathbf{P}}$ and $\eta_{\mathbf{Q}}$ are known, the GLS estimator of the treatment effect $\mathbf{R}\mathbf{X}_f\mathbf{X}_h\boldsymbol{\tau}$ is $(\mathbf{R}\mathbf{V}^{-1}\mathbf{R})^{-1}\mathbf{R}\mathbf{V}^{-1}\mathbf{Y}$, with variance matrix $(\mathbf{R}\mathbf{V}^{-1}\mathbf{R})^{-1}$. For a chain of randomizations, $\mathbf{R} = \mathbf{R}\mathbf{I}_{\mathcal{Q}} = \sum_{\mathbf{Q}} \mathbf{R}\mathbf{Q}$, so

$$\begin{aligned} \mathbf{R}\mathbf{V}^{-1} &= \sum_{\mathbf{P}} \sum_{\mathbf{Q}} \frac{1}{\xi_{\mathbf{P}}} \mathbf{R}\mathbf{Q}\mathbf{P} - \sum_{\mathbf{P}} \sum_{\mathbf{Q}} \sum_{\mathbf{P}^*} \left(\frac{r\eta_{\mathbf{Q}}}{1+r\eta_{\mathbf{Q}}\alpha_{\mathbf{Q}}} \right) \frac{1}{\xi_{\mathbf{P}}\xi_{\mathbf{P}^*}} \mathbf{R}\mathbf{Q}\mathbf{P}\mathbf{Q}\mathbf{P}^* \\ &= \sum_{\mathbf{P}} \sum_{\mathbf{Q}} \frac{1}{\xi_{\mathbf{P}}} \mathbf{R}\mathbf{Q}\mathbf{P} - \sum_{\mathbf{Q}} \sum_{\mathbf{P}^*} \left(\frac{r\eta_{\mathbf{Q}}\alpha_{\mathbf{Q}}}{1+r\eta_{\mathbf{Q}}\alpha_{\mathbf{Q}}} \right) \frac{1}{\xi_{\mathbf{P}^*}} \mathbf{R}\mathbf{Q}\mathbf{P}^* \\ &= \sum_{\mathbf{P}} \sum_{\mathbf{Q}} \frac{1}{\xi_{\mathbf{P}}} \left(\frac{1}{1+r\eta_{\mathbf{Q}}\alpha_{\mathbf{Q}}} \right) \mathbf{R}\mathbf{Q}\mathbf{P}. \end{aligned}$$

Hence

$$\mathbf{R}\mathbf{V}^{-1}\mathbf{R} = \sum_{\mathbf{P}} \sum_{\mathbf{Q}} \frac{1}{\xi_{\mathbf{P}}} \left(\frac{1}{1+r\eta_{\mathbf{Q}}\alpha_{\mathbf{Q}}} \right) \mathbf{R}\mathbf{Q}\mathbf{P}\mathbf{Q}\mathbf{R} = \sum_{\mathbf{Q}} \left(\frac{\alpha_{\mathbf{Q}}\lambda_{\mathbf{Q}\mathbf{R}}}{1+r\eta_{\mathbf{Q}}\alpha_{\mathbf{Q}}} \right) \mathbf{R} = \theta_{\mathbf{R}}\mathbf{R},$$

with $\theta_{\mathbf{R}} = \sum_{\mathbf{Q} \in \mathcal{Q}} \alpha_{\mathbf{Q}}\lambda_{\mathbf{Q}\mathbf{R}}(1+r\eta_{\mathbf{Q}}\alpha_{\mathbf{Q}})^{-1}$. Thus the GLS estimator of $\mathbf{R}\mathbf{X}_f\mathbf{X}_h\boldsymbol{\tau}$ is

$$\frac{1}{\theta_{\mathbf{R}}} \sum_{\mathbf{P}} \sum_{\mathbf{Q}} \frac{1}{\xi_{\mathbf{P}}} \left(\frac{1}{1+r\eta_{\mathbf{Q}}\alpha_{\mathbf{Q}}} \right) \mathbf{R}\mathbf{Q}\mathbf{P}\mathbf{Y},$$

with variance matrix $\theta_{\mathbf{R}}^{-1}\mathbf{R}$.

This estimator is a linear combination of the $\mathbf{R}\mathbf{Q}\mathbf{P}\mathbf{Y}$. There are no terms in $\mathbf{R}(\mathbf{P} \vdash \mathcal{Q})$, because all projectors of this form are zero for a chain of randomizations.

