

factorial but
constraints,
where
se experiments
 v_i is the
number of
levels of
factor i
The v_i th
factor

(1)

$$= V_1 V_2 \dots V_n$$

main

The
← When?

This ~~needs~~ ^{doesn't} explain how! ^{conditions, and}
 How does it ^{vector of} ~~inc~~ ^{allocate} the allocation? ^{where}

$$(x_1, x_2, \dots, x_n) : n\text{-tuple}$$

and $\beta_{jk} \sim \mathcal{N}(0, \sigma_j^2)$ ($j = 1, 2, \dots, b; k = 1, 2, \dots, m_j$). The block design matrix, \mathbf{Z} , in (1) can then be expressed as

- β_5 is not a ⁽⁴⁾block factor!

Same.

f why to q?

You need
to connect
q to
something
before
you write
equation

what??

Doesn't follow flow?

$$P_0 = Z_0^+ (Z_0^+ Z_0)^{-1} Z_0^+$$

$$P_1 =$$

elements in (6), i.e. V_0 and V_q , always denote the vector subspace for the grand mean and experimental error, respectively.

Since the decomposition is the separation of the known variation in the data, the variance structure of the data, y , can be expressed in spectral form as

his is like saying because — it follows that (6). Not the case! Re-word.

$$\text{Var}(y) = \sum_{l=0}^q \xi_l Q_l, \quad (6)$$

where Q_l is an $n \times n$ orthogonal projector matrix, which transforms vector y from vector space \mathbb{R}^n onto the vector subspace V_l (i.e. stratum l) and ξ_l is the l th stratum variance (~~the~~ $\xi_l = \text{Var}(Q_l y)$). Since the orthogonal projector is used to linear transform a vector onto a specific vector subspace, the orthogonal projector is a projection matrix which has the properties of being symmetric (i.e. $Q_l' = Q_l$), orthogonal (i.e. $Q_l Q_{l' \neq l} = 0$) and idempotent, (i.e. $Q_l^2 = Q_l$) (Hadi 1996).

It follows from (6) that the total unadjusted sum of squares (SS) of y , i.e. $y'y$, can be decomposed into $q+1$ components of the SS, i.e.

$$y'y = \sum_{l=0}^q y'Q_l y, \quad (7)$$

where $y'Q_l y$ denotes the total SS in the l th stratum. Equations (5), (6) and (7) thus give a basic illustration of the decomposition of the data vector space, total variability and SS without the treatment, which we refer to as the null decomposition. The remainder of this section describes each step of the null decomposition, particularly how the orthogonal projector, denoted by Q_0 , is computed in stratum l .

For any designed experiment, the initial step of null decomposition is to separate out the first term of the block structure formula, i.e. the grand mean, from the data vector, y . Since μ , in (1), is a vector of length 1, the grand mean vector spans a 1-dimensional grand mean vector subspace, denoted by V_0 in (5). Meanwhile, the orthogonal projector, Q_0 , is the projection matrix to project a vector onto vector subspace V_0 . This vector subspace can be generated by a set of vectors or a matrix. The grand mean vector subspace, V_0 , is thus generated by a $n \times n$ averaging matrix, denoted by K_n , with all elements equal to n^{-1} . The subscript n in K_n is again omitted for simplicity resulting in K . Hence, the projection of the vector y on to the grand mean vector subspace is given by

$$Q_0 y = P_K y$$

where P_K denotes the projection matrix of matrix K and is defined as

$$P_K = K(K'K)^{-1}K'$$

Since P_K can be shown to be the same as K , for simplicity, $P_K y$ is rewritten as Ky . The next step is to obtain the orthogonal complement of Ky by subtracting the Ky from y , i.e.

$$y - Ky = (I - K)y,$$

where $(I - K)y$ denotes the mean corrected observational vector, which spans V_0^\perp with dimension of $(n-1)$. The vector subspace V_0^\perp is also the orthogonal complement of V_0 . Furthermore, the adjusted total SS is computed by pre-multiplying the $(I - K)y$ by its transpose, i.e.

$$[(I - K)y]'[(I - K)y] = y'(I - K)y. \quad (8)$$

We refer to the decomposition which is $y'y$ as the null decomposition, as a null decomposition, treatment effects, as a null decomposition.

