CHAPTER 10

Bias in Regression Estimates, and Expected Values of Mean Squares and Sums of Squares

This chapter explores what can be said in situations where we fit one model (e.g., a straight line) but we fear that this model may be somewhat inadequate (e.g., there in fact may be a little quadratic curvature). We can talk in terms of the *fitted model* and the *true model* but it is better to think in terms of the fitted model and the *feared model* alternative. After all, if we knew we were fitting the *wrong* model, why would we do it? We are often interested in what might be wrong with the model fitted *if* some specified alternative were true, however. We first discuss possible biases in the estimates of the parameters of a possibly inadequate model and then see how the consequences of this go through to the analysis of variance table, via the expected values of the various mean squares. Details of how to compute the expected values of mean squares and sums of squares are then given.

10.1. BIAS IN REGRESSION ESTIMATES

We said earlier (Section 5.1) that the least squares estimate $\mathbf{b} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$ of $\boldsymbol{\beta}$ in the model $E(\mathbf{Y}) = \mathbf{X}\boldsymbol{\beta}$ is an unbiased estimate. This means that

$$E(\mathbf{b}) = \boldsymbol{\beta}.$$

That is, if we consider the distribution of $\mathbf{b}$ (obtained by taking repeated samples from the same Y-population keeping $\mathbf{X}$ fixed and estimating $\boldsymbol{\beta}$ for each sample), then the mean value of this distribution is $\boldsymbol{\beta}$.

We now emphasize that this is true *only if the postulated model is the correct model to consider.* If it is *not* the correct model, then the estimates are *biased*; that is, $E(\mathbf{b}) \neq \boldsymbol{\beta}$. The extent of the bias depends, as we shall show, not only on the postulated and the true models but also on the values of the X-variables that enter the regression calculations. When a designed experiment is used, the bias depends on the experimental design, as well as the models.

We shall deal with the general nonsingular regression model from the beginning, since once we have the necessary formulas in matrix terms, they can be applied universally. Special cases can be reworked in their algebraic detail as exercises if desired. Suppose we postulate the model

$$E(\mathbf{Y}) = \mathbf{X}_1\boldsymbol{\beta}_1. \tag{10.1.1}$$

This leads to the least squares estimates:

$$\mathbf{b}_1 = (\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{X}_1'\mathbf{Y}. \tag{10.1.2}$$

If the postulated model is correct, then, since $\mathbf{X}_1$ is a matrix of constants unaffected by expectation, and $\mathbf{b}_1$ and $\mathbf{Y}$ are the random variables,

$$E(\mathbf{b}_1) = (\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{X}_1'E(\mathbf{Y}) = (\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{X}_1'\mathbf{X}_1\boldsymbol{\beta}_1 = \boldsymbol{\beta}_1. \tag{10.1.3}$$

Thus $\mathbf{b}_1$ is an unbiased estimate of $\boldsymbol{\beta}_1$.

Now suppose we once again postulate the model given in Eq. (10.1.1) so that $\mathbf{b}_1$, as defined in Eq. (10.1.2), is still the vector of estimated regression coefficients. Suppose *now*, however, that the true response relationship is in fact not Eq. (10.1.1) but

$$E(\mathbf{Y}) = \mathbf{X}_1\boldsymbol{\beta}_1 + \mathbf{X}_2\boldsymbol{\beta}_2. \tag{10.1.4}$$

That is, there are terms $\mathbf{X}_2\boldsymbol{\beta}_2$ that we did not allow for in our estimation procedure. It now follows that

$$\begin{aligned} E(\mathbf{b}_1) &= (\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{X}_1'E(\mathbf{Y}) = (\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{X}_1'(\mathbf{X}_1\boldsymbol{\beta}_1 + \mathbf{X}_2\boldsymbol{\beta}_2) \\ &= (\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{X}_1'\mathbf{X}_1\boldsymbol{\beta}_1 + (\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{X}_1'\mathbf{X}_2\boldsymbol{\beta}_2 \\ &= \boldsymbol{\beta}_1 + \mathbf{A}\boldsymbol{\beta}_2, \end{aligned} \tag{10.1.5}$$

where

$$\mathbf{A} = (\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{X}_1'\mathbf{X}_2 \tag{10.1.6}$$

is called the *alias* or *bias* matrix. Note that the bias terms $\mathbf{A}\boldsymbol{\beta}_2$ depend not only on the postulated and the true models but also on the experimental design through the matrices $\mathbf{X}_1$ and $\mathbf{X}_2$. Thus a good choice of design may cause estimates to be less biased than they would otherwise be, even if the wrong model has been postulated and fitted.