In the special case that \mathcal{R} is orthogonal in relation to \mathcal{Q} there is a unique \mathbf{Q} such that $\mathbf{R}\mathbf{Q} = \mathbf{R}$ while $\mathbf{R}\mathbf{Q}^* = \mathbf{0}$ if $\mathbf{Q}^* \neq \mathbf{Q}$, so the estimator is a linear combination of the $\mathbf{R}\mathbf{P}\mathbf{Y}$, as shown in [48]. The scalar $\theta_{\mathbf{R}}$ specializes to that given in [48].

In the anova-applicable case, we have $\theta_{\mathbf{R}} = \sum_{\mathbf{Q} \in \mathcal{Q}} \lambda_{\mathbf{Q}\mathbf{R}}(\xi_{c(\mathbf{Q})} + r\eta_{\mathbf{Q}})^{-1}$ and

$$\mathbf{R}\mathbf{X}_f\mathbf{X}_h\hat{\boldsymbol{\tau}} = \theta_{\mathbf{R}}^{-1} \sum_{\mathbf{Q} \in \mathcal{Q}} (\xi_{c(\mathbf{Q})} + r\eta_{\mathbf{Q}})^{-1} \mathbf{R}\mathbf{Q}\mathbf{Y}.$$

If \mathbf{V} is unknown, canonical components need to be estimated using REML followed by estimation of the treatment effects using estimated GLS (EGLS).

10. Extension to more than two randomizations in a chain. We have seen that, even with structure balance, there can be difficulties with anova estimation for a three-tiered experiment. One solution can be to use software designed for fitting mixed models. This does not need to be restricted to designs with structure balance, or to experiments with three tiers, so we begin by generalizing Section 2.

As discussed in [11], Section 6, and [12], Section 7, more than two randomizations are possible. For example, a multiphase experiment can consist of p phases and involve p randomizations. Then there are p sets, Ω_i for $i = 1, \dots, p$, and another set Γ for the first phase. There is a design function $h: \Omega_p \rightarrow \Gamma$; if the objects in Γ are treatments then $h(\omega)$ is the treatment assigned to unit ω in Ω_p . A stratifiable group G_p of permutations of Ω_p is used to randomize h . For $i = 1, \dots, p-1$, there is a design function $f_i: \Omega_i \rightarrow \Omega_{i+1}$, so that $f_i(\omega)$ is the unit in Ω_{i+1} assigned to unit ω in Ω_i ; there is also a stratifiable group G_i of permutations of Ω_i which is used to

randomize f_i . It is assumed that f_i is equireplicate, with replication r_{i+1}/r_i , where $r_1 = 1$, so that each element in Ω_i is assigned to r_i elements in Ω_1 .

Let Y_ω be the response on unit ω in Ω_1 . For ω in Ω_1 , put $s_1(\omega) = \omega$, $s_{i+1}(\omega) = f_i(s_i(\omega))$ for $i = 1, \dots, p-1$ and $t(\omega) = h(s_p(\omega))$. The randomization-based model in equation (6) can be generalized to

$$Y_\omega = \sum_{i=1}^p Z_{i,s_i(\omega)} + \tau_{t(\omega)},$$

where $Z_{i,s_i(\omega)}$ is the random effect, under randomization by G_i , for unit $s_i(\omega)$ in Ω_i .

For this model, $E(\mathbf{Y}) = \mathbf{X}_s \mathbf{X}_h \boldsymbol{\tau}$, where \mathbf{X}_s is the $\Omega_1 \times \Omega_p$ design matrix for s_p and \mathbf{X}_h is the $\Omega_p \times \Gamma$ design matrix for h . Generalize $\mathbf{I}_{\mathcal{R}}$ to be the $\Omega_1 \times \Omega_1$ matrix of orthogonal projection onto $\text{Im}(\mathbf{X}_s \mathbf{X}_h)$. Also, $\mathbf{V} = \sum_{i=1}^p \mathbf{V}_i$, where $\mathbf{V}_i = r_i \sum_{\mathbf{P}_{ij} \in \mathcal{P}_i} \xi_{ij} \mathbf{P}_{ij}$ and each \mathbf{P}_{ij} is an idempotent of \mathbf{V}_i with spectral component ξ_{ij} .

