13 One-Way Analysis-of-Variance: Balanced Case

The one-way analysis-of-variance (ANOVA) model has been illustrated in Sections 12.1.1, 12.2.2, 12.3.1, 12.5, and 12.6. We now analyze this model more fully. To solve the normal equations in Section 13.3, we use side conditions as well as a generalized inverse approach. For hypothesis tests in Section 13.4, we use both the full-reduced-model approach and the general linear hypothesis. Expected mean squares are obtained in Section 13.5 using both a full-reduced-model approach and a general linear hypothesis approach. In Section 13.6, we discuss contrasts on the means, including orthogonal polynomials. Throughout this chapter, we consider only the balanced model. The unbalanced case is discussed in Chapter 15.

13.1 THE ONE-WAY MODEL

The one-way balanced model can be expressed as follows:

$$y_{ij} = \mu + \alpha_i + \varepsilon_{ij}, \quad i = 1, 2, \dots, k, j = 1, 2, \dots, n.$$
 (13.1)

If $\alpha_1, \alpha_2, \ldots, \alpha_k$ represent the effects of k treatments, each of which is applied to n experimental units, then y_{ij} is the response of the jth observation among the n units that receive the ith treatment. For example, in an agricultural experiment, the treatments may be different fertilizers or different amounts of a given fertilizer. On the other hand, in some experimental situations, the k groups may represent samples from k populations whose means we wish to compare, populations that are not created by applying treatments. For example, suppose that we wish to compare the average lifetimes of several brands of batteries or the mean grade-point averages for freshmen, sophomores, juniors, and seniors. Three additional assumptions that form part of the model in (13.1) are

1.
$$E(\varepsilon_{ij}) = 0$$
 for all i, j .

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- 2. $var(\varepsilon_{ii}) = \sigma^2$ for all i, j.
- 3. $cov(\varepsilon_{ij}, \varepsilon_{rs}) = 0$ for all $(i, j) \neq (r, s)$.
- 4. We sometimes add the assumption that ε_{ij} is distributed as $N(0, \sigma^2)$.
- 5. In addition, we often use the constraint (side condition) $\sum_{i=1}^{k} \alpha_i = 0$.

The mean for the *i*th treatment or population can be denoted by μ_i . Thus $E_{ij} = \mu_i$, and using assumption 1, we have $\mu_i = \mu + \alpha_i$. We can thus write (13.1) in the form

$$y_{ij} = \mu_i + \varepsilon_{ij}, \quad i = 1, 2, \dots, k, \ j = 1, 2, \dots, n.$$
 (13.2)

In this form of the model, the hypothesis H_0 : $\mu_1 = \mu_2 = \cdots = \mu_k$ is of interest.

In the context of design of experiments, the one-way layout is sometimes called a *completely randomized design*. In this design, the experimental units are assigned at random to the *k* treatments.

13.2 ESTIMABLE FUNCTIONS

To illustrate the model (13.1) in matrix form, let k = 3 and n = 2. The resulting six equations, $y_{ij} = \mu + \alpha_i + \varepsilon_{ij}$, i = 1, 2, 3, j = 1, 2, can be expressed as

$$\begin{pmatrix} y_{11} \\ y_{12} \\ y_{21} \\ y_{22} \\ y_{31} \\ y_{32} \end{pmatrix} = \begin{pmatrix} \mu + \alpha_1 \\ \mu + \alpha_2 \\ \mu + \alpha_2 \\ \mu + \alpha_3 \\ \mu + \alpha_3 \end{pmatrix} + \begin{pmatrix} \varepsilon_{11} \\ \varepsilon_{12} \\ \varepsilon_{21} \\ \varepsilon_{22} \\ \varepsilon_{31} \\ \varepsilon_{32} \end{pmatrix}$$

$$= \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \mu \\ \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{pmatrix} + \begin{pmatrix} \varepsilon_{11} \\ \varepsilon_{12} \\ \varepsilon_{21} \\ \varepsilon_{22} \\ \varepsilon_{31} \\ \varepsilon_{22} \end{pmatrix}, \quad (13.3)$$

or

$$y = X\beta + \varepsilon$$
.

In (13.3), **X** is 6×4 and is clearly of rank 3 because the first column is the sum of the other three columns. Thus $\beta = (\mu, \alpha_1, \alpha_2, \alpha_3)'$ is not unique and not estimable; hence

the individual parameters μ , α_1 , α_2 , α_3 cannot be estimated unless they are subject to constraints (side conditions). In general, the **X** matrix for the one-way balanced model is $kn \times (k+1)$ of rank k.

We discussed estimable functions $\lambda' \beta$ in Section 12.2.2. It was shown in Problem 12.10 that for the one-way balanced model, contrasts in the α 's are estimable. Thus $\sum_i c_i \alpha_i$ is estimable if and only if $\sum_i c_i = 0$. For example, contrasts such as $\alpha_1 - \alpha_2$ and $\alpha_1 - 2\alpha_2 + \alpha_3$ are estimable.

If we impose a side condition on the α_i 's and denote the constrained parameters as μ^* and α_i^* , then μ^* , α_1^* , ..., α_k^* are uniquely defined and estimable. Under the usual side condition, $\sum_{i=1}^k \alpha_i^* = 0$, the parameters are defined as $\mu^* = \bar{\mu}$ and $\alpha_i^* = \mu_i - \bar{\mu}$, where $\bar{\mu} = \sum_{i=1}^k \mu_i/k$. To see this, we rewrite (13.1) and (13.2) in the form $E(y_{ij}) = \mu_i = \mu^* + \alpha_i^*$ to obtain

$$\bar{\mu}_{\cdot} = \sum_{i=1}^{k} \frac{\mu_{i}}{k} = \sum_{i} \frac{\mu^{*} + \alpha_{i}^{*}}{k}$$

$$= \mu^{*} + \sum_{i} \frac{\alpha_{i}^{*}}{k} = \mu^{*}.$$
(13.4)

Then, from $\mu_i = \mu^* + \alpha_i^*$, we have

$$\alpha_i^* = \mu_i - \mu^* = \mu_i - \bar{\mu}. \tag{13.5}$$

13.3 ESTIMATION OF PARAMETERS

13.3.1 Solving the Normal Equations

Extending (13.3) to a general k and n, the one-way model can be written in matrix form as

$$\begin{pmatrix} \mathbf{y}_1 \\ \mathbf{y}_2 \\ \vdots \\ \mathbf{y}_k \end{pmatrix} = \begin{pmatrix} \mathbf{j} & \mathbf{j} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{j} & \mathbf{0} & \mathbf{j} & \cdots & \mathbf{0} \\ \vdots & \vdots & \vdots & & \vdots \\ \mathbf{j} & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{j} \end{pmatrix} \begin{pmatrix} \boldsymbol{\mu} \\ \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_k \end{pmatrix} + \begin{pmatrix} \boldsymbol{\varepsilon}_1 \\ \boldsymbol{\varepsilon}_2 \\ \vdots \\ \boldsymbol{\varepsilon}_k \end{pmatrix}, \tag{13.6}$$

or

$$\mathbf{v} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$$
,

where **j** and **0** are each of size $n \times 1$, and \mathbf{y}_i and $\boldsymbol{\varepsilon}_i$ are defined as

$$\mathbf{y}_i = egin{pmatrix} y_{i1} \ y_{i2} \ dots \ y_{in} \end{pmatrix}, \quad oldsymbol{arepsilon}_i = egin{pmatrix} arepsilon_{i1} \ arepsilon_{i2} \ dots \ arepsilon_{in} \end{pmatrix}.$$

For (13.6), the normal equations $\mathbf{X}'\mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{X}'\mathbf{y}$ take the form

$$\begin{pmatrix}
kn & n & n & \cdots & n \\
n & n & 0 & \cdots & 0 \\
n & 0 & n & \cdots & 0 \\
\vdots & \vdots & \vdots & & \vdots \\
n & 0 & 0 & \cdots & n
\end{pmatrix}
\begin{pmatrix}
\hat{\mu} \\
\hat{\alpha}_{1} \\
\hat{\alpha}_{2} \\
\vdots \\
\hat{\alpha}_{k}
\end{pmatrix} = \begin{pmatrix}
y_{.} \\
y_{1.} \\
y_{2.} \\
\vdots \\
y_{k.}
\end{pmatrix},$$
(13.7)

where $y_{..} = \sum_{ij} y_{ij}$ and $y_{i.} = \sum_{i} y_{ij}$.

In Section 13.3.1.1, we find a solution of (13.7) using side conditions, and in Section 13.3.1.2 we find another solution using a generalized inverse of X'X.

13.3.1.1 Side Conditions

The k + 1 normal equations in (13.7) can be expressed as

$$kn\hat{\mu} + n\hat{\alpha}_1 + n\hat{\alpha}_2 + \dots + n\hat{\alpha}_k = y_{..},$$

$$n\hat{\mu} + n\hat{\alpha}_i = y_i, \quad i = 1, 2, \dots, k.$$
(13.8)

Using the side condition $\sum_{i} \hat{\alpha}_{i} = 0$, the solution to (13.8) is given by

$$\hat{\mu} = \frac{y_{..}}{kn} = \bar{y}_{..},$$

$$\hat{\alpha}_i = \frac{y_{i.}}{n} - \hat{\mu} = \bar{y}_{i.} - \bar{y}_{..}, \quad i = 1, 2, ..., k.$$
(13.9)

In vector form, this solution $\hat{\boldsymbol{\beta}}$ for $\mathbf{X}'\mathbf{X}\hat{\boldsymbol{\beta}} = \mathbf{X}'\mathbf{y}$ is expressed as

$$\hat{\boldsymbol{\beta}} = \begin{pmatrix} \bar{y}_{..} \\ \bar{y}_{1.} - \bar{y}_{..} \\ \vdots \\ \bar{y}_{k.} - \bar{y}_{..} \end{pmatrix}. \tag{13.10}$$

If the side condition $\sum_i \alpha_i^* = 0$ is imposed on the parameters, then the elements of $\hat{\beta}$ are unique estimators of the (constrained) parameters $\mu^* = \bar{\mu}$ and

 $\alpha_i^* = \mu_i - \bar{\mu}_i$, i = 1, 2, ..., k, in (13.4) and (13.5). Otherwise, the estimators in (13.9) or (13.10) are to be used in estimable functions. For example, by Theorem 12.3a(i), the estimator of $\lambda' \beta = \alpha_1 - \alpha_2$ is given by $\lambda' \hat{\beta}$:

$$\lambda'\hat{\beta} = \alpha_1 - \alpha_2 = \hat{\alpha}_1 - \hat{\alpha}_2 = \bar{y}_1 - \bar{y}_2 - (\bar{y}_2 - \bar{y}_2) = \bar{y}_1 - \bar{y}_2$$

By Theorem 12.3d, such estimators are BLUE. If ε_{ij} is $N(0, \sigma^2)$, then, by Theorem 12.3h, the estimators are minimum variance unbiased estimators.

13.3.1.2 Generalized Inverse

By Corollary 1 to Theorem 2.8b, a generalized inverse of X'X in (13.7) is given by

$$(\mathbf{X}'\mathbf{X})^{-} = \begin{pmatrix} 0 & 0 & \cdots & 0 \\ 0 & \frac{1}{n} & \cdots & 0 \\ \vdots & \vdots & & \vdots \\ 0 & 0 & \cdots & \frac{1}{n} \end{pmatrix} .$$
 (13.11)

Then by (12.13) and (13.7), a solution to the normal equations is obtained as

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'\mathbf{y} = \begin{pmatrix} 0 \\ \bar{y}_{1.} \\ \vdots \\ \bar{y}_{k} \end{pmatrix}.$$
 (13.12)

The estimators in (13.12) are different from those in (13.10), but they give the same estimates of estimable functions. For example, using $\hat{\beta}$ from (13.12) to estimate $\lambda'\beta = \alpha_1 - \alpha_2$, we have

$$\boldsymbol{\lambda}'\hat{\boldsymbol{\beta}} = \widehat{\alpha_1 - \alpha_2} = \widehat{\alpha_1} - \widehat{\alpha_2} = \overline{y}_{1.} - \overline{y}_{2.},$$

which is the same estimate as that obtained above in Section 13.3.1.1 using $\hat{\beta}$ from (13.10).

13.3.2 An Estimator for σ^2

In assumption 2 for the one-way model in (13.1), we have $var(\varepsilon_{ij}) = \sigma^2$ for all i, j. To estimate σ^2 , we use (12.22)

$$s^2 = \frac{\text{SSE}}{k(n-1)},$$

where SSE is as given by (12.20) or (12.21):

$$SSE = \mathbf{y}'\mathbf{y} - \hat{\boldsymbol{\beta}}'\mathbf{X}'\mathbf{y} = \mathbf{y}'[\mathbf{I} - \mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}']\mathbf{y}.$$

The rank of the idempotent matrix $\mathbf{I} - \mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'$ is kn - k because $\mathrm{rank}(\mathbf{X}) = k$, $\mathrm{tr}(\mathbf{I}) = kn$, and $\mathrm{tr}[\mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'] = k$ (see Theorem 2.13d). Then $s^2 = \mathrm{SSE}/k(n-1)$ is an unbiased estimator of σ^2 [see Theorem 12.3e(i)].

Using $\hat{\beta}$ from (13.12), we can express SSE = $y'y - \hat{\beta}'Xy$ in the following form:

SSE =
$$\mathbf{y}'\mathbf{y} - \hat{\boldsymbol{\beta}}'\mathbf{X}'\mathbf{y} = \sum_{i=1}^{k} \sum_{j=1}^{n} y_{ij}^{2} - \sum_{i=1}^{k} \bar{y}_{i.} y_{i.}$$

= $\sum_{i} y_{ij}^{2} - \sum_{i} \frac{y_{i.}^{2}}{n}$. (13.13)

It can be shown (see Problem 13.4) that (13.13) can be written as

$$SSE = \sum_{ii} (y_{ij} - \bar{y}_{i.})^2.$$
 (13.14)

Thus s^2 is given by either of the two forms

$$s^{2} = \frac{\sum_{ij} (y_{ij} - \bar{y}_{i.})^{2}}{k(n-1)}$$
 (13.15)

$$=\frac{\sum_{ij} y_{ij}^2 - \sum_i y_{i.}^2 / n}{k(n-1)}.$$
 (13.16)

13.4 TESTING THE HYPOTHESIS $H_0: \mu_1 = \mu_2 = \cdots = \mu_k$

Using the model in (13.2), the hypothesis of equality of means can be expressed as $H_0: \mu_1 = \mu_2 = \cdots = \mu_k$. The alternative hypothesis is that at least two means are unequal. Using $\mu_i = \mu + \alpha_i$ [see (13.1) and (13.2)], the hypothesis can be expressed as $H_0: \alpha_1 = \alpha_2 = \cdots = \alpha_k$, which is testable because it can be written in terms of k-1 linearly independent estimable contrasts, for example, $H_0: \alpha_1 - \alpha_2 = \alpha_1 - \alpha_3 = \cdots = \alpha_1 - \alpha_k = 0$ (see the second paragraph in Section 12.7.1). In Section 13.4.1 we develop the test using the full-reduced-model approach, and in Section 13.4.2 we use the general linear hypothesis approach. In the model $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$, the vector \mathbf{y} is $kn \times 1$ [see (13.6)]. Throughout Section 13.4, we assume that \mathbf{y} is $N_{kn}(\mathbf{X}\boldsymbol{\beta}, \sigma^2\mathbf{I})$.