Note also that the observations Y_i do not appear in (10.1.5) so that the result can be used to examine potential experimental designs before they are actually performed.

The result (10.1.5) can also be viewed in another way. Look first at (10.1.6). If $\mathbf{X}_1'\mathbf{X}_2 = \mathbf{0}$, there is no bias because $\mathbf{A} = \mathbf{0}$. Suppose that $\mathbf{X}_1$ and $\mathbf{X}_2$ are not orthogonal, however. Then if we regress $\mathbf{X}_2$ on $\mathbf{X}_1$ (i.e., treat each of the columns of $\mathbf{X}_2$ as a "$\mathbf{Y}$ column") to give $\hat{\mathbf{X}}_2 = \mathbf{X}_1(\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{X}_1'\mathbf{X}_2$ for "fitted values," we get the "residuals"

$$\mathbf{X}_2 - \hat{\mathbf{X}}_2 = (\mathbf{I} - \mathbf{X}_1(\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{X}_1')\mathbf{X}_2 = \mathbf{Z}, \tag{10.1.7}$$

say. Note that $\mathbf{X}_1'\mathbf{Z} = \mathbf{0}$. We can thus rewrite the model (10.1.4) as

$$\begin{aligned} E(\mathbf{Y}) &= \mathbf{X}_1\boldsymbol{\beta}_1 + \mathbf{X}_1\mathbf{A}\boldsymbol{\beta}_2 + \mathbf{X}_2\boldsymbol{\beta}_2 - \mathbf{X}_1\mathbf{A}\boldsymbol{\beta}_2 \\ &= \mathbf{X}_1(\boldsymbol{\beta}_1 + \mathbf{A}\boldsymbol{\beta}_2) + (\mathbf{X}_2 - \mathbf{X}_1\mathbf{A})\boldsymbol{\beta}_2 \\ &= \mathbf{X}_1\boldsymbol{\beta}^* + \mathbf{Z}\boldsymbol{\beta}_2, \end{aligned} \tag{10.1.8}$$

say, where $\boldsymbol{\beta}^* = \boldsymbol{\beta}_1 + \mathbf{A}\boldsymbol{\beta}_2$. We have *orthogonalized the model* because $\mathbf{X}_1'\mathbf{Z} = \mathbf{0}$. Note that when we estimate $\boldsymbol{\beta}$, the coefficient of $\mathbf{X}_1$, we obtain an unbiased estimate because $\mathbf{X}_1'\mathbf{Z} = \mathbf{0}$, *but it is an estimate of* $\boldsymbol{\beta}_1 + \mathbf{A}\boldsymbol{\beta}_2$. So our two viewpoints are consistent! This orthogonalization procedure is used in Section 10.4, where $\mathbf{Z}$ is called $\mathbf{X}_{2\cdot 1}$, a common and meaningful notation indicating that we have obtained "the portion of $\mathbf{X}_2$ that is orthogonal to $\mathbf{X}_1$."

We now illustrate the application of Eq. (10.1.5) to some simple numerical cases.

Example 1. Suppose we postulate the model

$$E(Y) = \beta_0 + \beta_1 X,$$

but the model

$$E(Y) = \beta_0 + \beta_1 X + \beta_{11} X^2$$

is actually the true response function, unknown to us. If we use observations of Y at $X = -1$, 0, and 1 to estimate β_0 and β_1 in the postulated model, what bias will be introduced? That is, what will the estimates b_0 and b_1 actually estimate? The true model, in terms of the observations, is