6 **InfoDecompute**: an R package for information decomposition of two-phase experiments

The total adjusted SS can also be computed by subtracting the grand mean of data, $y'Ky$, from the total unadjusted total SS, $y'y$, i.e.

$$y'y - y'Ky = y'(I - K)y.$$

The vector $(I - K)y$ is then projected onto the vector subspace of stratum 1, i.e. V_1 , which results in Q_1y , where Q_1 is the orthogonal projector of the stratum that corresponds to the second term of the expanded block structure formula. The vector subspace, V_1 , is generated by the block design matrix corresponding to the second term of the expanded block structure formula, denoted by Z_1 . The orthogonal projector Q_1 is thus given by the $I - K$ pre-multiplied by P_{Z_1} , i.e. $P_{Z_1}(I - K)$, which can be re-written as

$$I_{q_1} - K \rightarrow P_{Z_1}(I - K)y = (P_{Z_1} - K)y$$

$$Q_1 = P_{Z_1}(I - K) \quad (9)$$

where vector $(P_{Z_1} - K)y$ represents estimates of effects associated with the second term of the expanded block structure formula. The orthogonal complement of $(P_{Z_1} - K)y$ is then derived by subtraction from the vector $(I - K)y$ as

$$(I - K)y - (P_{Z_1} - K)y = (I - P_{Z_1})y, \quad (10)$$

which corresponds to the elimination of the effects from the second term of the expanded block structure formula.

The SS are derived by pre-multiplying the vectors in (10) by their transpose, as described in (8), i.e.

$$y'(I - K)y - y'(P_{Z_1} - K)y = y'(I - P_{Z_1})y.$$

If the expanded block structure formula contains additional terms, the vector $(I - P_{Z_1})y$ is further projected onto the next vector subspace, V_2 , corresponding to the third term of the expanded block structure formula. Thus, in general, the projection of the data vector, y from V_l onto V_{l+1} can be written as $P_{Z_{l+1}}Q_ly$. The orthogonal complement of $P_{Z_{l+1}}Q_ly$ can be derived by subtraction from Q_ly , i.e.

$$\rightarrow Q_ly - P_{Z_{l+1}}Q_ly = (I - P_{Z_{l+1}})Q_ly = Q_{l+1}y, \quad (l = 0, 1, \dots, q; Q_0 = K). \quad (11)$$

The SS thus are derived by pre-multiplying the vector in (11) by their transpose, as follows:

$$y'Q_ly - y'Q_lP_{Z_{l+1}}Q_ly = y'Q_l(I - P_{Z_{l+1}})Q_ly = y'Q_{l+1}y, \quad (l = 0, 1, \dots, q; Q_0 = K).$$

Providing the SS for each stratum is defined using the orthogonal projectors, the EMS can be computed for the theoretical ANOVA table. The expected sum of squares (ESS) of the l th stratum without the treatment effects can be shown as

$$E(y'Q_ly) = \text{tr}(Q_l) \text{cov}(y), \quad (12)$$

where $\text{cov}(y)$ is the variance-covariance matrix and $\text{tr}(Q_l)$ is the trace of the matrix Q_l (Searle 1982).

Consider an experiment arranged in RCBD, then the null decomposition of the total SS can be expressed as

$$y'y = y'Ky + y'(P_{Z_1} - K)y + y'(I - P_{Z_1})y, \quad (13)$$

where \mathbf{K} , $(\mathbf{P}_{\mathbf{Z}_1} - \mathbf{K})$ and $(\mathbf{I} - \mathbf{P}_{\mathbf{Z}_1})$ denote the orthogonal projectors of the grand mean, Between and Within Blocks strata, i.e. \mathbb{V}_0 , \mathbb{V}_1 and \mathbb{V}_2 , respectively.