To this point, there is no need for structure balance, nor do any of the structures need to be defined by factors. However, if the randomization of f_i is based on a tier of factors \mathcal{H}_i defining a poset block structure on Ω_i then $\mathbf{V}_i = \sum_{H \in \mathcal{H}_i} \phi_H \mathbf{S}_H$, where \mathbf{S}_H is the $\Omega_1 \times \Omega_1$ relationship matrix for H considered as a factor on Ω_1 .

If all of f_1, \dots, f_p and h are structure-balanced then the results of Sections 3, 4, 7 and 8 can be extended to more than two randomizations. In particular, generalize \mathcal{Q}_1 be the set of idempotents \mathbf{Q} in \mathcal{P}_p for which there is an idempotent $\mathbf{P}_{c_i(\mathbf{Q})}$ in \mathcal{P}_i for $i = 1, \dots, p$ such that $\mathbf{P}_{c_p(\mathbf{Q})} \mathbf{Q} = \mathbf{Q}$ and $\mathbf{P}_{c_i(\mathbf{Q})} \mathbf{P}_{c_{i+1}(\mathbf{Q})} = \mathbf{P}_{c_{i+1}(\mathbf{Q})}$ for $i = 1, \dots, p-1$. The condition for anova-applicability becomes

$$\text{for every } \mathbf{Q} \text{ in } \mathcal{P}_p, \text{ if } \mathbf{Q} \mathbf{I}_{\mathcal{R}} \neq \mathbf{0} \text{ then } \mathbf{Q} \in \mathcal{Q}_1.$$

11. Obtaining estimates from data for experiments with a chain of randomizations. How can standard software be used to obtain, from data, estimates of treatment effects and their standard errors and/or estimates of canonical components, under randomization-based models? Assume that, for $i = 1, \dots, p$, \mathcal{P}_i is given by a poset block structure defined by a set \mathcal{H}_i of generalized factors on Ω_i , which are then expressed as factors on Ω_1 . Two possible procedures, based on mixed models, are anova and mixed-model fitting.

11.1. Analysis of variance. This is the method of choice for anova-applicable cases in which the structure \mathcal{R} on Γ is also orthogonal in relation to \mathcal{Q}_1 , and other cases in which it has been decided that each treatment effect is to be estimated from a single source, as might be done in Example 3. Other anova-applicable cases can be dealt with by anova followed by combination of information, as in Section 6.4.

Anova can also be used to estimate canonical components when there is CVS and \mathcal{R} is orthogonal in relation to \mathcal{Q} . If there is LDCVS then a generalized linear model (GLM) estimates the components. One fits a GLM to the observed mean squares involved in the estimation. The GLM has a gamma distribution, identity link, dispersion parameter equal to 2, weights equal to the degrees of freedom and an \mathbf{X} matrix that contains, in each row, the coefficients of the canonical components for the expected mean square corresponding to the observed mean square.

The advantage of anova is that it is a noniterative procedure in which all the quantities are well-defined. Further, nonnegativity constraints are easily implemented as a manual procedure applied after the anova has been obtained, and the inestimability of variance parameters is often inconsequential.

However, most anova software does not produce combined estimates of fixed effects, so that it is simpler to use mixed-model fitting. A further difficulty with anova for multitiered experiments is that software for it is not generally available, GenStat being the only package that has specific facilities [17]. However, it may be possible to specify a set of terms that will produce the correct decomposition by omitting some sources. For example, the correct decomposition is obtained for Example 2 from an anova or a regression model with the sources Operatives, Blocks, Treatments, Plots [Blocks] and Residual. This is akin to fitting a mixed model of convenience, as described in [14], because it does not contain terms for all the potential sources of variation that have been identified for the experiment.

11.2. *Classes of mixed models for structures defined by factors.* Most mixed-model software uses a conditional model ([25], Appendix A1, and [41], Section 4.6):

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\tau} + \mathbf{Z}\mathbf{U} + \mathbf{E},$$

with $E(\mathbf{Y} \mid \mathbf{U}) = \mathbf{X}\boldsymbol{\tau} + \mathbf{Z}\mathbf{U}$, $\text{Cov}(\mathbf{U}) = \mathbf{Z}\mathbf{G}\mathbf{Z}'$ and $\text{Cov}(\mathbf{Y} \mid \mathbf{U}) = \text{Cov}(\mathbf{E}) = \mathbf{R}$, where $\boldsymbol{\tau}$ is the vector of fixed-effects parameters, \mathbf{X} is an indicator-variable matrix for fixed effects with one row for each observation and a column for each fixed effect, \mathbf{Z} is an indicator-variable matrix with a row for each observation and a column for each random effect, \mathbf{U} is the vector of random effects, \mathbf{E} is the vector of random unit effects, and \mathbf{G} and \mathbf{R} are symmetric matrix functions of the variance parameters. This usage of \mathbf{R} is unrelated to its usage elsewhere in the paper.