$$\begin{aligned}
E(\mathbf{Y}) = E\begin{bmatrix} Y_1 \\ Y_2 \\ Y_3 \end{bmatrix} &= \begin{array}{c} \begin{array}{ccc} 1 & \mathbf{X} & \mathbf{X}^2 \end{array} \\ \begin{bmatrix} 1 & -1 & 1 \\ 1 & 0 & 0 \\ 1 & 1 & 1 \end{bmatrix} \end{array} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_{11} \end{bmatrix} \\
&= \begin{array}{c} \begin{array}{cc} 1 & \mathbf{X} \end{array} \\ \begin{bmatrix} 1 & -1 \\ 1 & 0 \\ 1 & 1 \end{bmatrix} \end{array} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} + \begin{array}{c} \mathbf{X}^2 \\ \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} \end{array} \beta_{11} \\
&= \mathbf{X}_1 \boldsymbol{\beta}_1 + \mathbf{X}_2 \boldsymbol{\beta}_2
\end{aligned}$$

to achieve the form of Eq. (10.1.4) with Eq. (10.1.1) as the postulated model. It follows that

$$(\mathbf{X}_1'\mathbf{X}_1)^{-1} = \begin{bmatrix} 3 & 0 \\ 0 & 2 \end{bmatrix}^{-1} = \begin{bmatrix} \frac{1}{3} & 0 \\ 0 & \frac{1}{2} \end{bmatrix},$$

$$\mathbf{X}_1'\mathbf{X}_2 = \begin{bmatrix} 1 & 1 & 1 \\ -1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 2 \\ 0 \end{bmatrix}.$$

Thus

$$\mathbf{A} = \begin{bmatrix} \frac{1}{3} & 0 \\ 0 & \frac{1}{2} \end{bmatrix} \begin{bmatrix} 2 \\ 0 \end{bmatrix} = \begin{bmatrix} \frac{2}{3} \\ 0 \end{bmatrix}.$$

Applying Eq. (10.1.5) we obtain

$$E\begin{bmatrix} b_0 \\ b_1 \end{bmatrix} = \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} + \begin{bmatrix} \frac{2}{3} \\ 0 \end{bmatrix} \beta_{11} = \begin{bmatrix} \beta_0 + \frac{2}{3}\beta_{11} \\ \beta_1 \end{bmatrix}$$

or

$$E(b_0) = \beta_0 + \tfrac{2}{3}\beta_{11}, \qquad E(b_1) = \beta_1.$$

Thus b_0 is *biased* by $\frac{2}{3}\beta_{11}$, and b_1 is unbiased.

Example 2. Suppose the postulated model is

$$E(Y) = \beta_0 + \beta_1 X,$$

but the true model is actually

$$E(Y) = \beta_0 + \beta_1 X + \beta_{11} X^2 + \beta_{111} X^3.$$

What biases are induced by taking observations at

$$X = -3, -2, -1, 0, 1, 2, 3?$$

We find

$$\mathbf{X}_1 = \begin{bmatrix} 1 & -3 \\ 1 & -2 \\ 1 & -1 \\ 1 & 0 \\ 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{bmatrix}, \qquad \mathbf{X}_2 = \begin{bmatrix} 9 & -27 \\ 4 & -8 \\ 1 & -1 \\ 0 & 0 \\ 1 & 1 \\ 4 & 8 \\ 9 & 27 \end{bmatrix}$$

$$(\mathbf{X}_1'\mathbf{X}_1)^{-1} = \begin{bmatrix} 7 & 0 \\ 0 & 28 \end{bmatrix}^{-1} = \begin{bmatrix} \frac{1}{7} & 0 \\ 0 & \frac{1}{28} \end{bmatrix},$$

$$\mathbf{X}_1'\mathbf{X}_2 = \begin{bmatrix} 28 & 0 \\ 0 & 196 \end{bmatrix},$$

$$\mathbf{A} = (\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{X}_1'\mathbf{X}_2 = \begin{bmatrix} 4 & 0 \\ 0 & 7 \end{bmatrix}.$$

Thus

$$E(b_0) = \beta_0 + 4\beta_{11},$$
$$E(b_1) = \beta_1 + 7\beta_{111}.$$

By using the general formula, Eq. (10.1.5), we can find the bias in any regression estimates once the postulated model, the feared model, and the design are established. This enables us to find, in specific situations, what effects will be transmitted to our estimates if a particular departure from the assumed model occurs. A sensible procedure in many situations where a polynomial model is postulated is to work on the basis that the postulated model may be wrong because it does not contain terms of one degree higher than those present.