13.4.1 Full-Reduced-Model Approach

The hypothesis

$$H_0: \alpha_1 = \alpha_2 = \dots = \alpha_k \tag{13.17}$$

is equivalent to

$$H_0: \alpha_1^* = \alpha_2^* = \dots = \alpha_k^*,$$
 (13.18)

where the α_i^* terms are subject to the side condition $\sum_i \alpha_i^* = 0$. With this constraint, H_0 in (13.18) is also equivalent to

$$H_0: \alpha_1^* = \alpha_2^* = \dots = \alpha_k^* = 0.$$
 (13.19)

The full model, $y_{ij} = \mu + \alpha_i + \varepsilon_{ij}$, i = 1, 2, ..., k, j = 1, 2, ..., n, is expressed in matrix form $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$ in (13.6). If the full model is written in terms of μ^* and α_i^* as $y_{ij} = \mu^* + \alpha_i^* + \varepsilon_{ij}$, then the reduced model under H_0 in (13.19) is $y_{ij} = \mu^* + \varepsilon_{ij}$. In matrix form, this becomes $\mathbf{y} = \mu^* \mathbf{j} + \boldsymbol{\varepsilon}$, where \mathbf{j} is $kn \times 1$. To be consistent with the full model $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$, we write the reduced model as

$$\mathbf{y} = \mu \mathbf{j} + \boldsymbol{\varepsilon}. \tag{13.20}$$

For the full model, the sum of squares $SS(\mu, \alpha) = \hat{\beta}' X' y$ is given as part of (13.13) as

$$SS(\mu, \alpha) = \hat{\boldsymbol{\beta}}' \mathbf{X}' \mathbf{y} = \sum_{i=1}^{k} \frac{y_{i.}^{2}}{n},$$

where the sum of squares $SS(\mu, \alpha_1, ..., \alpha_k)$ is abbreviated as $SS(\mu, \alpha)$. For the reduced model in (13.20), the estimator " $\hat{\beta} = (X'X)^{-1}X'y$ " and the sum of squares " $\hat{\beta}'X'y$ " become

$$\hat{\mu} = (\mathbf{j}'\mathbf{j})^{-1}\mathbf{j}'\mathbf{y} = \frac{1}{k_{P}}y_{..} = \bar{y}_{..},$$
 (13.21)

$$SS(\mu) = (\hat{\mu})' \mathbf{j}' \mathbf{y} = \bar{y}_{..} y_{..} = \frac{y_{..}^2}{kn},$$
(13.22)

where **j** is $kn \times 1$.

From Table 12.3, the sum of squares for the α 's adjusted for μ is given by

$$SS(\alpha|\mu) = SS(\mu, \alpha) - SS(\mu) = \hat{\boldsymbol{\beta}}' \mathbf{X}' \mathbf{y} - \frac{y_{..}^2}{kn}$$
$$= \frac{1}{n} \sum_{i=1}^{k} y_{i.}^2 - \frac{y_{..}^2}{kn}$$
(13.23)

$$= n \sum_{i=1}^{k} (\bar{y}_{i.} - \bar{y}_{..})^{2}. \tag{13.24}$$

Source of Variation	df	Sum of Squares	Mean Square	F Statistic
Treatments	k - 1	$SS(\alpha \mu) = \frac{1}{n} \sum_{i} y_{i.}^2 - \frac{y_{}^2}{kn}$	$SS\frac{(\alpha \mu)}{k-1}$	$\frac{\mathrm{SS}(\alpha \mu)/(k-1)}{\mathrm{SSE}/k(n-1)}$
Error	k(n-1)	$SSE = \sum_{ij} y_{ij}^2 - \frac{1}{n} \sum_{i} y_{i.}^2$	$\frac{\text{SSE}}{k(n-1)}$	_
Total	kn-1	$SST = \sum_{ij} y_{ij}^2 - \frac{y_{}^2}{kn}$		

TABLE 13.1 ANOVA for Testing $H_0: \alpha_1 = \alpha_2 = \cdots = \alpha_k$ in the One-Way Model

The test is summarized in Table 13.1 using $SS(\alpha|\mu)$ in (13.23) and SSE in (13.13). The chi-square and independence properties of $SS(\alpha|\mu)$ and SSE follow from results established in Section 12.7.2.

To facilitate comparison of (13.23) with the result of the general linear hypothesis approach in Section 13.4.2, we now express $SS(\alpha|\mu)$ as a quadratic form in y. By (12.13), $\hat{\beta} = (X'X)^-X'y$, and therefore $\hat{\beta}'X'y = y'X(X'X)^-X'y$. Then with (13.21) and (13.22), we can write

$$SS(\alpha|\mu) = \hat{\boldsymbol{\beta}}' \mathbf{X}' \mathbf{y} - \frac{y_{...}^{2}}{kn}$$

$$= \mathbf{y}' \mathbf{X} (\mathbf{X}' \mathbf{X})^{-} \mathbf{X}' \mathbf{y} - \mathbf{y}' \mathbf{j}_{kn} (\mathbf{j}'_{kn} \mathbf{j}_{kn})^{-1} \mathbf{j}'_{kn} \mathbf{y}$$

$$= \mathbf{y}' \mathbf{X} (\mathbf{X}' \mathbf{X})^{-} \mathbf{X}' \mathbf{y} - \mathbf{y}' \left(\frac{\mathbf{j}_{kn} \mathbf{j}'_{kn}}{kn} \right) \mathbf{y}$$

$$= \mathbf{y}' [\mathbf{X} (\mathbf{X}' \mathbf{X})^{-} \mathbf{X}' - \frac{1}{kn} \mathbf{J}_{kn}] \mathbf{y}.$$
(13.25)

Using some results in the answer to Problem 13.3, this can be expressed as

$$SS(\alpha|\mu) = \mathbf{y}' \begin{bmatrix} \mathbf{J} & \mathbf{O} & \cdots & \mathbf{O} \\ \mathbf{O} & \mathbf{J} & \cdots & \mathbf{O} \\ \vdots & \vdots & & \vdots \\ \mathbf{O} & \mathbf{O} & \cdots & \mathbf{J} \end{bmatrix} - \frac{1}{kn} \begin{pmatrix} \mathbf{J} & \mathbf{J} & \cdots & \mathbf{J} \\ \mathbf{J} & \mathbf{J} & \cdots & \mathbf{J} \\ \vdots & \vdots & & \vdots \\ \mathbf{J} & \mathbf{J} & \cdots & \mathbf{J} \end{pmatrix} \end{bmatrix} \mathbf{y}$$
(13.26)

$$= \frac{1}{kn} \mathbf{y}' \begin{pmatrix} (k-1)\mathbf{J} & -\mathbf{J} & \cdots & -\mathbf{J} \\ -\mathbf{J} & (k-1)\mathbf{J} & \cdots & -\mathbf{J} \\ \vdots & \vdots & & \vdots \\ -\mathbf{J} & -\mathbf{J} & \cdots & (k-1)\mathbf{J} \end{pmatrix} \mathbf{y},$$

where each **J** in (13.26) and (13.27) is $n \times n$.

Method	A	В	С
	14.29	20.06	20.04
	19.10	20.64	26.23
	19.09	18.00	22.74
	16.25	19.56	24.04
	15.09	19.47	23.37
	16.61	19.07	25.02
	19.63	18.38	23.27
Totals (y_i)	120.06	135.18	164.71
Means (\bar{y}_i)	17.15	19.31	23.53

TABLE 13.2 Ascorbic Acid (mg/100g) for Three Packaging Methods

Example 13.4. Three methods of packaging frozen foods were compared by Daniel (1974, p. 196). The response variable was ascorbic acid $(mg/100\,g)$. The data are in Table 13.2.

To make the test comparing the means of the three methods, we calculate

$$\frac{y_{...}^2}{kn} = \frac{(419.95)^2}{(3)(7)} = 8298.0001,$$

$$\frac{1}{7} \sum_{i=1}^3 y_{i.}^2 = \frac{1}{7} \left[(120.06)^2 + (135.18)^2 + (164.71)^2 \right]$$

$$= \frac{1}{7} (59, 817.4201) = 8545.3457,$$

$$\sum_{i=1}^3 \sum_{i=1}^7 y_{ij}^2 = 8600.3127.$$

The sums of squares for treatments, error, and total are then

$$SS(\alpha|\mu) = \frac{1}{7} \sum_{i=1}^{3} y_{i.}^{2} - \frac{y_{..}^{2}}{21} = 8545.3457 - 8398.0001 = 147.3456,$$

$$SSE = \sum_{ij} y_{ij}^{2} - \frac{1}{7} \sum_{i} y_{i.}^{2} = 8600.3127 - 8545.3457 = 54.9670,$$

$$SST = \sum_{ij} y_{ij}^{2} - \frac{y_{..}^{2}}{21} = 8600.3127 - 8398.0001 = 202.3126.$$

These sums of squares can be used to obtain an F test, as in Table 13.3. The p value for F = 24.1256 is 8.07×10^{-6} . Thus we reject $H_0: \mu_1 = \mu_2 = \mu_3$.

Source	df	Sum of Squares	Mean Square	F
Method	2	147.3456	73.6728	24.1256
Error	18	54.9670	3.0537	
Total	20	202.3126		

TABLE 13.3 ANOVA for the Ascorbic Acid Data in Table 13.2

13.4.2 General Linear Hypothesis

For simplicity of exposition, we illustrate all results in this section with k=4. In this case, $\beta = (\mu, \alpha_1, \alpha_2, \alpha_3, \alpha_4)'$, and the hypothesis is $H_0: \alpha_1 = \alpha_2 = \alpha_3 = \alpha_4$. Using three linearly independent estimable contrasts, the hypothesis can be written in the form

$$H_0: \begin{pmatrix} \alpha_1 - \alpha_2 \\ \alpha_1 - \alpha_3 \\ \alpha_1 - \alpha_4 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix},$$

which can be expressed as H_0 : $C\beta = 0$, where

$$\mathbf{C} = \begin{pmatrix} 0 & 1 & -1 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 & -1 \end{pmatrix}. \tag{13.28}$$

The matrix **C** in (13.28) used to express H_0 : $\alpha_1 = \alpha_2 = \alpha_3 = \alpha_4$ is not unique. Other contrasts could be used in **C**, for example

$$\mathbf{C}_1 = \begin{pmatrix} 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 1 & -1 \end{pmatrix} \quad \text{or} \quad \mathbf{C}_2 = \begin{pmatrix} 0 & 1 & 1 & -1 & -1 \\ 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 & -1 \end{pmatrix}.$$

From (12.13) and Theorem 12.7b(iii), we have

$$SSH = (\mathbf{C}\hat{\boldsymbol{\beta}})'[\mathbf{C}(\mathbf{X}'\mathbf{X})^{-}\mathbf{C}']^{-1}\mathbf{C}\hat{\boldsymbol{\beta}}$$

$$= \mathbf{y}'\mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{C}'[\mathbf{C}(\mathbf{X}'\mathbf{X})^{-}\mathbf{C}']^{-1}\mathbf{C}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'\mathbf{y}.$$
(13.29)

Using C in (13.28) and $(X'X)^-$ in (13.11), we obtain

$$\mathbf{C}(\mathbf{X}'\mathbf{X})^{-}\mathbf{C}' = \frac{1}{n} \begin{pmatrix} 0 & 1 & -1 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 1 & 1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$
$$= \frac{1}{n} \begin{pmatrix} 2 & 1 & 1 \\ 1 & 2 & 1 \\ 1 & 1 & 2 \end{pmatrix}. \tag{13.30}$$

To find the inverse of (13.30), we write it in the form

$$\mathbf{C}(\mathbf{X}'\mathbf{X})^{-}\mathbf{C}' = \frac{1}{n} \begin{bmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + \begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} \end{bmatrix} = \frac{1}{n} (\mathbf{I}_{3} + \mathbf{j}_{3} \mathbf{j}'_{3}).$$

Then by (2.53), the inverse is

$$[\mathbf{C}(\mathbf{X}'\mathbf{X})^{-}\mathbf{C}']^{-1} = n\left(\mathbf{I}_{3} - \frac{\mathbf{I}_{3}^{-1}\mathbf{j}_{3}\mathbf{j}_{3}'\mathbf{I}_{3}^{-1}}{1 + \mathbf{j}_{3}'\mathbf{I}_{3}^{-1}\mathbf{j}_{3}}\right)$$

$$= n\left(\mathbf{I}_{3} - \frac{1}{4}\mathbf{J}_{3}\right), \tag{13.31}$$

where J_3 is 3×3 .

For $C(X'X)^-X'$ in (13.29), we obtain

$$\mathbf{C}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}' = \frac{1}{n} \begin{pmatrix} \mathbf{j}'_{n} & -\mathbf{j}'_{n} & \mathbf{0}' & \mathbf{0}' \\ \mathbf{j}'_{n} & \mathbf{0}' & -\mathbf{j}'_{n} & \mathbf{0}' \\ \mathbf{j}'_{n} & \mathbf{0}' & \mathbf{0}' & -\mathbf{j}'_{n} \end{pmatrix} = \frac{1}{n}\mathbf{A},$$
 (13.32)

where \mathbf{j}'_n and $\mathbf{0}'$ are $1 \times n$.