This conditional model can be re-expressed in the following marginal form:

$$(14) \quad E(\mathbf{Y}) = \mathbf{X}\boldsymbol{\tau} \text{ and } \text{Cov}(\mathbf{Y}) = \mathbf{V} = \mathbf{Z}\mathbf{G}\mathbf{Z}' + \mathbf{R}.$$

The model for the variance matrix in equation (14) is referred to as the unstructured variance model; the only condition imposed is that \mathbf{V} is p.s.d.

We are concerned with models for the $\Omega_1 \times \Omega_1$ variance matrix \mathbf{V} that are based on sets \mathcal{H}_i of generalized factors on Ω_1 . Put $\mathcal{H} = \bigcup_{i=1}^p \mathcal{H}_i$. Let \mathcal{E} be the set of those generalized factors in \mathcal{H} that uniquely index the units in Ω_1 , and let $\mathcal{U} = \mathcal{H} \setminus \mathcal{E}$. This allows us to write $\text{Cov}(\mathbf{U}) = \mathbf{Z}\mathbf{G}\mathbf{Z}' = \sum_{U \in \mathcal{U}} \mathbf{Z}_U \mathbf{G}_U \mathbf{Z}'_U$ and $\mathbf{R} = \sum_{E \in \mathcal{E}} \mathbf{R}_E$.

All software allows the fitting of variance models based on variance components, for which $\mathbf{G}_U = \sigma_U^2 \mathbf{I}_{m(U)}$, where $m(U)$ is the number of levels of U , and $\mathbf{R}_E = \sigma_E^2 \mathbf{I}_{\Omega_1}$. The variance-components model for the matrix \mathbf{V} in equation (14) is $\mathbf{V} = \sum_{U \in \mathcal{U}} \sigma_U^2 \mathbf{S}_U + \sum_{E \in \mathcal{E}} \sigma_E^2 \mathbf{I}_{\Omega_1}$, where $\mathbf{Z}_U \mathbf{Z}'_U = \mathbf{S}_U$. For such models, it is required that all variance components are nonnegative, which implies that \mathbf{V} is p.s.d.

Some software allows negative estimates of the variance components: this is essentially fitting a canonical-components model for the variance matrix, whose general form is obtained by replacing each σ^2 -parameter with a ϕ -parameter:

$$(15) \quad \mathbf{V} = \sum_{U \in \mathcal{U}} \phi_U \mathbf{S}_U + \sum_{E \in \mathcal{E}} \phi_E \mathbf{I}_{\Omega_1}.$$

This differs from the variance-components model in that the ϕ_U , for U in \mathcal{U} , are not required to be nonnegative, although \mathbf{V} is required to be p.s.d.

Randomization-based models are inherently marginal linear mixed models. The expectation is as given in equation (14), with \mathbf{X} replaced by $\mathbf{X}_s \mathbf{X}_h$. For the variance

part of the model, equation (8) is generalized to

$$\mathbf{V} = \sum_{i=1}^p \mathbf{V}_i = \sum_{i=1}^p \sum_{H \in \mathcal{H}_i} \phi_H \mathbf{S}_H,$$

which is of the form given in equation (15).

The particular features of randomization-based models are:

- (R.a) For $i = 1, \dots, p$, all the factors initially defined on Ω_i are deemed random.
- (R.b) For $i = 1, \dots, p$, \mathbf{V}_i is p.s.d., so that linear combinations of the canonical components corresponding to its spectral components must be nonnegative. This implies that $\phi_{\Omega_i} \geq 0$ for $i = 1, \dots, p$ but that other canonical components can be negative.
- (R.c) The factors on Γ , the treatment factors, are usually regarded as fixed.

