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WHEN IS A SUM OF SQUARES AN ANALYSIS OF VARIANCE?

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A sum of squares can be partitioned into sums of quadratic forms whose kernels are projections. If these projections are mutually orthogonal and add to the identity, then, under the classical fixed effects linear model, the terms of the decomposition are mutually independent and are distributed as multiples of chi-square. In this paper we exhibit necessary and sufficient conditions for a specified sum of squares decomposition to have this property in the case of the mixed model.

1. Introduction. Suppose y is a normally distributed random vector that can be expressed in the form

$$y = m + \sum_{r=1}^{p} H_r x_r + v \tag{1.1}$$

where $(v, x_1, x_2, \cdots, x_p)$ are jointly distributed random vectors with mean zero and

$$\begin{aligned} \text{Cov}(x_r, v) &= 0 , \\ \text{Cov}(v, v) &= \sigma_0^2 I , \\ \text{Cov}(x_i, x_k) &= \sigma_i^2 I \qquad \text{if} \quad i = k \\ &= 0 \qquad\quad \text{otherwise.} \end{aligned}$$

The H's are specified matrices and m is an unknown (deterministic) vector parameter. If $p = 0$ (or $p = 1$ and $H_1 = 0$) the model described above describes the so-called *fixed effects linear model*. If $p > 0$ and $m = 0$, it describes the *random effects model* and in general it describes the so-called *mixed model*.

In [1], Graybill and Hultquist make the following

DEFINITION. An analysis of variance is said to exist (under the assumption that y is a normal vector whose components all have the same mean and whose covariance is $W = \sigma_0^2 I + \sum_{r=1}^{p} \sigma_r^2 H_r H_r'$) if matrices, B_i, of known constants exist such that

(1) $y'y = \sum_{i=0}^{p+1} y' B_i y$,

(2) $y' B_i y$ are distributed as constant multiples of (possibly noncentral) chi-square rv's,

(3) $B_0 = jj'/||j||^2$ (where j is the vector of ones),

(4) the $B_i y$ are pairwise independent,

(5) the constants of proportionality in (2) can be expressed as linear functions of the unknown parameters of the model.

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Defining $A_0 = jj'$ and $A_k = H_k H_k'$ (for $k = 1, \cdots, p$), Theorem 6 of [1] states that a necessary and sufficient condition for the existence of an analysis of variance is that the A's all commute with one another and that $\mathrm{E}yy'$ have $p+2$ distinct characteristic roots.

This theorem is an existence theorem and does not help one to decide whether a proposed sum of squares decomposition

$$y'y = \textstyle\sum_i y'P_i y \tag{1.2}$$

is an analysis of variance. This issue arises in connection with "Henderson's Method I," sometimes referred to as the "analysis of variance method" for estimating variance components (see Chapter 10 of [3]).

The present main result is intended to cast light on this latter issue.

2. The main result.

DEFINITION. Suppose $\{P_0, P_1, \cdots, P_n\}$ are a collection of symmetric idempotent matrices (projections) such that $P_i P_k = 0$ if $i \neq k$ and $\sum_{i=0}^n P_i = I$. We will call such a collection a *complete set of orthogonal projections.*

THEOREM 1. *Suppose* $\{P_0, P_1, \cdots, P_n\}$ *is a complete set of orthogonal projections so that*

$$y'y = \textstyle\sum_{i=0}^n y'P_i y\,. \tag{2.1}$$

If $y \sim N(m, W)$ *where* W *is nonsingular, then*

(a) *All terms on the right side of* (2.1) *are mutually independent and are distributed as scalar multiples of* (*possibly noncentral*) *chi-square* rv's *if and only if there are scalars*, γ_k, *such that*

$$WP_k = \gamma_k P_k \qquad (k = 0, 1, \cdots, n)\,. \tag{2.2}$$

In this case:

(b) *Each* $\gamma_k > 0$ *and the distribution of* $y'P_k y/\gamma_k$ *is chi-square with degrees of freedom equal to the rank of* P_k *and noncentrality parameter*

$$\delta_k = m'P_k m/\gamma_k\,. \tag{2.3}$$

(c) *The mean square value of* $P_k y$ *is*

$$Ey'P_k y = m'P_k m + \gamma_k \cdot \operatorname{rank}(P_k)\,. \tag{2.4}$$

PROOF (sufficiency of (a) and (b)). If (2.2) holds, $\operatorname{Cov}(P_i y, P_k y) = P_i W P_k = \gamma_k P_i P_k$, which establishes the independence of the terms on the right side of (2.1).