10.2. THE EFFECT OF BIAS ON THE LEAST SQUARES ANALYSIS OF VARIANCE

Note: In this section we shall write $\mathbf{X}$ for the matrix previously called $\mathbf{X}_1$ and $\boldsymbol{\beta}$ for the vector previously called $\boldsymbol{\beta}_1$. The notation $\mathbf{X}_2\boldsymbol{\beta}_2$ will still denote the extra terms of the true models, however. We now summarize the effect bias has on the usual least squares analysis.

Suppose that:

1. The postulated model $E(\mathbf{Y}) = \mathbf{X}\boldsymbol{\beta}$ contains p parameters; $\mathbf{V}(\mathbf{Y}) = \mathbf{I}\sigma^2$.
2. The true model is $E(\mathbf{Y}) = \mathbf{X}\boldsymbol{\beta} + \mathbf{X}_2\boldsymbol{\beta}_2$, where $\boldsymbol{\beta}_2$ may be $\mathbf{0}$, in which case the postulated model is correct.
3. The total number of observations taken is n and there are f degrees of freedom

available for lack of fit and e degrees of freedom for pure error, so that $n = p + f + e$. (This means there are $p + f$ distinct points in the design.)

4. The estimates $\mathbf{b} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$ and the fitted values $\hat{\mathbf{Y}} = \mathbf{X}\mathbf{b}$ are obtained as usual.

5. $\mathbf{A} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{X}_2$.

Then a number of results are true as given below.

1. The matrix $(\mathbf{X}'\mathbf{X})^{-1}\sigma^2$ is always the correct variance–covariance matrix, $V(\mathbf{b})$, of estimated coefficients $\mathbf{b}$.

2. $E(\mathbf{b}) = \boldsymbol{\beta} + \mathbf{A}\boldsymbol{\beta}_2$.

3. $E(\hat{\mathbf{Y}}) = \mathbf{X}\boldsymbol{\beta} + \mathbf{X}\mathbf{A}\boldsymbol{\beta}_2$.

4. The analysis of variance table takes the form below:

Source	df	SS	Expected Value of MS
b_0	1	$\mathbf{Y}'\mathbf{1}\mathbf{1}'\mathbf{Y}/n$	$\sigma^2 + (\mathbf{X}\boldsymbol{\beta} + \mathbf{X}_2\boldsymbol{\beta}_2)'\mathbf{1}\mathbf{1}'(\mathbf{X}\boldsymbol{\beta} + \mathbf{X}_2\boldsymbol{\beta}_2)/n$
Other estimates $\mid b_0$	$p - 1$	$\mathbf{b}'\mathbf{X}'\mathbf{Y} - \mathbf{Y}'\mathbf{1}\mathbf{1}'\mathbf{Y}/n$	$\sigma^2 + (\mathbf{X}\boldsymbol{\beta} + \mathbf{X}_2\boldsymbol{\beta}_2)'\{\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}X' - \mathbf{1}\mathbf{1}'/n\}(\mathbf{X}\boldsymbol{\beta} + \mathbf{X}_2\boldsymbol{\beta}_2)/(p - 1)$
Lack of fit	f	By difference	$\sigma^2 + \boldsymbol{\beta}_2'(\mathbf{X}_2 - \mathbf{X}\mathbf{A})'(\mathbf{X}_2 - \mathbf{X}\mathbf{A})\boldsymbol{\beta}_2/f$
Pure error	e	es_e^2	σ^2
Total	n	$\mathbf{Y}'\mathbf{Y}$	

5. When $\boldsymbol{\beta}_2 = \mathbf{0}$, that is, when the postulated model is correct, the results above reduce to the following:

$$E(\mathbf{b}) = \boldsymbol{\beta}, \qquad E(\hat{\mathbf{Y}}) = \mathbf{X}\boldsymbol{\beta},$$

E(mean square due to other estimates $\mid b_0$) $= \sigma^2 + \boldsymbol{\beta}'\mathbf{X}'(\mathbf{I} - \mathbf{1}\mathbf{1}'/n)\mathbf{X}\boldsymbol{\beta}/(p - 1)$. This is why the mean square due to estimates is compared with an estimate of σ^2 to test H_0: all parameters in β, except β_0, are zero, when the fitted model is not rejected out of hand as a result of a nonsignificant lack of fit test. If the lack of fit test *did* indicate the presence of lack of fit, so that $\boldsymbol{\beta}_2 \neq \mathbf{0}$, then it is useless to carry out a test using the regression mean square, even if we use the pure error mean square s_e^2 to estimate σ^2 rather than the residual mean square. In this case, under H_0, E(mean square due to other estimates $\mid b_0$) $= \sigma^2 + \boldsymbol{\beta}_2'\mathbf{X}_2'[\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}' - \mathbf{1}\mathbf{1}'/n]\mathbf{X}_2\beta_2/(p - 1)$, and the F-ratio we would use has a noncentral F-distribution, rather than the ordinary central F-distribution that we assume when we make the (erroneous) test in the usual way.