The set \mathcal{V} of possible estimates of a model for \mathbf{V} is a subset of the set \mathcal{M} of $\Omega_1 \times \Omega_1$ real symmetric matrices. If \mathcal{F} is any subset of \mathcal{H} , put $\mathcal{M}(\mathcal{F}) = \{\sum_{F \in \mathcal{F}} a_F \mathbf{S}_F : a_F \in \mathbb{R} \text{ for } F \text{ in } \mathcal{F}\}$. For the models described above, the sets of possible estimates are:

Unstructured: $\mathcal{V}_{\text{US}} = \{\mathbf{M} \in \mathcal{M} : \mathbf{M} \text{ is p.s.d.}\}$;

Canonical-components: $\mathcal{V}_{\text{CC}}(\mathcal{H}) = \mathcal{M}(\mathcal{H}) \cap \mathcal{V}_{\text{US}}$;

Variance-components: $\mathcal{V}_{\text{VC}}(\mathcal{H}) = \{\sum_{H \in \mathcal{H}} a_H \mathbf{S}_H : a_H \in \mathbb{R}_0^+ \text{ for } H \text{ in } \mathcal{H}\}$;

Randomization-based: $\mathcal{V}_{\text{RB}}(\mathcal{H}_1, \dots, \mathcal{H}_p) = \{\sum_{i=1}^p \mathbf{V}_i : \mathbf{V}_i \in \mathcal{V}_{\text{CC}}(\mathcal{H}_i) \text{ for } i = 1, \dots, p\}$.

Clearly, $\mathcal{V}_{\text{VC}}(\mathcal{H}) \subset \mathcal{V}_{\text{RB}}(\mathcal{H}_1, \dots, \mathcal{H}_p) \subset \mathcal{V}_{\text{CC}}(\mathcal{H}) \subset \mathcal{V}_{\text{US}}$.

11.3. *Mixed-model fitting.* By mixed-model fitting, in the case where variances are unknown, we mean REML estimation of variance parameters followed by EGLS estimation of the fixed effects. It is preferred for estimation of effects in cases that are not anova-applicable, including all those without structure balance, and for estimation of canonical components when there is not OVS. It might also be deployed in anova-applicable cases because of software availability or because it is convenient to use a method that covers virtually all the cases. Mixed-model fitting can also be used when \mathbf{V} is known: the variance parameters are fixed at their known values. It cannot be used for those anova-applicable cases in which \mathcal{R} is not orthogonal in relation to \mathcal{Q}_1 and separate analyses are required for different parts of \mathcal{Q}_1 . Further advantages of mixed-model fitting are that pseudofactors are unnecessary and that combined estimates of treatment effects are obtained when \mathcal{R} is not orthogonal to the other structures. A disadvantage of mixed-model fitting is that it is an iterative procedure that can have computational difficulties. Using anova estimates of canonical components as initial values helps surmount these.

In obtaining the fitted values for a randomization-based model using data from an experiment, a problem is that mixed-model software usually fits only variance-components models and perhaps canonical-components models. The default for GenStat directives [36] is to fit canonical-components models and it is an option in both ASReML-R [18], a commercial package for R [39], and in PROC MIXED in SAS [40]. The R packages `lme4` [8] and `nlme` [38] fit variance-components models only. Because $\mathcal{V}_{\text{RB}}(\mathcal{H}_1, \dots, \mathcal{H}_p) \not\subseteq \mathcal{V}_{\text{VC}}(\mathcal{H})$, we recommend fitting canonical-components models. Even so, a number of difficulties arise: (i) all canonical components in the

given model must be estimable, (ii) software does not allow the separate specification of the factor sets \mathcal{H}_i and so cannot impose the constraint that each \mathbf{V}_i is p.s.d., and (iii) software requires the fitted canonical components to be nonzero to avoid singularities in the matrices involved in the computations.

For some variance models, it is inherently impossible to estimate all variance parameters, as required in (i). This should be investigated when designing an experiment so that any problems can be identified and rectified before the experiment is run. The anova table is extremely useful for this and, in particular, we advocate the use of ‘dummy analyses’ in which anova is applied to randomly generated data to check the properties of designs. These analyses are implemented in GenStat for structure-balanced three-tier experiments; they can be achieved in R, in many cases including those with \mathcal{R} not structure balanced in relation to \mathcal{P}_p , by judicious specification of the **Error** function in a call to the **aov** function. Another possibility is to perform a dummy mixed-model analysis, although this requires that the generated data are a reasonable fit to the model to be tested.