If x is a vector with $\|P_k x\| = 1$, then $\gamma_k = (P_k x)'W(P_k x) > 0$ because W is positive definite. Thus $P_k W/\gamma_k = P_k$ is idempotent and by Theorem 9.2.1 of [2], $y'P_k y/\gamma_k$ has a chi-square distribution with the asserted properties.

PROOF (necessity of (a)). If each $y'P_k y/\gamma_k$ has a (possibly noncentral) chi-square distribution then by Theorem 9.2.1 of [2], $P_k W/\gamma_k$ is idempotent and hence

$$P_k W P_k/\gamma_k = P_k \tag{2.5}$$

since W is assumed to be nonsingular. If $y'P_k y/\gamma_k$ is independent of $y'P_i y/\gamma_i$, then by Theorem 9.4.1 of [2], $P_i W P_k = 0$. The last implies that $(I - P_k)WP_k = (\sum_{i\neq k} P_i)WP_k = 0$ and so

$$\frac{WP_k}{\gamma_k} = \frac{P_k W P_k}{\gamma_k}.$$

From (2.5), we conclude

$$WP_k = \gamma_k P_k \qquad k = 0, 1, \cdots, n,$$

as claimed. □

The application to Henderson's Method I is implicit in the following:

COROLLARY. *Suppose*

$$W = \sigma_0^2 I + \sum_{r=1}^{p} \sigma_r^2 H_r H_r'.$$

All terms on the right of (2.1) *are mutually independent and are distributed as scalar multiples of* (*possibly noncentral*) *chi-square* rv's *and this statement holds for all choices of* $\sigma_0^2 > 0$, $\sigma_1^2 \geqq 0, \cdots, \sigma_p^2 \geqq 0$ *if and only if there are scalars,* λ_{kr} *such that*

$$H_r H_r' P_k = \lambda_{kr} P_k \qquad k = 0, 1, \cdots, n; r = 1, \cdots, p. \tag{2.6}$$

In this case (2.2) *holds for each such choice of the* σ's *and*

$$\gamma_k = \gamma_k(\sigma_0^2, \sigma_1^2, \cdots, \sigma_p^2) = \sigma_0^2 + \sum_{r=1}^{p} \lambda_{kr}\sigma_r^2. \tag{2.7}$$

PROOF. If (2.6) holds, then (2.2) holds with γ_k defined as in (2.7). Conversely, if (2.2) holds for all $\sigma_0^2 > 0$, $\sigma_1^2 \geqq 0, \cdots, \sigma_p^2 \geqq 0$ then, setting $\sigma_0^2 = \sigma_r^2 = 1$ and all the other σ's $= 0$, we see that (2.6) will hold.

COMMENT. Under the hypotheses of Theorem 1, the mean value vector, m, can be arbitrary. The Graybill–Hultquist condition (that m's components are all the same) is overly restrictive and we have dispensed with it.

3. Balanced designs. In many ANOVA models of the form (1.1), the matrices, H_r, satisfy the condition

$$H_r' H_r = \nu_r^2 I_{m_r} \qquad r = 1, 2, \cdots, p \tag{3.1}$$

where m_r is the number of columns in H_r. The results of Theorem 1 can be sharpened in this case:

THEOREM 2. *Suppose* (2.6) *holds for a complete set of orthogonal projections. If* (3.1) *holds, then* γ_k, *defined by* (2.7), *satisfies*

$$\gamma_k = \sigma_0^2 + \sum_{r \in \mathscr{S}_k} \nu_r^2 \sigma_r^2. \tag{3.2}$$

Here,

$$\mathscr{S}_k = \{r \geqq 1 : H_r' P_k \neq 0\} \qquad k = 0, 1, \cdots, n. \tag{3.3}$$

PROOF. The nonzero eigenvalues of $H_r H_r'$ are the same as the nonzero eigenvalues of $H_r' H_r$, namely ν_r^2. Thus, either $H_r H_r' P_k = 0$ or $H_r H_r' P_k = \nu_r^2 P_k$ if (2.6) holds. The conclusion follows since $H_r H_r' P = 0$ if and only if $H_r' P = 0$.

COMMENTS. If H_r is an incidence matrix satisfying (3.1), ν_r^2 is an integer equal to the number of nonzero entries in a typical column of H_r. In fact, ν_r^2 is equal to the number of observations involving each component of the "main effect" x_r in such a "balanced design."

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