Since the SS of the Between Blocks stratum is $\mathbf{y}'(\mathbf{P}_{\mathbf{Z}_1} - \mathbf{K})\mathbf{y}$, the ESS of the Between Blocks stratum can be shown as

$$\begin{aligned} E[\mathbf{y}'(\mathbf{P}_{\mathbf{Z}_1} - \mathbf{K})\mathbf{y}] &= \text{tr}(\mathbf{P}_{\mathbf{Z}_1} - \mathbf{K}) \text{cov}(\mathbf{y}) \\ &= \text{tr}(\mathbf{P}_{\mathbf{Z}_1} - \mathbf{K}) \text{cov}(\epsilon) + \text{tr}[\mathbf{Z}'(\mathbf{P}_{\mathbf{Z}_1} - \mathbf{K})\mathbf{Z}] \text{cov}(\beta) \\ &= (m_1 - 1)\sigma^2 + (m_1 - 1)m_2\sigma_1^2 \\ &= (m_1 - 1)(\sigma^2 + m_2\sigma_1^2), \end{aligned} \quad (14)$$

where m_1 and m_2 denote the block number and block size, respectively. Subsequently, the EMS is calculated by dividing the ESS by the corresponding DF. Hence, the EMS of the Between Blocks stratum is $\sigma^2 + m_2\sigma_1^2$. Similarly, the EMS of the Within Blocks stratum can be shown as σ^2 . Table 1 shows the theoretical ANOVA table without the treatment components for RCBD.

Table 1: ANOVA with the coefficients of variance components of the EMS from an experiment arranged with RCBD.

Source of Variation	Vector (Sub)space	DF	SS	EMS
Between Blocks	\mathbb{V}_1	$m_1 - 1$	$\mathbf{y}'(\mathbf{P}_{\mathbf{Z}_1} - \mathbf{K})\mathbf{y}$	$\sigma^2 + m_2\sigma_1^2$
Within Blocks	$\mathbb{V}_1^\perp = \mathbb{V}_2$	$m_1(m_2 - 1)$	$\mathbf{y}'(\mathbf{I} - \mathbf{P}_{\mathbf{Z}_1})\mathbf{y}$	σ^2
Adjusted Total	\mathbb{V}_0^\perp	$n - 1$	$\mathbf{y}'(\mathbf{I} - \mathbf{K})\mathbf{y}$	
Grand Mean	\mathbb{V}_0	1	$\mathbf{y}'\mathbf{K}\mathbf{y}$	
Total	\mathbb{R}^n	n	$\mathbf{y}'\mathbf{y}$	

2.3. Computing the treatment SS

The previous section presented an overview of the process used to compute the SS and EMS from the null decomposition. The next step is to compute the treatment SS and EMS within each stratum. To compute the treatment SS, the treatment design matrix, \mathbf{X} , must be defined in (1) with another set of matrices. This set of matrices are known as the treatment contrast matrices, and are denoted by \mathbf{C}_x (John and Williams 1987). These matrices can be generated based on the treatment structure and yield identity, which describes how the treatment effects are partitioned into orthogonal components.

Consider an example where the treatment structure comprises a single treatment factor, the effect of treatment f_1 is denoted by α_{f_1} , $f_1 = 1, \dots, t_1$, then the yield identity is given by

$$\alpha_{f_1} = \bar{\alpha}_{f_1} + (\alpha_{f_1} - \bar{\alpha}_{f_1}) \quad (15)$$

The dot in the subscript denotes the summation over the subscript it replaces and the over-line, also known as bar, indicates the average of the terms associated with the nominal subscript. Thus, $\bar{\alpha}_{f_1}$ denotes the overall mean of the α_{f_1} and $\alpha_{f_1} - \bar{\alpha}_{f_1}$ denotes the effect of treatment f_1 corrected for the mean. In matrix notation, (15) can be written as

$$\alpha = \mathbf{C}_0\alpha + \mathbf{C}_1\alpha$$

grand mean
over all levels of the
treatments (at levels)

where

$$\begin{aligned} \mathbf{C}_0 &= \mathbf{K}_{t_1} \\ \mathbf{C}_1 &= \mathbf{I}_{t_1} - \mathbf{K}_{t_1} \end{aligned}$$

where \mathbf{I}_{t_1} is the $t_1 \times t_1$ identity matrix and \mathbf{K}_{t_1} is the $t_1 \times t_1$ averaging matrix with all elements equal t_1^{-1} . The contrast matrix $\mathbf{C}_0\alpha$, corresponding to $\bar{\alpha}$, can be seen as an operation that averages over the α_i . The contrast matrix $\mathbf{C}_1\alpha$, corresponds to $\alpha_{f_1} - \bar{\alpha}$, represents the effect of treatment i after correction for the mean.