Inestimability of variance parameters can arise in two ways. First, a variance parameter is not estimable if it is completely confounded by one or more fixed effects. For example, if there is some H in \mathcal{H} for which $\mathbf{S}_H \mathbf{I}_{\mathcal{R}} = \mathbf{S}_H$ then neither ϕ_H nor ξ_H is estimable. In particular, as pointed out in Section 8.2.1, components corresponding to the overall mean are never estimable and mixed-model-fitting software usually excludes them; if not, they must be dropped. However, if other canonical components are inestimable for this reason then this is usually a sign that the experiment suffers from some form of pseudoreplication; dropping such components results in incorrect estimates of standard errors and so is inadvisable. The avoidance of such design deficiencies is one reason we urge the use of dummy analyses to check proposed designs.

Let $\tilde{\mathcal{H}}$ be the set of all factors in \mathcal{H} which do not correspond to the overall mean. The other cause of inestimability is linear dependence among the matrices \mathbf{S}_H for H in $\tilde{\mathcal{H}}$. Then canonical components need to be dropped so that those remaining correspond to a linearly independent set of \mathbf{S}_H for H in \mathcal{H}^* , where $\mathcal{H}^* \subset \tilde{\mathcal{H}}$ and $\mathcal{V}_{\text{CC}}(\mathcal{H}^*) = \mathcal{V}_{\text{CC}}(\tilde{\mathcal{H}})$. The model based on \mathcal{H}^* is a ‘model of convenience’. There is a choice about which canonical components to drop in forming \mathcal{H}^* . When all the structures on Ω_i , $i = 1, \dots, p$, exhibit structure balance then a skeleton anova table can aid in detecting the cause of inestimability of the type outlined in Section 8.2.1 and so in determining which canonical components to drop.

Section 8.2.1 shows that in Example 1 the canonical components for Sessions and Blocks are inestimable. The term for one or other must be omitted from the mixed model. This should not be taken to imply that the designer or the analyser of the experiment is assuming that either does not contribute to the variability. Indeed, the estimated component should be regarded as estimating the sum of these two canonical components. Also, the spectral components for Sessions and Blocks are confounded and so it is not possible to check that each is nonnegative, although the nonnegativity of $\xi_S + 12\eta_B$ should be checked. All the other spectral components except ξ_0 and η_0 are estimable and so their nonnegativity can be verified.

For Example 2, the symbolic mixed model, derived using Step 1 in [14], is:

$$\begin{aligned} & \text{K} \mid \text{Operatives} + \text{Operatives} \wedge \text{Tests} \\ & + \text{Blocks} + \text{Blocks} \wedge \text{Plots} + \text{Blocks} \wedge \text{Plots} \wedge \text{Fibres}. \end{aligned}$$

As outlined in Section 8.2.1, none of the spectral components is estimable and so their nonnegativity cannot be checked, although the nonnegativity of sums such as $\xi_{OT} + \eta_B$ should be. However, all canonical components other than ϕ_0 and ψ_0 are estimable, except that only $\phi_{OT} + \psi_{BPF}$ is estimable. One of these two terms needs to be omitted. Omitting `Blocks^Plots^Fibres` is, in effect, setting $\psi_{BPF} = 0$, and hence $\eta_{BPF} = 0$. Again, it is not assumed that this is the true value of the components. The constraint is imposed merely to obtain a solution, and the supposed estimate of ϕ_{OT} is actually an estimate of $\phi_{OT} + \psi_{BPF}$.

For (ii), a check that the spectral components are nonnegative is the only option to ensure that the constraints on them are met. A GenStat procedure for this has been developed. Equation (5) is used to obtain the estimated spectral components from the estimated canonical components. If any spectral component is negative then the linear combination of canonical components on the right-hand side of equation (5) has to be constrained to zero in a refit of the model. If there are several negative spectral components, it may be that some canonical components are constrained to zero.

Difficulty (iii) occurs because the estimate of some canonical component happens to be zero. It has to be addressed by removing this canonical component from the model, which implies that a pair of spectral components are equal. It is not something that can be anticipated ahead of having the data.