Using (13.31) and (13.32), the matrix of the quadratic form for SSH in (13.29) can be expressed as

$$\mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{C}'[\mathbf{C}(\mathbf{X}'\mathbf{X})^{-}\mathbf{C}']^{-1}\mathbf{C}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}' = \frac{1}{n}\mathbf{A}'n\left(\mathbf{I}_{3} - \frac{1}{4}\mathbf{J}_{3}\right)\frac{1}{n}\mathbf{A}$$

$$= \frac{1}{n}\mathbf{A}'\mathbf{I}_{3}\mathbf{A} - \frac{1}{4n}\mathbf{A}'\mathbf{J}_{3}\mathbf{A}. \tag{13.33}$$

The first term of (13.33) is given by

$$\frac{1}{n}\mathbf{A}'\mathbf{A} = \frac{1}{n} \begin{pmatrix} \mathbf{j}_{n} & \mathbf{j}_{n} & \mathbf{j}_{n} \\ -\mathbf{j}_{n} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & -\mathbf{j}_{n} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & -\mathbf{j}_{n} \end{pmatrix} \begin{pmatrix} \mathbf{j}'_{n} & -\mathbf{j}'_{n} & \mathbf{0}' & \mathbf{0}' \\ \mathbf{j}'_{n} & \mathbf{0}' & -\mathbf{j}'_{n} & \mathbf{0}' \\ \mathbf{j}'_{n} & \mathbf{0}' & \mathbf{0}' & -\mathbf{j}'_{n} \end{pmatrix}$$

$$= \frac{1}{n} \begin{pmatrix} 3\mathbf{J}_{n} & -\mathbf{J}_{n} & -\mathbf{J}_{n} & -\mathbf{J}_{n} \\ -\mathbf{J}_{n} & \mathbf{J}_{n} & \mathbf{O} & \mathbf{O} \\ -\mathbf{J}_{n} & \mathbf{O} & \mathbf{J}_{n} & \mathbf{O} \\ -\mathbf{J}_{n} & \mathbf{O} & \mathbf{O} & \mathbf{J}_{n} \end{pmatrix}, \tag{13.34}$$

since $\mathbf{j}_n \mathbf{j}'_n = \mathbf{J}_n$ and $\mathbf{j}_n \mathbf{0}' = \mathbf{O}$, where \mathbf{O} is $n \times n$. Similarly (see Problem 13.10), the second term of (13.33) is given by

$$\frac{1}{4n}\mathbf{A}'\mathbf{J}_{3}\mathbf{A} = \frac{1}{4n} \begin{pmatrix} 9\mathbf{J}_{n} & -3\mathbf{J}_{n} & -3\mathbf{J}_{n} & -3\mathbf{J}_{n} \\ -3\mathbf{J}_{n} & \mathbf{J}_{n} & \mathbf{J}_{n} & \mathbf{J}_{n} \\ -3\mathbf{J}_{n} & \mathbf{J}_{n} & \mathbf{J}_{n} & \mathbf{J}_{n} \end{pmatrix}.$$
(13.35)

Then (13.33) becomes

$$\frac{1}{4n}(4\mathbf{A}'\mathbf{A}) - \frac{1}{4n}\mathbf{A}'\mathbf{J}_{3}\mathbf{A} = \frac{1}{4n} \begin{pmatrix} 12\mathbf{J}_{n} & -4\mathbf{J}_{n} & -4\mathbf{J}_{n} & -4\mathbf{J}_{n} \\ -4\mathbf{J}_{n} & \mathbf{O} & \mathbf{O} \\ -4\mathbf{J}_{n} & \mathbf{O} & 4\mathbf{J}_{n} & \mathbf{O} \\ -4\mathbf{J}_{n} & \mathbf{O} & \mathbf{O} & 4\mathbf{J}_{n} \end{pmatrix}$$

$$-\frac{1}{4n} \begin{pmatrix} 9\mathbf{J}_{n} & -3\mathbf{J}_{n} & -3\mathbf{J}_{n} & -3\mathbf{J}_{n} \\ -3\mathbf{J}_{n} & \mathbf{J}_{n} & \mathbf{J}_{n} & \mathbf{J}_{n} \\ -3\mathbf{J}_{n} & \mathbf{J}_{n} & \mathbf{J}_{n} & \mathbf{J}_{n} \end{pmatrix}$$

$$= \frac{1}{4n} \begin{pmatrix} 3\mathbf{J}_{n} & -\mathbf{J}_{n} & -\mathbf{J}_{n} & -\mathbf{J}_{n} \\ -\mathbf{J}_{n} & 3\mathbf{J}_{n} & -\mathbf{J}_{n} & -\mathbf{J}_{n} \\ -\mathbf{J}_{n} & -\mathbf{J}_{n} & -\mathbf{J}_{n} & -\mathbf{J}_{n} \end{pmatrix} = \frac{1}{4n} \mathbf{B}. \quad (13.36)$$

Note that the matrix for SSH in (13.36) is the same as the matrix for $SS(\alpha|\mu)$ in (13.27) with k=4.

For completeness, we now express SSH in (13.29) in terms of the y_{ij} 's. We begin by writing (13.36) in the form

$$\frac{1}{4n}\mathbf{B} = \frac{1}{4n} \begin{pmatrix} 4\mathbf{J}_{n} & \mathbf{O} & \mathbf{O} & \mathbf{O} \\ \mathbf{O} & 4\mathbf{J}_{n} & \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} & 4\mathbf{J}_{n} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} & 4\mathbf{J}_{n} & \mathbf{O} \end{pmatrix} - \frac{1}{4n} \begin{pmatrix} \mathbf{J}_{n} & \mathbf{J}_{n} & \mathbf{J}_{n} & \mathbf{J}_{n} \\ \mathbf{J}_{n} & \mathbf{J}_{n} & \mathbf{J}_{n} & \mathbf{J}_{n} \\ \mathbf{J}_{n} & \mathbf{J}_{n} & \mathbf{J}_{n} & \mathbf{J}_{n} \end{pmatrix}$$

$$= \frac{1}{n} \begin{pmatrix} \mathbf{J}_{n} & \mathbf{O} & \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{J}_{n} & \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} & \mathbf{J}_{n} & \mathbf{O} \end{pmatrix} - \frac{1}{4n} \mathbf{J}_{4n}.$$

Using $y' = (y'_1, y'_2, y'_3, y'_4)$ as defined in (13.6), SSH in (13.29) becomes

$$SSH = \mathbf{y}' \mathbf{X} (\mathbf{X}' \mathbf{X})^{-} \mathbf{C}' [\mathbf{C} (\mathbf{X}' \mathbf{X})^{-} \mathbf{C}']^{-1} \mathbf{C} (\mathbf{X}' \mathbf{X})^{-} \mathbf{X}' \mathbf{y}$$

$$= \mathbf{y}' \left(\frac{1}{4n} \mathbf{B} \right) \mathbf{y}$$

$$= \frac{1}{n} (\mathbf{y}'_{1}, \mathbf{y}'_{2}, \mathbf{y}'_{3}, \mathbf{y}'_{4}) \begin{pmatrix} \mathbf{J}_{n} & \mathbf{O} & \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{J}_{n} & \mathbf{O} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} & \mathbf{J}_{n} & \mathbf{O} \\ \mathbf{O} & \mathbf{O} & \mathbf{O} & \mathbf{J}_{n} \end{pmatrix} \begin{pmatrix} \mathbf{y}_{1} \\ \mathbf{y}_{2} \\ \mathbf{y}_{3} \\ \mathbf{y}_{4} \end{pmatrix} - \frac{1}{4n} \mathbf{y}' \mathbf{J}_{4n} \mathbf{y}$$

$$= \frac{1}{n} \sum_{i=1}^{4} \mathbf{y}'_{i} \mathbf{J}_{n} \mathbf{y}_{i} - \frac{1}{4n} \mathbf{y}' \mathbf{J}_{4n} \mathbf{y}$$

$$= \frac{1}{n} \sum_{i=1}^{4} \mathbf{y}'_{i} \mathbf{J}_{n} \mathbf{j}'_{n} \mathbf{y}_{i} - \frac{1}{4n} \mathbf{y}' \mathbf{J}_{4n} \mathbf{y}'$$

$$= \frac{1}{n} \sum_{i=1}^{4} \mathbf{y}'_{i} \mathbf{J}_{n} \mathbf{y}'_{i} - \frac{1}{4n} \mathbf{y}'_{i} \mathbf{J}_{n} \mathbf{y}'_{i},$$

which is the same as $SS(\alpha|\mu)$ in (13.23).

13.5 EXPECTED MEAN SQUARES

The expected mean squares for a one-way ANOVA are given in Table 13.4. The expected mean squares are defined as $E[SS(\alpha|\mu)/(k-1)]$ and E[SSE/k(n-1)]. The result is given in terms of parameters α_i^* such that $\sum_i \alpha_i^* = 0$.

Source of Variation	df	Sum of Squares	Mean Square	Expected Mean Squares
Treatments	k-1	$\mathrm{SS}(lpha \mu)$	$\frac{\mathrm{SS}(\alpha \mu)}{k-1}$	$\sigma^2 + \frac{n}{k-1} \sum_{i=1}^k \alpha_i^{*2}$
Error	k(n-1)	SSE	$\frac{\text{SSE}}{k(n-1)}$	σ^2
Total	kn-1	$\sum_{ij} y_{ij}^2 - \frac{y^2}{kn}$	$\kappa(n-1)$	

TABLE 13.4 Expected Mean Squares for One-Way ANOVA

If $H_0: \alpha_1^* = \alpha_2^* = \cdots = \alpha_k^* = 0$ is true, both of the expected mean squares are equal to σ^2 , and we expect F to be close to 1. On the other hand, if H_0 is false, $E[SS(\alpha|\mu)/(k-1)] > E[SSE/k(n-1)]$, and we expect F to exceed 1. We therefore reject H_0 for large values of F.

The expected mean squares in Table 13.4 can be derived using the model $y_{ij} = \mu^* + \alpha_i^* + \varepsilon_{ij}$ in $E[SS(\alpha|\mu)]$ and E(SSE) (see Problem 13.11). In Sections 13.5.1 and 13.5.2, we obtain the expected mean squares using matrix methods similar to those in Sections 13.4.1 and 13.4.2.

13.5.1 Full-Reduced-Model Approach

For the error term in Table 13.4, we have

$$E(SSE) = E\{\mathbf{y}'[\mathbf{I} - \mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}']\mathbf{y}\} = k(n-1)\sigma^{2}, \tag{13.37}$$

which was proved in Theorem 12.3e(i).

Using a full-reduced-model approach the sum of squares for the α 's adjusted for μ is given by (13.25) as $SS(\alpha|\mu) = \mathbf{y}'\mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'\mathbf{y} - \mathbf{y}'[(1/kn)\mathbf{J}_{kn}]\mathbf{y}$. Thus

$$E[SS(\alpha|\mu)] = E[\mathbf{y}'\mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'\mathbf{y}] - E\left[\mathbf{y}'\left(\frac{1}{kn}\mathbf{J}_{kn}\right)\mathbf{y}\right]. \tag{13.38}$$

Using Theorem 5.2a, the first term on the right side of (13.38) becomes

$$E[\mathbf{y}'\mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'\mathbf{y}] = \text{tr}[\mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'\sigma^{2}\mathbf{I}] + (\mathbf{X}\boldsymbol{\beta})'\mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'(\mathbf{X}\boldsymbol{\beta})$$

$$= \sigma^{2}\text{tr}[\mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'] + \boldsymbol{\beta}'\mathbf{X}'\mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'\mathbf{X}\boldsymbol{\beta}$$

$$= \sigma^{2}\text{tr}[\mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'] + \boldsymbol{\beta}'\mathbf{X}'\mathbf{X}\boldsymbol{\beta} \quad \text{[by (2.58)]}. \quad (13.39)$$

By Theorem 2.13f, the matrix $\mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'$ is idempotent. Hence, by Theorems 2.13d and 2.8c(v), we obtain

$$tr[\mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'] = rank[\mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}] = rank(\mathbf{X}) = k.$$
 (13.40)

To evaluate the second term on the right side of (13.39), we use $\mathbf{X}'\mathbf{X}$ in (13.7) and use $\boldsymbol{\beta}' = (\mu^*, \alpha_1^*, \dots, \alpha_k^*)$ subject to $\sum_i \alpha_i^* = 0$. Then

$$\beta' \mathbf{X}' \mathbf{X} \boldsymbol{\beta} = n(\mu^*, \alpha_1^*, \dots, \alpha_k^*) \begin{pmatrix} k & 1 & 1 & \dots & 1 \\ 1 & 1 & 0 & \dots & 0 \\ 1 & 0 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & 0 & 0 & \dots & 1 \end{pmatrix} \begin{pmatrix} \mu^* \\ \alpha_1^* \\ \vdots \\ \alpha_k^* \end{pmatrix}$$

$$= n \left(k \mu^* + \sum_i \alpha_i^*, \mu^* + \alpha_1^*, \dots, \mu^* + \alpha_k^* \right) \begin{pmatrix} \mu^* \\ \alpha_1^* \\ \vdots \\ \alpha_k^* \end{pmatrix}$$

$$= n \left[k \mu^{*2} + \sum_i (\mu^* + \alpha_i^*) \alpha_i^* \right]$$

$$= n \left(k \mu^{*2} + \mu^* \sum_i \alpha_i^* + \sum_i \alpha_i^{*2} \right)$$

$$= k n \mu^{*2} + n \sum_i \alpha_i^{*2}. \tag{13.41}$$

Hence, using (13.40) and (13.41), $E[y'X(X'X)^{-}X'y]$ in (13.39) becomes

$$E[\mathbf{y}'\mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'\mathbf{y}] = k\sigma^{2} + kn\mu^{*2} + n\sum_{i}\alpha_{i}^{*2}.$$
 (13.42)

For the second term on the right side of (13.38), we obtain

$$E\left[\mathbf{y}'\left(\frac{1}{kn}\mathbf{J}_{kn}\right)\mathbf{y}\right] = \sigma^{2}\operatorname{tr}\left(\frac{1}{kn}\mathbf{J}_{kn}\right) + \boldsymbol{\beta}'\mathbf{X}'\left(\frac{1}{kn}\mathbf{J}_{kn}\right)\mathbf{X}\boldsymbol{\beta}$$

$$= \frac{\sigma^{2}kn}{kn} + \frac{1}{kn}\boldsymbol{\beta}'\mathbf{X}'\mathbf{j}_{kn}\mathbf{j}'_{kn}\mathbf{X}\boldsymbol{\beta}$$

$$= \sigma^{2} + \frac{1}{kn}(\boldsymbol{\beta}'\mathbf{X}'\mathbf{j}_{kn})(\mathbf{j}'_{kn}\mathbf{X}\boldsymbol{\beta}). \tag{13.43}$$