Consider a factorial experiment with two factors, f_1 and f_2 , with levels t_1 and t_2 , respectively, where the yield identity of $\alpha_{f_1 f_2}$, $f_1 = 1, \dots, t_1$; $f_2 = 1, \dots, t_2$, can be written as,

$$\alpha_{f_1 f_2} = \bar{\alpha}_{..} + (\bar{\alpha}_{f_1.} - \bar{\alpha}_{..}) + (\bar{\alpha}_{.f_2} - \bar{\alpha}_{..}) + (\alpha_{f_1 f_2} + \bar{\alpha}_{f_1.} + \bar{\alpha}_{.f_2} - \bar{\alpha}_{..}), \quad (16)$$

where $\bar{\alpha}_{..}$ denotes the overall mean of $\alpha_{f_1 f_2}$, $\bar{\alpha}_{f_1.} - \bar{\alpha}_{..}$ denotes the main effects of factor f_1 , $\bar{\alpha}_{.f_2} - \bar{\alpha}_{..}$ represents the main effects of factor f_2 and $\alpha_{f_1 f_2} + \bar{\alpha}_{f_1.} + \bar{\alpha}_{.f_2} - \bar{\alpha}_{..}$ is the interaction of two treatment factors. In the matrix notation, (16) can be written as

$$\alpha = \mathbf{C}_{00}\alpha + \mathbf{C}_{10}\alpha + \mathbf{C}_{01}\alpha + \mathbf{C}_{11}\alpha$$

where

$$\begin{aligned} \mathbf{C}_{00} &= \mathbf{K}_{t_1} \otimes \mathbf{K}_{t_2} &= \mathbf{K}_{t_1 t_2} \\ \mathbf{C}_{10} &= \mathbf{I}_{t_1} \otimes \mathbf{K}_{t_2} - \mathbf{K}_{t_1 t_2} &= (\mathbf{I}_{t_1} - \mathbf{K}_{t_1}) \otimes \mathbf{K}_{t_2} \\ \mathbf{C}_{01} &= \mathbf{K}_{t_1} \otimes \mathbf{I}_{t_2} - \mathbf{K}_{t_1 t_2} &= \mathbf{K}_{t_1} \otimes (\mathbf{I}_{t_2} - \mathbf{K}_{t_2}) \\ \mathbf{C}_{11} &= \mathbf{I}_{t_1 t_2} - \mathbf{I}_{t_1} \otimes \mathbf{K}_{t_2} - \mathbf{K}_{t_1} \otimes \mathbf{I}_{t_2} + \mathbf{K}_{t_1 t_2} &= (\mathbf{I}_{t_1} - \mathbf{K}_{t_1}) \otimes (\mathbf{I}_{t_2} - \mathbf{K}_{t_2}), \end{aligned}$$

where denotes \otimes an operator for the Kronecker product.

To summarise, for a v -factor experiment with each treatment factor f_i at t_i levels, $i = 1, \dots, v$, the treatment structure is given by

$$\alpha = \sum_x \mathbf{C}_x \alpha \quad (17)$$

where x is a string of binary numbers, $(x_1 x_2 \dots x_v)$, and

$$\mathbf{C}_x = \mathbf{C}_{x_1} \otimes \mathbf{C}_{x_2} \otimes \dots \otimes \mathbf{C}_{x_v} = \bigotimes_{i=1}^v \mathbf{C}_{x_i},$$

where

$$\mathbf{C}_{x_i} = \begin{cases} \mathbf{K}_{t_i}, & x_i = 0 \\ \mathbf{I}_{t_i} - \mathbf{K}_{t_i}, & x_i = 1, \end{cases} \quad (18)$$

where x_i is a binary number. For example, in a 2-factor $t_1 \times t_2$ factorial experiment, the treatment contrast matrix is represented by

$$\mathbf{C}_x = \mathbf{C}_{x_1 x_2} = \mathbf{C}_{x_1} \otimes \mathbf{C}_{x_2}.$$

Thus, the main effects of factors f_1 and f_2 are represented by the two sets of contrasts $\mathbf{C}_{10}\alpha$ and $\mathbf{C}_{01}\alpha$, respectively, and the $f_1 f_2$ interaction is represented by the set of contrasts $\mathbf{C}_{11}\alpha$.