12. Statistical inference. In order to perform hypothesis tests or compute confidence intervals one has to assume that the response follows a multivariate normal distribution whose expectation and variance are those described in Section 10 for the randomization-based model. Some justification for this approach is that, over all possible randomizations, the distribution of the data has this expectation and variance. The only further assumption that is required for inference is that of multivariate normality, although the guarantee for the associated expectation and covariance strictly applies only over future re-runs of the experiment. The role for randomization in an analysis based on this model is to ensure that the sources of variation taken into account by the designer have terms in the model; that is, it links the model to the design. Irrespective of the number of tiers, the randomization does not itself produce distributions whose third and higher-order moments are those of a multivariate normal distribution.

13. Other Models. Steps 2 and 3 of the method in [14] suggest changes that could be made to the expectation and variance of randomization-based models. Here we concentrate on changing treatment factors from fixed to random and changing unrandomized factors from random to fixed. The first of these produces a randomization-based model, but the second does not; the latter does not preserve the variance matrix under randomization as part of the model.

13.1. *Treatment factors regarded as random.* The simplest modification to the model in equation (1) is to assume that the τ_i , for i in Γ , are random variables with common mean μ and variance matrix \mathbf{C}_Γ , which may be as simple as $\sigma_\Gamma^2 \mathbf{I}_\Gamma$ or may be based on a poset block structure on Γ . So long as h is equireplicate, \mathbf{C}_Γ translates easily to add an extra variance matrix to \mathbf{V} .

Varieties in early generation variety trials are often regarded as random: see [42].

If Lines are designated random in Example 4 then the variance matrix becomes

$$\begin{aligned} \mathbf{V} = & \xi_0 \mathbf{P}_0 + \xi_O \mathbf{P}_O + \xi_{OIR} \mathbf{P}_{OIR} + \xi_{OIT} \mathbf{P}_{OIT} + \xi_{OIRT} \mathbf{P}_{OIRT} \\ & + \eta_0 \mathbf{Q}_0 + \eta_B \mathbf{Q}_B + \eta_{BP} \mathbf{Q}_{BP} + \eta_{BPS} \mathbf{Q}_{BPS} \\ & + 8\sigma_L^2 \mathbf{I}_{\mathcal{R}}. \end{aligned}$$

13.2. *Unrandomized factors regarded as fixed.* Sometimes it is appropriate to classify unrandomized factors such as Sites, Centres, Laboratories, Sex or Judges as fixed. It requires that there is no confounding between fixed sources. It results in the exclusion of the corresponding subspaces from the REML estimation of variance parameters, with canonical components effectively being set to zero and effects added to the expectation, so the variance matrix may have LDCVS. In the expected mean squares, $q(H)$ replaces $r_i k_H \phi_H$ if generalized factor H on Ω_i is designated as fixed.

Suppose that Operatives in Example 2 is to be considered fixed. This removes ϕ_O from the expression for the variance matrix, and $\text{Im}(\mathbf{P}_0 + \mathbf{P}_O)$ is excluded from the REML estimation of the canonical components. The effect on the expected mean squares in Table 2 is to replace ξ_O by $\xi_{OT} + q(O)$ and $15\phi_O$ by $q(O)$.

14. Discussion. This paper extends randomization-based models to multi-tiered experiments with two or more randomizations in a chain, and discusses the estimation of treatment effects and their standard errors, and canonical components, under the assumption of such a model. There are novel aspects to the estimability of spectral and canonical components in such experiments, including that the variance matrix can exhibit LDCVS.

We have emphasised the usefulness of a skeleton anova in checking the properties of a design and of anova in analysing anova-applicable experiments and for supplying initial estimates for mixed-model fitting. A limitation is software availability.

Otherwise, mixed-model fitting software is used to fit a randomization-based model. In this, one has to ensure that estimates of ‘variance components’ can be negative and be vigilant that estimates of spectral components are nonnegative.

While potentially negative canonical components are mandated for randomization-based models, they have the additional benefit of allowing for negative correlation, which is realistic in some circumstances: see [28]. Littell et al. [25], Section 4.7, recommend that unconstrained estimates be allowed in order to control Type I error, and show that they can achieve greater power; this agrees with the conclusions of Wolde-Tsadik and Afifi [47]. However, caution is required in ascribing a negative estimate for a component to negative population correlation. As Searle, Casella and McCulloch [41], Section 3.5, show, for a variance component just above zero, there can be a high probability of a negative estimate if the number of treatments is less than 5 and the number of replicates less than 25. Gilmour and Goos [21] demonstrate that simply allowing negative variance components is not a panacea, especially in small experiments.

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