Using **X** as given in (13.6), $\mathbf{j}'_{kn}\mathbf{X}\boldsymbol{\beta}$ becomes

$$\mathbf{j}'_{kn}\mathbf{X}\boldsymbol{\beta} = (\mathbf{j}'_{n}, \mathbf{j}'_{n}, \dots, \mathbf{j}'_{n}) \begin{pmatrix} \mathbf{j}_{n} & \mathbf{j}_{n} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{j}_{n} & \mathbf{0} & \mathbf{j}_{n} & \cdots & \mathbf{0} \\ \vdots & \vdots & \vdots & & \vdots \\ \mathbf{j}_{n} & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{j}_{n} \end{pmatrix} \begin{pmatrix} \boldsymbol{\mu}^{*} \\ \boldsymbol{\alpha}_{1}^{*} \\ \vdots \\ \boldsymbol{\alpha}_{k}^{*} \end{pmatrix}$$

$$= (kn, n, n, \dots, n) \begin{pmatrix} \boldsymbol{\mu}^{*} \\ \boldsymbol{\alpha}_{1}^{*} \\ \vdots \\ \boldsymbol{\alpha}_{k}^{*} \end{pmatrix} \qquad (\text{since } \mathbf{j}'_{n}\mathbf{j}_{n} = n)$$

$$= kn\boldsymbol{\mu}^{*} + n \sum_{i=1}^{k} \alpha_{i}^{*} = kn\boldsymbol{\mu}^{*} \qquad \left(\text{since } \sum_{i} \alpha_{i}^{*} = \mathbf{0} \right).$$

The second term on the right side of (13.43) is then given by

$$\frac{1}{kn}(\boldsymbol{\beta}'\mathbf{X}'\mathbf{j}_{kn})(\mathbf{j}'_{kn}\mathbf{X}\boldsymbol{\beta}) = \frac{1}{kn}(\mathbf{j}'\mathbf{X}\boldsymbol{\beta})^2 = \frac{k^2n^2\mu^{*2}}{kn} = kn\mu^{*2},$$

so that (13.43) becomes

$$E\left[\mathbf{y}'\left(\frac{1}{kn}\mathbf{J}_{kn}\right)\mathbf{y}\right] = \sigma^2 + kn\mu^{*2}.$$
 (13.44)

Now, using (13.42) and (13.44), $E[SS(\alpha|\mu)]$ in (13.38) becomes

$$E[SS(\alpha|\mu)] = k\sigma^2 + kn\mu^{*2} + n\sum_{i=1}^k \alpha_i^{*2} - (\sigma^2 + kn\mu^{*2})$$
$$= (k-1)\sigma^2 + n\sum_i \alpha_i^{*2}.$$
 (13.45)

13.5.2 General Linear Hypothesis

To simplify exposition, we use k=4 to illustrate results in this section, as was done in Section 13.4.2. It was shown in Section 13.4.2 that SSH = $(\mathbf{C}\hat{\boldsymbol{\beta}})'[\mathbf{C}(\mathbf{X}'\mathbf{X})^{-}\mathbf{C}']^{-1}\mathbf{C}\hat{\boldsymbol{\beta}}$ is the same as SS($\alpha|\mu$) = $\sum_{i} y_{i.}^{2}/n - y_{...}^{2}/kn$ in (13.23). Note that for k=4, \mathbf{C} is 3×5 [see (13.28)] and $\mathbf{C}(\mathbf{X}'\mathbf{X})^{-}\mathbf{C}'$ is 3×3 [see (13.30)]. To obtain $E[SS(\alpha|\mu)]$, we first note that by (12.44), (12.45), and (13.31), $E(\mathbf{C}\hat{\boldsymbol{\beta}}) = \mathbf{C}\boldsymbol{\beta}$, $\operatorname{cov}(\mathbf{C}\hat{\boldsymbol{\beta}}) = \sigma^{2}\mathbf{C}(\mathbf{X}'\mathbf{X})^{-}\mathbf{C}'$, and $[\mathbf{C}(\mathbf{X}'\mathbf{X})^{-}\mathbf{C}']^{-1} = n(\mathbf{I}_{3} - \frac{1}{4}\mathbf{J}_{3})$.

Then, by Theorem 5.2a, we have

$$E[SS(\alpha|\mu)] = E\{(\mathbf{C}\hat{\boldsymbol{\beta}})'[\mathbf{C}(\mathbf{X}'\mathbf{X})^{-}\mathbf{C}']^{-1}\mathbf{C}\hat{\boldsymbol{\beta}}\}$$

$$= tr\{[\mathbf{C}(\mathbf{X}'\mathbf{X})^{-}\mathbf{C}']^{-1}cov(\mathbf{C}\hat{\boldsymbol{\beta}})\} + [E(\mathbf{C}\hat{\boldsymbol{\beta}})]'[\mathbf{C}(\mathbf{X}'\mathbf{X})^{-}\mathbf{C}']^{-1}E(\mathbf{C}\hat{\boldsymbol{\beta}})$$

$$= tr\{[\mathbf{C}(\mathbf{X}'\mathbf{X})^{-}\mathbf{C}']^{-1}\sigma^{2}\mathbf{C}(\mathbf{X}'\mathbf{X})^{-}\mathbf{C}'\} + n(\mathbf{C}\boldsymbol{\beta})'[\mathbf{I}_{3} - \frac{1}{4}\mathbf{J}_{3}]\mathbf{C}\boldsymbol{\beta}$$

$$= \sigma^{2}tr(\mathbf{I}_{3}) + n\boldsymbol{\beta}'\mathbf{C}'(\mathbf{I}_{3} - \frac{1}{4}\mathbf{J}_{3})\mathbf{C}\boldsymbol{\beta}$$

$$= 3\sigma^{2} + n\boldsymbol{\beta}'(\mathbf{C}'\mathbf{C} - \frac{1}{4}\mathbf{C}'\mathbf{J}_{3}\mathbf{C})\boldsymbol{\beta}. \tag{13.46}$$

Using C in (13.28), we obtain

$$\mathbf{C}'\mathbf{C} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & -1 & -1 & -1 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 & 1 \end{pmatrix}, \tag{13.47}$$

$$\mathbf{C}'\mathbf{J}_{3}\mathbf{C} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 9 & -3 & -3 & -3 \\ 0 & -3 & 1 & 1 & 1 \\ 0 & -3 & 1 & 1 & 1 \\ 0 & -3 & 1 & 1 & 1 \end{pmatrix}. \tag{13.48}$$

From (13.47) and (13.48), we have

$$\begin{split} \mathbf{C'C} - \frac{1}{4}\mathbf{C'J_3C} &= \frac{1}{4}(4\mathbf{C'C} - \mathbf{C'J_3C}) \\ &= \frac{1}{4} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 3 & -1 & -1 & -1 \\ 0 & -1 & 3 & -1 & -1 \\ 0 & -1 & -1 & 3 & -1 \\ 0 & -1 & -1 & -1 & 3 \end{pmatrix} \\ &= \frac{1}{4} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 4 & 0 & 0 & 0 \\ 0 & 0 & 4 & 0 & 0 \\ 0 & 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 0 & 4 \end{pmatrix} - \frac{1}{4} \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 & 1 \end{pmatrix} \\ &= \begin{pmatrix} 0 & \mathbf{0'} \\ \mathbf{0} & \mathbf{I_4} \end{pmatrix} - \frac{1}{4} \begin{pmatrix} 0 & \mathbf{0'} \\ \mathbf{0} & \mathbf{J_4} \end{pmatrix}. \end{split}$$

Thus the second term on the right side of (13.46) is given by

$$n\boldsymbol{\beta}'(\mathbf{C}'\mathbf{C} - \frac{1}{4}\mathbf{C}'\mathbf{J}_{3}\mathbf{C})\boldsymbol{\beta}$$

$$= n\boldsymbol{\beta}'\begin{pmatrix} 0 & \mathbf{0}' \\ \mathbf{0} & \mathbf{I}_{4} \end{pmatrix} \boldsymbol{\beta} - \frac{1}{4}n\boldsymbol{\beta}'\begin{pmatrix} 0 & \mathbf{0}' \\ \mathbf{0} & \mathbf{J}_{4} \end{pmatrix} \boldsymbol{\beta}$$

$$= n(\boldsymbol{\mu}^{*}, \alpha_{1}^{*}, \alpha_{2}^{*}, \alpha_{3}^{*}, \alpha_{4}^{*})\begin{pmatrix} 0 & \mathbf{0}' \\ \mathbf{0} & \mathbf{I}_{4} \end{pmatrix}\begin{pmatrix} \boldsymbol{\mu}^{*} \\ \alpha_{1}^{*} \\ \alpha_{2}^{*} \\ \alpha_{3}^{*} \\ \alpha_{4}^{*} \end{pmatrix}$$

$$- \frac{1}{4}n(\boldsymbol{\mu}^{*}, \alpha_{1}^{*}, \alpha_{2}^{*}, \alpha_{3}^{*}, \alpha_{4}^{*})\begin{pmatrix} 0 & \mathbf{0}' \\ \mathbf{0} & \mathbf{J}_{4} \end{pmatrix}\begin{pmatrix} \boldsymbol{\mu}^{*} \\ \alpha_{1}^{*} \\ \alpha_{2}^{*} \\ \alpha_{3}^{*} \\ \alpha_{4}^{*} \end{pmatrix}$$

$$= n \sum_{i=1}^{4} \alpha_{i}^{*2} - \frac{1}{4}n\begin{pmatrix} 0, \sum_{i} \alpha_{i}^{*}, \sum_{i} \alpha_{i}^{*}, \sum_{i} \alpha_{i}^{*}, \sum_{i} \alpha_{i}^{*}, \sum_{i} \alpha_{i}^{*} \end{pmatrix}\begin{pmatrix} \boldsymbol{\mu}^{*} \\ \alpha_{1}^{*} \\ \alpha_{2}^{*} \\ \alpha_{3}^{*} \\ \alpha_{4}^{*} \end{pmatrix}$$

$$= n \sum_{i=1}^{4} \alpha_{i}^{*2}.$$

Hence, (13.46) becomes

$$E[SS(\alpha|\mu)] = 3\sigma^2 + n\sum_{i=1}^{4} \alpha_i^{*2}.$$
 (13.49)

This result is for the special case k = 4. For a general k, (13.49) becomes

$$E[SS(\alpha|\mu)] = (k-1)\sigma^2 + n\sum_{i=1}^{k} \alpha_i^{*2}.$$

For the case in which $\beta' = (\mu, \alpha_1, \dots, \alpha_k)$ is not subject to $\sum_i \alpha_i = 0$, see Problem 13.14.

13.6 CONTRASTS

We noted in Section 13.2 that a linear combination $\sum_{i=1}^k c_i \alpha_i$ in the α 's is estimable if and only if $\sum_{i=1}^k c_i = 0$. In Section 13.6.1, we develop a test of significance for such contrasts. In Section 13.6.2, we show that if the contrasts are formulated appropriately, the sum of squares for treatments can be partitioned into k-1 independent sums of squares for contrasts. In Section 13.6.3, we develop orthogonal polynomial contrasts for the special case in which the treatments have equally spaced quantitative levels.

13.6.1 Hypothesis Test for a Contrast

For the one-way model, a contrast $\sum_i c_i \alpha_i$, where $\sum_i c_i = 0$, is equivalent to $\sum_i c_i \mu_i$ since

$$\sum c_i \mu_i = \sum_i c_i (\mu + \alpha_i) = \mu \sum_i c_i + \sum_i c_i \alpha_i = \sum_i c_i \alpha_i.$$

A hypothesis of interest is

$$H_0: \sum c_i \alpha_i = 0 \quad \text{or} \quad H_0: \sum c_i \mu_i = 0,$$
 (13.50)

which represents a comparison of means if $\sum_i c_i = 0$. For example, the hypothesis

$$H_0: 3\mu_1 - \mu_2 - \mu_3 - \mu_4 = 0$$

can be written as

$$H_0: \mu_1 = \frac{1}{3}(\mu_2 + \mu_3 + \mu_4),$$

which compares μ_1 with the average of μ_2 , μ_3 , and μ_4 .

The hypothesis in (13.50) can be expressed as $H_0: \mathbf{c'}\boldsymbol{\beta} = 0$, where $\mathbf{c'} = (0, c_1, c_2, \ldots, c_k)$ and $\boldsymbol{\beta} = (\mu, \alpha_1, \ldots, \alpha_k)'$. Assuming that \mathbf{y} is $N_{kn}(\mathbf{X}\boldsymbol{\beta}, \sigma^2\mathbf{I})$, H_0 can be tested using Theorem 12.7c. In this case, we have m = 1, and the test statistic becomes

$$F = \frac{(\mathbf{c}'\hat{\boldsymbol{\beta}})'[\mathbf{c}'(\mathbf{X}'\mathbf{X})^{-}\mathbf{c}]^{-1}\mathbf{c}'\hat{\boldsymbol{\beta}}}{\mathrm{SSE}/k(n-1)}$$
$$= \frac{(\mathbf{c}'\hat{\boldsymbol{\beta}})^{2}}{s^{2}\mathbf{c}'(\mathbf{X}'\mathbf{X})^{-}\mathbf{c}}$$
(13.51)

$$= \frac{\left(\sum_{i=1}^{k} c_{i} \bar{y}_{i}\right)^{2}}{s^{2} \sum_{i=1}^{k} c_{i}^{2} / n},$$
(13.52)

where $s^2 = \text{SSE}/k(n-1)$, and $(\mathbf{X}'\mathbf{X})^-$ and $\hat{\boldsymbol{\beta}}$ are as given by (13.11) and (13.12). The sum of squares for the contrast is $(\mathbf{c}'\hat{\boldsymbol{\beta}})^2/\mathbf{c}'(\mathbf{X}'\mathbf{X})^-\mathbf{c}$ or $n(\sum_i c_i \bar{y}_i)^2/(\sum_i c_i^2)$.

13.6.2 Orthogonal Contrasts

Two contrasts $\mathbf{c}_i'\hat{\boldsymbol{\beta}}$ and $\mathbf{c}_j'\hat{\boldsymbol{\beta}}$ are said to be *orthogonal* if $\mathbf{c}_i'\mathbf{c}_j = 0$. We now show that if $\mathbf{c}_i'\hat{\boldsymbol{\beta}}$ and $\mathbf{c}_j'\hat{\boldsymbol{\beta}}$ are orthogonal, they are independent. Since we are assuming normality, $\mathbf{c}_i'\hat{\boldsymbol{\beta}}$ and $\mathbf{c}_j'\hat{\boldsymbol{\beta}}$ are independent if

$$cov(\mathbf{c}_i'\hat{\boldsymbol{\beta}}, \mathbf{c}_i'\hat{\boldsymbol{\beta}}) = 0 \tag{13.53}$$

(see Problem 13.16). By Theorem 12.3c, $\operatorname{cov}(\mathbf{c}_i'\hat{\boldsymbol{\beta}}, \mathbf{c}_j'\hat{\boldsymbol{\beta}}) = \sigma^2 \mathbf{c}_i'(\mathbf{X}'\mathbf{X})^- \mathbf{c}_j$. By (13.11), $(\mathbf{X}'\mathbf{X})^- = \operatorname{diag}[0, (1/n), \dots, (1/n)]$, and therefore

$$\operatorname{cov}(\mathbf{c}_{i}'\hat{\boldsymbol{\beta}}, \mathbf{c}_{i}'\hat{\boldsymbol{\beta}}) = \mathbf{c}_{i}'(\mathbf{X}'\mathbf{X})^{-}\mathbf{c}_{i} = 0 \quad \text{if} \quad \mathbf{c}_{i}'\mathbf{c}_{i} = 0$$
 (13.54)

(assuming that the first element of \mathbf{c}_i is 0 for all i). By an argument similar to that used in the proofs of Corollary 1 to Theorem 5.6b and in Theorem 12.7b(v), the sums of squares $(\mathbf{c}_i'\hat{\boldsymbol{\beta}})^2/\mathbf{c}_i'(\mathbf{X}'\mathbf{X})^-\mathbf{c}_i$ and $(\mathbf{c}_j'\hat{\boldsymbol{\beta}})^2/\mathbf{c}_j'(\mathbf{X}'\mathbf{X})^-\mathbf{c}_j$ are also independent. Thus, if two contrasts are orthogonal, they are independent and their corresponding sums of squares are independent.

We now show that if the rows of **C** (Section 13.4.2) are mutually orthogonal contrasts, SSH is the sum of $(\mathbf{c}_i'\hat{\boldsymbol{\beta}})^2/\mathbf{c}_i'(\mathbf{X}'\mathbf{X})^-\mathbf{c}_i$ for all rows of **C**.

Theorem 13.6a. In the balanced one-way model, if **y** is $N_{kn}(\mathbf{X}\boldsymbol{\beta}, \sigma^2\mathbf{I})$ and if $H_0: \alpha_1 = \alpha_2 = \cdots = \alpha_k$ is expressed as $\mathbf{C}\boldsymbol{\beta} = \mathbf{0}$, where the rows of

$$\mathbf{C} = \left(egin{array}{c} \mathbf{c}_1' \ \mathbf{c}_2' \ dots \ \mathbf{c}_{k-1}' \end{array}
ight)$$

are mutually orthogonal contrasts, then SSH = $(C\hat{\beta})'[C(X'X)^-C']^{-1}C\hat{\beta}$ can be expressed (partitioned) as

$$SSH = \sum_{i=1}^{k-1} \frac{(\mathbf{c}_i' \hat{\boldsymbol{\beta}})^2}{\mathbf{c}_i' (\mathbf{X}' \mathbf{X})^{-} \mathbf{c}_i},$$
 (13.55)

where the sums of squares $(\mathbf{c}_i'\hat{\boldsymbol{\beta}})^2/\mathbf{c}_i'(\mathbf{X}'\mathbf{X})^{-}\mathbf{c}_i$, $i=1,2,\ldots,k-1$, are independent.

PROOF. By (13.54), $\mathbf{C}(\mathbf{X}'\mathbf{X})^{-}\mathbf{C}'$ is a diagonal matrix with $\mathbf{c}'_{i}(\mathbf{X}'\mathbf{X})^{-}\mathbf{c}_{i}$, $i=1,2,\ldots,k-1$, on the diagonal. Thus, with $(\mathbf{C}\hat{\boldsymbol{\beta}})'=(\mathbf{c}'_{1}\hat{\boldsymbol{\beta}},\mathbf{c}'_{2}\hat{\boldsymbol{\beta}},\ldots,\mathbf{c}'_{k-1}\hat{\boldsymbol{\beta}})$, (13.55) follows. Since the rows $\mathbf{c}'_{1},\mathbf{c}'_{2},\ldots,\mathbf{c}'_{k-1}$ of \mathbf{C} are orthogonal, the independence of the sums of squares for the contrasts follows from (13.53) and (13.54). \square

An interesting implication of Theorem 13.6a is that the overall F for treatments (Table 13.1) is the average of the F statistics for each of the orthogonal contrasts:

$$F = \frac{\text{SSH}/(k-1)}{s^2} = \frac{1}{k-1} \sum_{i=1}^{k-1} \frac{(\mathbf{c}_i \hat{\boldsymbol{\beta}})^2}{s^2 \mathbf{c}_i' (\mathbf{X} \mathbf{X})^- \mathbf{c}_i}$$
$$= \frac{1}{k-1} \sum_{i=1}^{k-1} F_i.$$

It is possible that the overall F would lead to rejection of the overall H_0 while some of the F_i 's for individual contrasts would not lead to rejection of the corresponding H_0 's. Likewise, since one or more of the F_i 's will be larger than the overall F, it is possible that an individual H_0 would be rejected, while the overall H_0 is not rejected.

Example 13.6a. We illustrate the use of orthogonal contrasts with the ascorbic acid data of Table 13.2. Consider the orthogonal contrasts $2\mu_1 - \mu_2 - \mu_3$ and $\mu_2 - \mu_3$. By (13.50), these can be expressed as

$$2\mu_1 - \mu_2 - \mu_3 = 2\alpha_1 - \alpha_2 - \alpha_3 = (0, 2, -1, -1)\boldsymbol{\beta} = \mathbf{c}_1'\boldsymbol{\beta},$$

$$\mu_2 - \mu_3 = \alpha_2 - \alpha_3 = (0, 0, 1, -1)\boldsymbol{\beta} = \mathbf{c}_2'\boldsymbol{\beta}.$$

The hypotheses $H_{01}: \mathbf{c}_1' \boldsymbol{\beta} = 0$ and $H_{02}: \mathbf{c}_2' \boldsymbol{\beta} = 0$ compare the first treatment versus the other two and the second treatment versus the third.

The means are given in Table 13.2 as $\bar{y}_{1.} = 17.15$, $\bar{y}_{2.} = 19.31$, and $\bar{y}_{3.} = 23.53$. Then by (13.52), the sums of squares for the two contrasts are

$$SS_{1} = \frac{n(\sum_{i=1}^{3} c_{i}\bar{y}_{i})^{2}}{\sum_{i=1}^{3} c_{i}^{2}} = \frac{7[2(17.15) - 19.31 - 23.53]^{2}}{4 + 1 + 1} = 85.0584,$$

$$SS_{2} = \frac{7(19.31 - 23.53)^{2}}{1 + 1} = 62.2872.$$

By (13.52), the corresponding F statistics are

$$F_1 = \frac{\text{SS}_1}{s^2} = \frac{85.0584}{3.0537} = 27.85, \qquad F_2 = \frac{\text{SS}_2}{s^2} = \frac{62.2872}{3.0537} = 20.40,$$

where $s^2=3.0537$ is from Table 13.3. Both F_1 and F_2 exceed $F_{.05,1,18}=4.41$. The p values are .0000511and .000267, respectively.

Note that the sums of squares for the two orthogonal contrasts add to the sum of squares for treatments given in Example 13.4; that is, 147.3456 = 85.0584 + 62.2872, as in (13.55).

The partitioning of the treatment sum of squares in Theorem 13.6a is always possible. First note that $SSH = \mathbf{y}'\mathbf{A}\mathbf{y}$ as in (13.29), where \mathbf{A} is idempotent. We now show that any such quadratic form can be partitioned into independent components.

Theorem 13.6b. Let \mathbf{y}' $\mathbf{A}\mathbf{y}$ be a quadratic form, let \mathbf{A} be symmetric and idempotent of rank r, let N = kn, and let the $N \times 1$ random vector \mathbf{y} be $N_N(\mathbf{X}\boldsymbol{\beta}, \sigma^2\mathbf{I})$. Then there exist r idempotent matrices $\mathbf{A}_1, \mathbf{A}_2, \ldots, \mathbf{A}_r$ such that $\mathbf{A} = \sum_{i=1}^r \mathbf{A}_i$, rank $(\mathbf{A}_i) = 1$ for $i = 1, 2, \ldots, r$, and $\mathbf{A}_i \mathbf{A}_j = \mathbf{O}$ for $i \neq j$. Furthermore, $\mathbf{y}' \mathbf{A} \mathbf{y}$ can be partitioned as

$$\mathbf{y}'\mathbf{A}\mathbf{y} = \sum_{i=1}^{r} \mathbf{y}'\mathbf{A}_{i}\mathbf{y}, \tag{13.56}$$

where each $\mathbf{y}'\mathbf{A}_i\mathbf{y}$ in (13.56) is $\chi^2(1, \lambda_i)$ and $\mathbf{y}'\mathbf{A}_i\mathbf{y}$ and $\mathbf{y}'\mathbf{A}_j\mathbf{y}$ are independent for $i \neq j$ (note that λ_i is a noncentrality parameter).

PROOF. Since **A** is $N \times N$ of rank r and is symmetric and idempotent, then by Theorem 2.13c, r of its eigenvalues are equal to 1 and the others are 0. Using the spectral decomposition (2.104), we can express **A** in the form

$$\mathbf{A} = \sum_{i=1}^{r} \mathbf{v}_i \mathbf{v}_i' = \sum_{i=1}^{r} \mathbf{A}_i, \tag{13.57}$$

where $\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_r$ are normalized orthogonal eigenvectors corresponding to the nonzero eigenvalues and $\mathbf{A}_i = \mathbf{v}_i \mathbf{v}_i'$. It is easily shown that $\mathrm{rank}(\mathbf{A}_i) = 1$, $\mathbf{A}_i \mathbf{A}_j = \mathbf{O}$ for $i \neq j$, and \mathbf{A}_i is symmetric and idempotent (see Problem 13.17). Then by Corollary 2 to Theorem 5.5 and Corollary 1 to Theorem 5.6b, $\mathbf{y}'\mathbf{A}_i\mathbf{y}$ is $\chi^2(1,\lambda_i)$ and $\mathbf{y}'\mathbf{A}_i\mathbf{y}$ and $\mathbf{y}'\mathbf{A}_i\mathbf{y}$ are independent.

If $\mathbf{y'Ay}$ in Theorem 13.6b is used to represent SSH, the eigenvectors corresponding to nonzero eigenvalues of \mathbf{A} always define contrasts of the cell means. In other words, the partitioning of $\mathbf{y'Ay}$ in (13.56) is always in terms of orthogonal contrasts. To see this, note that

$$SST = SSH + SSE$$
,

which, in the case of the one-way balanced model, implies that

$$\mathbf{y}'\left(\mathbf{I} - \frac{1}{kn}\mathbf{J}\right)\mathbf{y} = \sum_{i=1}^{k} \mathbf{y}'\mathbf{A}_{i}\mathbf{y} + \mathbf{y}'[\mathbf{I} - \mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}']\mathbf{y}.$$
 (13.58)

If we let

$$\mathbf{K} = \frac{1}{n} \begin{pmatrix} \mathbf{J} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \mathbf{J} & \cdots & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \cdots & \mathbf{J} \end{pmatrix}$$

as in (13.26), then (13.58) can be rewritten as

$$\mathbf{y}'\mathbf{y} = \mathbf{y}'\frac{1}{kn}\mathbf{J}\mathbf{y} + \sum_{i=1}^{k} \mathbf{y}'(\mathbf{v}_{i}\mathbf{v}'_{i})\mathbf{y} + \mathbf{y}'(\mathbf{I} - \mathbf{K})\mathbf{y}.$$
 (13.59)

By Theorem 2.13h, each \mathbf{v}_i must be orthogonal to the columns of $(1/n)\mathbf{J}$ and $\mathbf{I} - \mathbf{K}$. Orthogonality to $(1/n)\mathbf{J}$ implies that $\mathbf{v}_i\mathbf{j} = 0$; that is, \mathbf{v}_i defines a contrast

in the elements of \mathbf{y} . Orthogonality to $\mathbf{I} - \mathbf{K}$ implies that the elements of \mathbf{v}_i corresponding to units associated with a particular treatment are constants. Together these results imply that \mathbf{v}_i defines a contrast of the estimated treatment means.

Example 13.6b. Using a one-way model, we demonstrate that orthogonal contrasts in the treatment means can be expressed in terms of contrasts in the observations and that the coefficients in these contrasts form eigenvectors. For simplicity of exposition, let k = 4. The model is then

$$y_{ij} = \mu + \alpha_i + \varepsilon_{ij}, \quad i = 1, 2, 3, 4, \quad j = 1, 2, \ldots, n.$$

The sums of squares in (13.59) can be written in the form

$$\mathbf{y}'\mathbf{y} = SS(\mu) + SS(\alpha|\mu) + SSE$$
$$= \frac{y_{..}^2}{kn} + \left(\hat{\boldsymbol{\beta}}'\mathbf{X}'\mathbf{y} - \frac{y_{..}^2}{kn}\right) + (\mathbf{y}'\mathbf{y} - \hat{\boldsymbol{\beta}}'\mathbf{X}'\mathbf{y}).$$

With k=4, the sum of squares for treatments, $\mathbf{y}'\mathbf{A}\mathbf{y} = \hat{\boldsymbol{\beta}}'\mathbf{X}'\mathbf{y} - y_{...}^2/4n$, has 3 degrees of freedom. Any set of three orthogonal contrasts in the treatment means will serve to illustrate. As an example, consider $\mathbf{c}_1'\boldsymbol{\beta} = (0, 1, -1, 0, 0)\boldsymbol{\beta}$, $\mathbf{c}_2'\boldsymbol{\beta} = (0, 1, 1, -2, 0)\boldsymbol{\beta}$, and $\mathbf{c}_3'\boldsymbol{\beta} = (0, 1, 1, 1, -3)\boldsymbol{\beta}$, where $\boldsymbol{\beta} = (\mu, \alpha_1, \alpha_2, \alpha_3, \alpha_4)'$. Thus, we are comparing the first mean to the second, the first two means to the third, and the first three to the fourth (see a comment at the beginning of Section 13.4 for the equivalence of $H_0: \alpha_1 = \alpha_2 = \alpha_3 = \alpha_4$ and $H_0: \mu_1 = \mu_2 = \mu_3 = \mu_4$). Using the format in (13.55), we can write the three contrasts as

$$\frac{\mathbf{c}_{1}'\hat{\boldsymbol{\beta}}}{\sqrt{\mathbf{c}_{1}'(\mathbf{X}'\mathbf{X})^{-}\mathbf{c}_{1}}} = \frac{\bar{y}_{1.} - \bar{y}_{2.}}{\sqrt{2/n}}$$

$$\frac{\mathbf{c}_{2}'\hat{\boldsymbol{\beta}}}{\sqrt{\mathbf{c}_{2}'(\mathbf{X}'\mathbf{X})^{-}\mathbf{c}_{2}}} = \frac{\bar{y}_{1.} + \bar{y}_{2.} - 2\bar{y}_{3.}}{\sqrt{6/n}}$$

$$\frac{\mathbf{c}_{3}'\hat{\boldsymbol{\beta}}}{\sqrt{\mathbf{c}_{3}'(\mathbf{X}'\mathbf{X})^{-}\mathbf{c}_{3}}} = \frac{\bar{y}_{1.} + \bar{y}_{2.} + \bar{y}_{3.} - 3\bar{y}_{4.}}{\sqrt{12/n}},$$

where $(\mathbf{X}'\mathbf{X})^- = \text{diag}[0, (1/n), \dots, (1/n)]$ is given in (13.11) and $\hat{\boldsymbol{\beta}} = (0, \bar{y}_1, \dots, \bar{y}_{4.})'$ is from (13.12).

To write these in the form $\mathbf{v}_1'\mathbf{y}$, $\mathbf{v}_2'\mathbf{y}$, and $\mathbf{v}_3'\mathbf{y}$ [as in (13.59)] we start with the first:

$$\frac{\bar{y}_{1.} - \bar{y}_{2.}}{\sqrt{2/n}} = \frac{1}{\sqrt{2/n}} \left(\frac{\sum_{j=1}^{n} y_{1j}}{n} - \frac{\sum_{j=1}^{n} y_{2j}}{n} \right)
= \frac{1/n}{\sqrt{2/n}} (1, 1, \dots, 1, -1, -1, \dots, -1, 0, 0, \dots, 0) \mathbf{y}
= \mathbf{v}_{1}' \mathbf{y},$$

where the number of 1s is n, the number of -1s is n, and the number of 0s is 2n. Thus $\mathbf{v}'_1 = (1/\sqrt{2n})(\mathbf{j}'_n, -\mathbf{j}'_n, \mathbf{0}', \mathbf{0}')$, and

$$\mathbf{v}_1'\mathbf{v}_1 = \frac{2n}{2n} = 1.$$

Similarly, \mathbf{v}_2' and \mathbf{v}_3' can be expressed as $\mathbf{v}_2' = (1/\sqrt{6n})(\mathbf{j}_n', \mathbf{j}_n' - 2\mathbf{j}_n', \mathbf{0}')$ and $\mathbf{v}_3' = (1/\sqrt{12n})(\mathbf{j}_n', \mathbf{j}_n', \mathbf{j}_n', \mathbf{j}_n', -3\mathbf{j}_n')$. We now show that $\mathbf{v}_1, \mathbf{v}_2$, and \mathbf{v}_3 serve as eigenvectors in the spectral decomposition [see (2.104)] of the matrix \mathbf{A} in $SS(\alpha|\mu) = \mathbf{y}'\mathbf{A}\mathbf{y}$. Since \mathbf{A} is idempotent of rank 3, it has three nonzero eigenvalues, each equal to 1. Thus the spectral decomposition of \mathbf{A} is

$$\mathbf{A} = \mathbf{v}_{1}\mathbf{v}_{1}' + \mathbf{v}_{2}\mathbf{v}_{2}' + \mathbf{v}_{3}\mathbf{v}_{3}'$$

$$= \frac{1}{2n} \begin{pmatrix} \mathbf{j}_{n} \\ -\mathbf{j}_{n} \\ \mathbf{0} \\ \mathbf{0} \end{pmatrix} (\mathbf{j}_{n}', -\mathbf{j}_{n}', \mathbf{0}', \mathbf{0}') + \frac{1}{6n} \begin{pmatrix} \mathbf{j}_{n} \\ \mathbf{j}_{n} \\ -2\mathbf{j}_{n} \\ \mathbf{0} \end{pmatrix} (\mathbf{j}_{n}', \mathbf{j}_{n}', -2\mathbf{j}_{n}', \mathbf{0}')$$

$$+ \frac{1}{12n} \begin{pmatrix} \mathbf{j}_{n} \\ \mathbf{j}_{n} \\ \mathbf{j}_{n} \\ -3\mathbf{j}_{n} \end{pmatrix} (\mathbf{j}_{n}', \mathbf{j}_{n}', \mathbf{j}_{n}', -3\mathbf{j}_{n}')$$

$$= \frac{1}{2n} \begin{pmatrix} \mathbf{J}_{n} & -\mathbf{J}_{n} & \mathbf{O} & \mathbf{O} \\ -\mathbf{J}_{n} & \mathbf{J}_{n} & -\mathbf{O} & \mathbf{O} \\ -2\mathbf{J}_{n} & -2\mathbf{J}_{n} & -2\mathbf{J}_{n} & \mathbf{O} \\ -2\mathbf{J}_{n} & -2\mathbf{J}_{n} & -3\mathbf{J}_{n} \\ -3\mathbf{J}_{n} & -3\mathbf{J}_{n} & -3\mathbf{J}_{n} \\ -3\mathbf{J}_{n} & -3\mathbf{J}_{n} & -3\mathbf{J}_{n} \\ -3\mathbf{J}_{n} & -3\mathbf{J}_{n} & -3\mathbf{J}_{n} & -3\mathbf{J}_{n} \\ -3\mathbf{J}_{n} & -3$$

which is the matrix of the quadratic form for $SS(\alpha|\mu)$ in (13.27) with k=4. For $SS(\mu) = y^2/4n$, we have

$$\frac{\mathbf{y}_{\cdot \cdot}^2}{4n} = \mathbf{y}' \left(\frac{\mathbf{j}_{4n} \mathbf{j}'_{4n}}{4n} \right) \mathbf{y} = (\mathbf{v}'_0 \mathbf{y})^2,$$

where $\mathbf{v}_0' = \mathbf{j}_{4n}'/2\sqrt{n}$. It is easily shown that $\mathbf{v}_0'\mathbf{v}_0 = 1$ and that $\mathbf{v}_0'\mathbf{v}_1 = 0$. It is also clear that \mathbf{v}_0 is an eigenvector of $\mathbf{j}_{4n}\mathbf{j}_{4n}'/4n$, because $\mathbf{j}_{4n}\mathbf{j}_{4n}'/4n$ has one eigenvalue equal to 1 and the others equal to 0, so that $\mathbf{j}_{4n}\mathbf{j}_{4n}'/4n$ is already in the form of a spectral decomposition with $\mathbf{j}_{4n}/2\sqrt{n}$ as the eigenvector corresponding to the eigenvalue 1 (see Problem 13.18b).

13.6.3 Orthogonal Polynomial Contrasts

Suppose the treatments in a one-way analysis of variance have equally spaced quantitative levels, for example, 5, 10, 15, and 20lb of fertilizer per plot of ground. The researcher may then wish to investigate how the response varies with the level of fertilizer. We can check for a linear trend, a quadratic trend, or a cubic trend by fitting a third-order polynomial regression model

$$y_{ij} = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \beta_3 x_i^3 + \varepsilon_{ij},$$

$$i = 1, 2, 3, 4, \quad j = 1, 2, \dots, n,$$
(13.60)

where $x_1 = 5$, $x_2 = 10$, $x_3 = 15$, and $x_4 = 20$. We now show that tests on the β 's in (13.60) can be carried out using orthogonal contrasts on the means \bar{y}_i that are estimates of μ_i in the ANOVA model

$$y_{ij} = \mu + \alpha_i + \varepsilon_{ij} = \mu_i + \varepsilon_{ij}, \quad i = 1, 2, 3, 4, \quad j = 1, 2, \dots, n.$$
 (13.61)

The sum of squares for the full-reduced-model test of H_0 : $\beta_3 = 0$ is

$$\hat{\boldsymbol{\beta}}'\mathbf{X}'\mathbf{y} - \hat{\boldsymbol{\beta}}_1^{*'}\mathbf{X}_1'\mathbf{y}, \tag{13.62}$$

where $\hat{\beta}$ is from the full model in (13.60) and $\hat{\beta}_1^*$ is from the reduced model with $\beta_3 = 0$ [see (8.9), (8.20), and Table 8.3]. The **X** matrix is of the form

$$\mathbf{X} = \begin{pmatrix} 1 & x_1 & x_1^2 & x_1^3 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_1 & x_1^2 & x_1^3 \\ 1 & x_2 & x_2^2 & x_2^3 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_2 & x_2^2 & x_2^3 \\ 1 & x_3 & x_3^2 & x_3^3 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_3 & x_3^2 & x_3^3 \\ 1 & x_4 & x_4^2 & x_4^3 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & x_4 & x_4^2 & x_4^3 \end{pmatrix}.$$

$$(13.63)$$

For testing H_0 : $\beta_3 = 0$, we can use (8.37)

$$F = \frac{\hat{\boldsymbol{\beta}}' \mathbf{X}' \mathbf{y} - \hat{\boldsymbol{\beta}}_1^{*'} \mathbf{X}_1' \mathbf{y}}{s^2},$$

or (8.39)

$$F = \frac{\hat{\beta}_3^2}{s^2 g_{33}},\tag{13.64}$$

where \mathbf{X}_1 consists of the first three columns of \mathbf{X} in (13.63), $s^2 = \text{SSE}/(n-3-1)$, and g_{33} is the last diagonal element of $(\mathbf{X}'\mathbf{X})^{-1}$. We now carry out this full-reduced-model test using contrasts.

Since the columns of **X** are not orthogonal, the sums of squares for the β 's analogous to $\hat{\beta}_3^2/g_{33}$ in (13.64) are not independent. Thus, the interpretation in terms of the degree of curvature for $E(y_{ij})$ is more difficult. We therefore orthogonalize the columns of **X** so that the sums of squares become independent.

To simplify computations, we first transform $x_1 = 5$, $x_2 = 10$, $x_3 = 15$, and $x_4 = 20$ by dividing by 5, the common distance between them. The x's then become $x_1 = 1$, $x_2 = 2$, $x_3 = 3$, and $x_4 = 4$. The transformed $4n \times 4$ matrix **X** in (13.63) is given by

$$\mathbf{X} = \begin{pmatrix} 1 & 1 & 1^{2} & 1^{3} \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 1 & 1^{2} & 1^{3} \\ 1 & 2 & 2^{2} & 2^{3} \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 2 & 2^{2} & 2^{3} \\ 1 & 3 & 3^{2} & 3^{3} \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 3 & 3^{2} & 3^{3} \\ 1 & 4 & 4^{2} & 4^{3} \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 4 & 4^{2} & 4^{3} \end{pmatrix} = (\mathbf{j}, \mathbf{x}_{1}, \mathbf{x}_{2}, \mathbf{x}_{3}),$$

where \mathbf{j} is $4n \times 1$. Note that by Theorem 8.4c, the resulting F statistics such as (13.64) will be unaffected by this transformation.

To obtain orthogonal columns, we use the orthogonalization procedure in Section 7.10 based on regressing columns of \mathbf{X} on other columns and taking residuals. We begin by orthogonalizing \mathbf{x}_1 . Denoting the first column by \mathbf{x}_0 , we use

(7.97) to obtain

$$\mathbf{x}_{1\cdot0} = \mathbf{x}_1 - \mathbf{x}_0(\mathbf{x}_0'\mathbf{x}_0)^{-1}\mathbf{x}_0'\mathbf{x}_1$$

$$= \mathbf{x}_1 - \mathbf{j}(\mathbf{j}'\mathbf{j})^{-1}\mathbf{j}'\mathbf{x}_1 = \mathbf{x}_1 - \mathbf{j}(4n)^{-1}n\sum_{i=1}^4 x_i$$

$$= \mathbf{x}_1 - \bar{x}\mathbf{j}.$$
(13.65)

The residual vector $\mathbf{x}_{1\cdot 0}$ is orthogonal to $\mathbf{x}_0 = \mathbf{j}$:

$$\mathbf{j}'\mathbf{x}_{1\cdot 0} = \mathbf{j}'(\mathbf{x}_1 - \bar{x}\mathbf{j}) = \mathbf{j}'\mathbf{x}_1 - \bar{x}\mathbf{j}'\mathbf{j} = 4n\bar{x} - 4n\bar{x} = 0.$$
 (13.66)

We apply this procedure successively to the other two columns of X. To transform the third column, x_2 , so that it is orthogonal to the first two columns, we use (7.97) to obtain

$$\mathbf{x}_{2\cdot 01} = \mathbf{x}_2 - \mathbf{Z}_1(\mathbf{Z}_1'\mathbf{Z}_1)^{-1}\mathbf{Z}_1'\mathbf{x}_2, \tag{13.67}$$

where $\mathbf{Z}_1 = (\mathbf{j}, \mathbf{x}_{1 \cdot 0})$. We use the notation \mathbf{Z}_1 instead of \mathbf{X}_1 because $\mathbf{x}_{1 \cdot 0}$, the second column of \mathbf{Z}_1 , is different from \mathbf{x}_1 , the second column of \mathbf{X}_1 . The matrix $\mathbf{Z}_1'\mathbf{Z}_1$ is given by

$$\mathbf{Z}_{1}'\mathbf{Z}_{1} = \begin{pmatrix} \mathbf{j}' \\ \mathbf{x}_{1\cdot0}' \end{pmatrix} (\mathbf{j}, \mathbf{x}_{1\cdot0})$$

$$= \begin{pmatrix} \mathbf{j}'\mathbf{j} & 0 \\ 0 & \mathbf{x}_{1\cdot0}' \mathbf{x}_{1\cdot0} \end{pmatrix} \quad \text{[by (13.66)]},$$

and (13.67) becomes

$$\mathbf{x}_{2\cdot01} = \mathbf{x}_{2} - \mathbf{Z}_{1}(\mathbf{Z}_{1}'\mathbf{Z}_{1})^{-1}\mathbf{Z}_{1}'\mathbf{x}_{2}$$

$$= \mathbf{x}_{2} - (\mathbf{j}, \mathbf{x}_{1\cdot0}) \begin{pmatrix} \mathbf{j}'\mathbf{j} & 0\\ 0 & \mathbf{x}_{1\cdot0}'\mathbf{x}_{1\cdot0} \end{pmatrix}^{-1} \begin{pmatrix} \mathbf{j}'\\ \mathbf{x}_{1\cdot0}' \end{pmatrix} \mathbf{x}_{2}$$

$$= \mathbf{x}_{2} - \frac{\mathbf{j}'\mathbf{x}_{2}}{\mathbf{j}'\mathbf{j}} \mathbf{j} - \frac{\mathbf{x}_{1\cdot0}'\mathbf{x}_{2}}{\mathbf{x}_{1\cdot0}'\mathbf{x}_{1\cdot0}} \mathbf{x}_{1\cdot0}.$$
(13.68)

The residual vector $\mathbf{x}_{2\cdot01}$ is orthogonal to $\mathbf{x}_0 = \mathbf{j}$ and to $\mathbf{x}_{1\cdot0}$:

$$\mathbf{j}'\mathbf{x}_{2\cdot01} = 0, \quad \mathbf{x}'_{1\cdot0}\mathbf{x}_{2\cdot01} = 0.$$
 (13.69)

The fourth column of **Z** becomes

$$\mathbf{x}_{3\cdot012} = \mathbf{x}_3 - \frac{\mathbf{j}'\mathbf{x}_3}{\mathbf{j}'\mathbf{j}}\mathbf{j} - \frac{\mathbf{x}'_{1\cdot0}\mathbf{x}_3}{\mathbf{x}'_{1\cdot0}\mathbf{x}_{1\cdot0}}\mathbf{x}_{1\cdot0} - \frac{\mathbf{x}'_{2\cdot01}\mathbf{x}_3}{\mathbf{x}'_{2\cdot01}\mathbf{x}_{2\cdot01}}\mathbf{x}_{2\cdot01},$$
 (13.70)

which is orthogonal to the first three columns, \mathbf{j} , $\mathbf{x}_{1\cdot 0}$, and $\mathbf{x}_{2\cdot 01}$.

We have thus transformed $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$ to

$$\mathbf{y} = \mathbf{Z}\boldsymbol{\theta} + \boldsymbol{\varepsilon},\tag{13.71}$$

where the columns of **Z** are mutually orthogonal and the elements of θ are functions of the β 's. The columns of **Z** are given in (13.65), (13.68), and (13.70):

$$\mathbf{z}_0 = \mathbf{j}, \quad \mathbf{z}_1 = \mathbf{x}_{1.0}, \quad \mathbf{z}_2 = \mathbf{x}_{2.01}, \quad \mathbf{z}_3 = \mathbf{x}_{3.012}.$$

We now evaluate \mathbf{z}_1 , \mathbf{z}_2 , and \mathbf{z}_3 for our illustration, in which $x_1 = 1$, $x_2 = 2$, $x_3 = 3$, and $x_4 = 4$. By (13.65), we obtain

$$\mathbf{z}_1 = \mathbf{x}_{1 \cdot 0} = \mathbf{x}_1 - \bar{\mathbf{x}} \mathbf{j} = \mathbf{x}_1 - 2.5 \mathbf{j}$$

= $(-1.5, \dots, -1.5, -.5, \dots, -.5, .5, \dots, 5, 1.5, \dots, 1.5)'$,

which we multiply by 2 so as to obtain integer values:

$$\mathbf{z}_1 = \mathbf{x}_{1\cdot 0} = (-3, \ldots, -3, -1, \ldots, -1, 1, \ldots, 1, 3, \ldots, 3)'.$$
 (13.72)

Note that multiplying by 2 preserves the orthogonality and does not affect the F values.

To obtain \mathbf{z}_2 , by (13.68), we first compute

$$\frac{\mathbf{j}'\mathbf{x}_2}{\mathbf{j}'\mathbf{j}} = \frac{n\sum_{i=1}^4 x_i^2}{4n} = \frac{\sum_{i=1}^4 i^2}{4} = \frac{30}{4} = 7.5,$$

$$\frac{\mathbf{x}'_{1:0}\mathbf{x}_2}{\mathbf{x}'_{1:0}\mathbf{x}_{1:0}} = \frac{n[-3(1^2) - 1(2^2) + 1(3^2) + 3(4^2)]}{n[(-3)^2 + (-1)^2 + 1^2 + 3^2]} = \frac{50}{20} = 2.5.$$

Then, by (13.68), we obtain

$$\mathbf{z}_{2} = \mathbf{x}_{2} - \frac{\mathbf{j}' \mathbf{x}_{2}}{\mathbf{j}' \mathbf{j}} \mathbf{j} - \frac{\mathbf{x}'_{1.0} \mathbf{x}_{2}}{\mathbf{x}'_{1.0} \mathbf{x}_{1.0}} \mathbf{x}_{1.0}$$

$$= \mathbf{x}_{2} - 7.5 \mathbf{j} - 2.5 \mathbf{x}_{1.0}$$

$$\begin{pmatrix} 1^{2} \\ \vdots \\ 1^{2} \\ 2^{2} \\ \vdots \\ 3^{2} \\ 4^{2} \\ \vdots \\ 4^{2} \end{pmatrix} \begin{pmatrix} 1 \\ \vdots \\ 1 \\ 1 \\ \vdots \\ 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} \begin{pmatrix} -3 \\ \vdots \\ -3 \\ -1 \\ \vdots \\ -1 \\ 1 \\ \vdots \\ 1 \\ 3 \end{pmatrix} \begin{pmatrix} 1 \\ \vdots \\ 1 \\ -1 \\ \vdots \\ -1 \\ 1 \\ \vdots \\ 1 \\ 3 \end{pmatrix} . \qquad (13.73)$$

Similarly, using (13.70), we obtain

$$\mathbf{z}_3 = (-1, \ldots, -1, 3, \ldots, 3, -3, \ldots, -3, 1, \ldots, 1)'.$$
 (13.74)

Thus **Z** is given by

$$\mathbf{Z} = \begin{pmatrix} 1 & -3 & 1 & -1 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & -3 & 1 & -1 \\ 1 & -1 & -1 & 3 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & -1 & -1 & 3 \\ 1 & 1 & -1 & -3 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 1 & -1 & -3 \\ 1 & 3 & 1 & 1 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 3 & 1 & 1 \end{pmatrix}.$$

Since

$$X\beta = Z\theta$$
,

we can find the θ 's in terms of the β 's or the β 's in terms of the θ 's. For our illustration, these relationships are given by (see Problem 13.24)

$$\beta_0 = \theta_0 - 5\theta_1 + 5\theta_2 - 35\theta_3, \quad \beta_1 = 2\theta_1 - 5\theta_2 + \frac{16.7}{.3}\theta_3,$$

$$\beta_2 = \theta_2 - 25\theta_3, \quad \beta_3 = \frac{\theta_3}{3}.$$
(13.75)

Since the columns of $\mathbf{Z} = (\mathbf{j}, \mathbf{z}_1, \mathbf{z}_2, \mathbf{z}_3)$ are orthogonal $(\mathbf{z}_i'\mathbf{z}_j = 0 \text{ for all } i \neq j)$, we have $\mathbf{Z}'\mathbf{Z} = \text{diag}(\mathbf{j}'\mathbf{j}, \mathbf{z}_1'\mathbf{z}_1, \mathbf{z}_2'\mathbf{z}_2, \mathbf{z}_3'\mathbf{z}_3)$. Thus

$$\hat{\boldsymbol{\theta}} = (\mathbf{Z}'\mathbf{Z})^{-1}\mathbf{Z}'\mathbf{y} = \begin{pmatrix} \mathbf{j}'\mathbf{y}/\mathbf{j}'\mathbf{j} \\ \mathbf{z}'_1\mathbf{y}/\mathbf{z}'_1\mathbf{z}_1 \\ \mathbf{z}'_2\mathbf{y}/\mathbf{z}'_2\mathbf{z}_2 \\ \mathbf{z}'_3\mathbf{y}/\mathbf{z}'_3\mathbf{z}_3 \end{pmatrix}.$$
 (13.76)

The regression sum of squares (uncorrected for θ_0) is

$$SS(\boldsymbol{\theta}) = \hat{\boldsymbol{\theta}}' \mathbf{Z}' \mathbf{y} = \sum_{i=0}^{3} \frac{(\mathbf{z}_{i}' \mathbf{y})^{2}}{\mathbf{z}_{i}' \mathbf{z}_{i}},$$
(13.77)

where $\mathbf{z}_0 = \mathbf{j}$. By an argument similar to that following (13.54), the sums of squares on the right side of (13.77) are independent.

Since the sums of squares $SS(\theta_i) = (\mathbf{z}_i'\mathbf{y})^2/\mathbf{z}_i'\mathbf{z}_i$, i = 1, 2, 3, are independent, each $SS(\theta_i)$ tests the significance of $\hat{\theta}_i$ by itself (regressing y on \mathbf{z}_i alone) as well as in the presence of the other $\hat{\theta}_i$'s; that is, for a general k, we have

$$\begin{aligned} \operatorname{SS}(\theta_i | \theta_0, \dots, \theta_{i-1}, \theta_{i+1}, \dots, \theta_k) &= \operatorname{SS}(\theta_0, \dots, \theta_k) - \operatorname{SS}(\theta_0, \dots, \theta_{i-1}, \theta_{i+1}, \dots, \theta_k) \\ &= \sum_{j=0}^k \frac{(\mathbf{z}_j' \mathbf{y})^2}{\mathbf{z}_j' \mathbf{z}_j} - \sum_{j \neq i} \frac{(\mathbf{z}_j' \mathbf{y})^2}{\mathbf{z}_j' \mathbf{z}_j} \\ &= \frac{(\mathbf{z}_i' \mathbf{y})^2}{\mathbf{z}_i' \mathbf{z}_i} = \operatorname{SS}(\theta_i). \end{aligned}$$

In terms of the $\hat{\beta}_i$'s, it can be shown that each $SS(\theta_i)$ tests the significance of $\hat{\beta}_i$ in the presence of $\hat{\beta}_0, \hat{\beta}_1, \dots, \hat{\beta}_{i-1}$. For example, for β_k (the last β), the sum of squares

can be written as

$$SS(\theta_k) = \frac{(\mathbf{z}_k' \mathbf{y})^2}{\mathbf{z}_k' \mathbf{z}_k} = \hat{\boldsymbol{\beta}}' \mathbf{X}' \mathbf{y} - \hat{\boldsymbol{\beta}}_1^{*'} \mathbf{X}_1' \mathbf{y}$$
(13.78)

(see Problem 13.26), where $\hat{\boldsymbol{\beta}}$ is from the full model $\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$ and $\hat{\boldsymbol{\beta}}_1^*$ is from the reduced model $\mathbf{y} = \mathbf{X}_1\boldsymbol{\beta}_1^* + \boldsymbol{\varepsilon}$, in which $\boldsymbol{\beta}_1$ contains all the $\boldsymbol{\beta}$'s except $\boldsymbol{\beta}_k$ and \mathbf{X}_1 consists of all columns of \mathbf{X} except the last.

The sum of squares $SS(\theta_i) = (\mathbf{z}_i'\mathbf{y})^2/\mathbf{z}_i'\mathbf{z}_i$ is equivalent to a sum of squares for a contrast on the means $\bar{y}_1, \bar{y}_2, \dots, \bar{y}_k$ as in (13.52). For example

$$\mathbf{z}_{1}'\mathbf{y} = -3y_{11} - 3y_{12} - \dots - 3y_{1n} - y_{21} - \dots - y_{2n} + y_{31} + \dots + y_{3n} + 3y_{41} + \dots + 3y_{4n}$$

$$= -3\sum_{j=1}^{n} y_{1j} - \sum_{j=1}^{n} y_{2j} + \sum_{j=1}^{n} y_{3j} + 3\sum_{j=1}^{n} y_{4j}$$

$$= -3y_{1.} - y_{2.} + y_{3.} + 3y_{4.}$$

$$= n(-3\bar{y}_{1.} - \bar{y}_{2.} + \bar{y}_{3.} + 3\bar{y}_{4.})$$

$$= n\sum_{i=1}^{4} c_{i}\bar{y}_{i.},$$

where $c_1 = -3$, $c_2 = -1$, $c_3 = 1$, and $c_4 = 3$. Similarly

$$\mathbf{z}_{1}'\mathbf{z}_{1} = n(-3)^{2} + n(-1)^{2} + n(1)^{2} + n(3)^{2}$$

$$= n[(-3)^{2} + (-1)^{2} + 1^{2} + 3^{2}]$$

$$= n\sum_{i=1}^{4} c_{i}^{2}.$$

Then

$$\frac{(\mathbf{z}_{1}'\mathbf{y})^{2}}{\mathbf{z}_{1}'\mathbf{z}_{1}} = \frac{(n\sum_{i=1}^{4}c_{i}\bar{\mathbf{y}}_{i.})^{2}}{n\sum_{i=1}^{4}c_{i}^{2}} = \frac{n(\sum_{i=1}^{4}c_{i}\bar{\mathbf{y}}_{i.})^{2}}{\sum_{i=1}^{4}c_{i}^{2}},$$

which is the sum of squares for the contrast in (13.52). Note that the coefficients -3, -1, 1, and 3 correspond to a linear trend.

Likewise, $\mathbf{z}_2'\mathbf{y}$ becomes

$$\mathbf{z}_{2}'\mathbf{y} = n(\bar{y}_{1.} - \bar{y}_{2.} - \bar{y}_{3.} + \bar{y}_{4.}),$$

whose coefficients show a quadratic trend, and $\mathbf{z}_{3}'\mathbf{y}$ can be written as

$$\mathbf{z}_{3}'\mathbf{y} = n(-\bar{y}_{1.} + 3\bar{y}_{2.} - 3\bar{y}_{3.} + \bar{y}_{4.})$$

with coefficients that exhibit a cubic pattern.

These contrasts in the \bar{y}_i 's have a meaningful interpretation in terms of the shape of the response curve. For example, suppose that the \bar{y}_i 's fall on a straight line. Then, for some b_0 and b_1 , we have

$$\bar{y}_i = b_0 + b_1 x_i = b_0 + b_1 i, i = 1, 2, 3, 4,$$

since $x_i = i$. In this case, the linear contrast is nonzero and the quadratic and cubic contrasts are zero:

$$-3\bar{y}_{1.} - \bar{y}_{2.} + \bar{y}_{3.} + 3\bar{y}_{4.} =$$

$$-3(b_0 + b_1) - (b_0 + 2b_1) + b_0 + 3b_1 + 3(b_0 + 4b_1) = 10b_1,$$

$$b_0 + b_1 - (b_0 + 2b_1) - (b_0 + 3b_1) + (b_0 + 4b_1) = 0,$$

$$-(b_0 + b_1) + 3(b_0 + 2b_1) - 3(b_0 + 3b_1) + (b_0 + 4b_1) = 0.$$

This demonstration could be simplified by choosing the linear trend $\bar{y}_{1.} = 1$, $\bar{y}_{2.} = 2$, $\bar{y}_{3.} = 3$, and $\bar{y}_{4.} = 4$.

Similarly, if the \bar{y}_i 's follow a quadratic trend, say

$$\bar{y}_1 = 1$$
, $\bar{y}_2 = 2$, $\bar{y}_3 = 2$, $\bar{y}_4 = 1$,

then the linear and cubic contrasts are zero.

In many cases it is not necessary to find the orthogonal polynomial coefficients by the orthogonalization process illustrated in this section. Tables of orthogonal polynomials are available [see, e.g., Rencher (2002, p. 587) or Guttman (1982, pp. 349-354)]. We give a brief illustration of some orthogonal polynomial coefficients in Table 13.5, including those we found above for k=4.

TABLE 13.5 Orthogonal Polynomial Coefficients for k = 3, 4, 5

-		k = 3			k =	4				k = 5		
Linear	-1	0	1	-3	-1	1	3	-2	-1	0	1	2
Quadratic	1	-2	1	1	-1	-1	1	2	-1	-2	-1	2
Cubic				-1	3	-3	1	-1	2	0	-2	1
Quartic								1	-4	6	-4	1

In Table 13.5, we can see some relationships among the coefficients for each value of k. For example, if k=3 and the three means \bar{y}_1 , \bar{y}_2 , \bar{y}_3 have a linear relationship, then $\bar{y}_2 - \bar{y}_1$ is equal to $\bar{y}_3 - \bar{y}_2$; that is

$$\bar{y}_{3.} - \bar{y}_{2.} = \bar{y}_{2.} - \bar{y}_{1.}$$

or

$$\bar{y}_{3.} - \bar{y}_{2.} - (\bar{y}_{2.} - \bar{y}_{1.}) = 0,$$

 $\bar{y}_{3.} - 2\bar{y}_{2.} + \bar{y}_{1.} = 0.$

If this relationship among the three means fails to hold, we have a quadratic component of curvature.

Similarly, for k=4, the cubic component, $-\bar{y}_{1.}+3\bar{y}_{2.}-3\bar{y}_{3.}+\bar{y}_{4.}$, is equal to the difference between the quadratic component for $\bar{y}_{1.},\bar{y}_{2.},\bar{y}_{3.}$ and the quadratic component for $\bar{y}_{2.},\bar{y}_{3.},\bar{y}_{4.}$:

$$-\bar{y}_{1.}+3\bar{y}_{2.}-3\bar{y}_{3.}+\bar{y}_{4.}=\bar{y}_{2.}-2\bar{y}_{3.}+\bar{y}_{4.}-(\bar{y}_{1.}-2\bar{y}_{2.}+\bar{y}_{3.}).$$

PROBLEMS

- **13.1** Obtain the normal equations in (13.7) from the model in (13.6).
- **13.2** Obtain $\hat{\beta}$ in (13.12) using $(X'X)^-$ in (13.11) and X'y in (13.7).
- **13.3** Show that SSE = $\mathbf{y}'[\mathbf{I} \mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}']\mathbf{y}$ in (12.21) is equal to SSE = $\sum_{ij} y_{ij}^2 \sum_i y_i^2/n$ in (13.13).
- **13.4** Show that the expressions for SSE in (13.13) and (13.14) are equal.
- **13.5** (a) Show that $H_0: \alpha_1 = \alpha_2 = \cdots = \alpha_k$ in (13.17) is equivalent to $H_0: \alpha_1^* = \alpha_2^* = \cdots = \alpha_k^*$ in (13.18).
 - **(b)** Show that $H_0: \alpha_1^* = \alpha_2^* = \cdots = \alpha_k^*$ in (13.18) is equivalent to $H_0: \alpha_1^* = \alpha_2^* = \cdots = \alpha_k^* = 0$ in (13.19).
- **13.6** Show that $n \sum_{i=1}^{k} (\bar{y}_{i.} \bar{y}_{..})^2$ in (13.24) is equal to $\sum_{i} y_{i.}^2 / n y_{..}^2 / kn$ in (13.23).
- **13.7** Using (13.6) and (13.11), show that $\mathbf{X}(\mathbf{X}'\mathbf{X})^{-}\mathbf{X}'$ in (13.25) can be written in terms of **J** and **O** as in (13.26).
- **13.8** Show that for **C** in (13.28), $C(X'X)^-C'$ is given by (13.30).
- 13.9 Show that $C(X'X)^{-}X'$ is given by the matrix in (13.32).
- **13.10** Show that the matrix $(1/4n)\mathbf{A}'\mathbf{J}_3\mathbf{A}$ in (13.33) has the form shown in (13.35).

- **13.11** Using the model $y_{ij} = \mu^* + \alpha_i^* + \varepsilon_{ij}$ with the assumptions $E(\varepsilon_{ij}) = 0$, $var(\varepsilon_{ij}) = \sigma^2$, $cov(\varepsilon_{ij}, \varepsilon_{i'j'}) = 0$, and the side condition $\sum_{i=1}^k \alpha_i^* = 0$, obtain the following results used in Table 13.4:
 - (a) $E(\varepsilon_{ii}^2) = \sigma^2$ for all i, j and $E(\varepsilon_{ij}\varepsilon_{i'j'}) = 0$ for $i, j \neq i', j'$.
 - **(b)** $E[SS(\alpha|\mu)] = (k-1)\sigma^2 + n\sum_{i=1}^k \alpha_i^{*2}$.
 - (c) (SSE) = $k(n-1)\sigma^2$.
- **13.12** Using C in (13.28), show that C'C is given by the matrix in (13.47)
- 13.13 Show that $C'J_3C$ has the form shown in (13.48).
- **13.14** Show that if the constraint $\sum_{i=1}^{4} \alpha_i = 0$ is not imposed, (13.49) becomes

$$E[SS(\alpha|\mu)] = 3\sigma^2 + 4\sum_{i=1}^4 (\alpha_i - \bar{\alpha})^2.$$

- **13.15** Show that F in (13.52) can be obtained from (13.51).
- **13.16** Express the sums of squares $(\mathbf{c}_i'\hat{\boldsymbol{\beta}})^2/\mathbf{c}_i'(\mathbf{X}'\mathbf{X})^-\mathbf{c}_i$ and $(\mathbf{c}_j'\hat{\boldsymbol{\beta}})^2/\mathbf{c}_j'(\mathbf{X}'\mathbf{X})^-\mathbf{c}_j$ below (13.54) in Section 13.6.2 as quadratic forms in \mathbf{y} , and show that these sums of squares are independent if $\text{cov}(\mathbf{c}_i'\hat{\boldsymbol{\beta}}, \mathbf{c}_i'\hat{\boldsymbol{\beta}}) = 0$ as in (13.53).
- 13.17 In the proof of Theorem 13.6b, show that A_i is symmetric and idempotent that rank(A_i) = 1, and that $A_iA_j = 0$.
- 13.18 (a) Show that J/kn in the first term on the right side of (13.59) is idempotent with one eigenvalue equal to 1 and the others equal to 0.
 - (b) Show that \mathbf{j} is an eigenvector corresponding to the nonzero eigenvalue of \mathbf{J}/kn .
- **13.19** In Example 13.6b, show that $\mathbf{v}_0'\mathbf{v}_0 = 1$ and $\mathbf{v}_0'\mathbf{v}_1 = 0$.
- **13.20** Show that $\mathbf{j}'\mathbf{x}_{2\cdot01} = 0$ and $\mathbf{x}'_{0\cdot1}\mathbf{x}_{2\cdot01} = 0$ as in (13.69).
- **13.21** Show that $\mathbf{x}_{3.012}$ has the form given in (13.70).
- **13.22** Show that $\mathbf{x}_{3.012}$ is orthogonal to each of \mathbf{j} , $\mathbf{x}_{1.0}$, and $\mathbf{x}_{2.01}$, as noted following (13.70).
- **13.23** Show that $\mathbf{z}_3 = (-1, \dots, -1, 3, \dots, 3, -3, \dots, -3, 1, \dots, 1)'$ as in (13.74).
- **13.24** Show that $\beta_0 = \theta_0 5\theta_1 + 5\theta_2 35\theta_3$, $\beta_1 = 2\theta_1 5\theta_2 + (16.7/.3)\theta_3$, $\beta_2 = \theta_2 25\theta_3$, and $\beta_3 = \theta_3/.3$, as in (13.75).
- 13.25 Show that the elements of $\hat{\boldsymbol{\theta}} = (\mathbf{Z}'\mathbf{Z})^{-1}\mathbf{Z}'\mathbf{y}$ are of the form $\mathbf{z}_i'\mathbf{y}/\mathbf{z}_i'\mathbf{z}_i$ as in (13.76).
- 13.26 Show that $SS(\theta_k) = \hat{\boldsymbol{\beta}}' \mathbf{X}' \mathbf{y} \hat{\boldsymbol{\beta}}^{*'} \mathbf{X}'_1 \mathbf{y}$ as in (13.78).
- 13.27 If the means $\bar{y}_1, \bar{y}_2, \bar{y}_3$, and \bar{y}_4 have the quadratic trend $\bar{y}_1 = 1$, $\bar{y}_2 = 2$, $\bar{y}_3 = 2$, $\bar{y}_4 = 1$, show that the linear and cubic contrasts are zero, but the quadratic contrast is not zero.

			` /	
A	В	С	D	Е
124	111	117	104	142
116	101	142	128	139
101	130	121	130	133
118	108	123	103	120
118	127	121	121	127
120	129	148	119	149
110	122	141	106	150
127	103	122	107	149
106	122	139	107	120
130	127	125	115	116

TABLE 13.6 Blood Sugar Levels (mg/100 g) for 10 Animals from Each of Five Breeds (A–E)

- **13.28** Blood sugar levels (mg/100g) were measured on 10 animals from each of five breeds (Daniel 1974, p. 197). The results are presented in Table 13.6.
 - (a) Test the hypothesis of equality of means for the five breeds.
 - **(b)** Make the following comparisons by means of orthogonal contrasts:

- **13.29** In Table 13.7, we have the amount of insulin released from specimens of pancreatic tissue treated with five concentrations of glucose (Daniel 1974, p. 182).
 - (a) Test the hypothesis of equality of means for the five glucose concentrations.
 - (b) Assuming that the levels of glucose concentration are equally spaced, use orthogonal polynomial contrasts to test for linear, quadratic, cubic, and quartic trends.
- **13.30** A different stimulus was given to each of three groups of 14 animals (Daniel 1974, p. 196). The response times in seconds are given in Table 13.8.
 - (a) Test the hypothesis of equal mean response times.
 - **(b)** Using orthogonal contrasts, make the two comparisons of stimuli: 1 versus 2, 3; and 2 versus 3.
- 13.31 The tensile strength (kg) was measured for 12 wires from each of nine cables (Hald 1952, p. 434). The results are given in Table 13.9.
 - (a) Test the hypothesis of equal mean strengths for the nine cables.
 - **(b)** The first four cables were made from one type of raw material and the other five from another type. Compare these two types by means of a contrast.

TABLE 13.7	Insulin	Released	at Five	Different	Glucose
Concentration	s (1-5)				

1	2	3	4	5
1.53	3.15	3.89	8.18	5.86
1.61	3.96	4.80	5.64	5.46
3.75	3.59	3.69	7.36	5.96
2.89	1.89	5.70	5.33	6.49
3.26	1.45	5.62	8.82	7.81
2.83	3.49	5.79	5.26	9.03
2.86	1.56	4.75	8.75	7.49
2.59	2.44	5.33	7.10	8.98

TABLE 13.8 Response Times (in seconds) to Three Stimuli

Stimulus				Stimulus	,
1	2	3	1	2	3
16	6	8	17	6	9
14	7	10	7	8	11
14	7	9	17	6	11
13	8	10	19	4	9
13	4	6	14	9	10
12	8	7	15	5	9
12	9	10	20	5	5

TABLE 13.9 Tensile Strength (kg) of Wires from Nine Cables (1-9)

1	2	3	4	5	6	7	8	9
345	329	340	328	347	341	339	339	342
327	327	330	344	341	340	340	340	346
335	332	325	342	345	335	342	347	347
338	348	328	350	340	336	341	345	348
330	337	338	335	350	339	336	350	355
334	328	332	332	346	340	342	348	351
335	328	335	328	345	342	347	341	333
340	330	340	340	342	345	345	342	347
333	328	335	337	330	346	336	340	348
335	330	329	340	338	347	342	345	341

TABLE 13.10	Scores for Physical Therapy Patients
Subjected to Fo	ur Treatment Programs (1-14)

1	2	3	4
64	76	58	95
88	70	74	90
72	90	66	80
80	80	60	87
79	75	82	88
71	82	75	85

TABLE 13.11 Weight Gain of Pigs Subjected to Five Treatments (1–5)

1	2	3	4	5
165	168	164	185	201
156	180	156	195	189
159	180	156	195	189
159	180	189	184	173
167	166	138	201	193
170	170	153	165	164
146	161	190	175	160
130	171	160	187	200
151	169	172	177	142
164	179	142	166	184
158	191	155	165	149

- **13.32** Four groups of physical therapy patients were given different treatments (Daniel 1974, p. 195). The scores measuring treatment effectiveness are given in Table 13.10.
 - (a) Test the hypothesis of equal mean treatment effects.
 - **(b)** Using contrasts, compare treatments 1, 2 versus 3, 4; 1 versus 2; and 3 versus 4.
- **13.33** Weight gains in pigs subjected to five different treatments are given in Table 13.11 (Crampton and Hopkins 1934).
 - (a) Test the hypothesis of equal mean treatment effects.
 - **(b)** Using contrasts, compare treatments 1, 2, 3 versus 4; 1, 2 versus 3; and 1 versus 2.