10.3. FINDING THE EXPECTED VALUES OF MEAN SQUARES

To find the expectation of mean squares, certain special matrix results are useful. Suppose $\mathbf{Q}$ is an $n \times n$ matrix so that $\mathbf{Y}'\mathbf{Q}\mathbf{Y}$ is a quadratic form in the elements of $\mathbf{Y}$. Then if E denotes expectation

$$E(\mathbf{Y}'\mathbf{Q}\mathbf{Y}) = E(\mathbf{Y})'\mathbf{Q}E(\mathbf{Y}) + \text{trace}(\mathbf{Q}\boldsymbol{\Sigma}),$$

where "trace" means "take the sum of the diagonal elements of the square matrix indicated," and $\boldsymbol{\Sigma} = \mathbf{V}(\mathbf{Y})$ is the $n \times n$ variance–covariance matrix of the vector $\mathbf{Y}$. Furthermore, if $\mathbf{M}_1$ and $\mathbf{M}_2$ are any two square matrices of the same size,

$$\text{trace}(\mathbf{M}_1 + \mathbf{M}_2) = \text{trace } \mathbf{M}_1 + \text{trace } \mathbf{M}_2.$$

In addition, if $\mathbf{T}$ is a $t \times s$ matrix and $\mathbf{S}$ is an $s \times t$ matrix so that both products $\mathbf{TS}$ and $\mathbf{ST}$ are feasible, then

$$\text{trace}(\mathbf{TS}) = \text{trace}(\mathbf{ST}).$$

This last result is a remarkably useful result and often leads to quite fantastic simplification. For example, if $\mathbf{X}$ is $n \times p$ and we take $\mathbf{T} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}$, $\mathbf{S} = \mathbf{X}'$, we can quickly evaluate

$$\text{trace}\{\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\} = \text{trace}\{\mathbf{X}'\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\} = \text{trace}\{\mathbf{I}_p\} = p.$$

We use this particular result in the next example.

Example. Find $E(\mathbf{b}'\mathbf{X}'\mathbf{Y}/p)$, when $E(\mathbf{Y}) = \mathbf{X}\boldsymbol{\beta} + \mathbf{X}_2\boldsymbol{\beta}_2$ and $\mathbf{V}(\mathbf{Y}) = \mathbf{I}\sigma^2$.

$$\begin{aligned}
E(\mathbf{b}'\mathbf{X}'\mathbf{Y}) &= E(\mathbf{Y}'\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}) \\
&= (\mathbf{X}\boldsymbol{\beta} + \mathbf{X}_2\boldsymbol{\beta}_2)'\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'(\mathbf{X}\boldsymbol{\beta} + \mathbf{X}_2\boldsymbol{\beta}_2) \\
&\quad + \text{trace}(\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{I}\sigma^2) \\
&= \{(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{X}\boldsymbol{\beta} + (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{X}_2\boldsymbol{\beta}_2\}'(\mathbf{X}'\mathbf{X})(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{X} \\
&\quad \times \{(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{X}\boldsymbol{\beta} + (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{X}_2\boldsymbol{\beta}_2\} + p\sigma^2 \\
&= (\boldsymbol{\beta} + \mathbf{A}\boldsymbol{\beta}_2)'\mathbf{X}'\mathbf{X}(\boldsymbol{\beta} + \mathbf{A}\boldsymbol{\beta}_2) + p\sigma^2.
\end{aligned}$$

Dividing each side by p provides the df-weighted average of the first two entries in the foregoing table. Note, in the manipulations shown, the insertion of the unit matrices $\mathbf{I} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{X}$ and $\mathbf{I} = \mathbf{X}'\mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}$ to lead to the desired form.

For another example in a different context, see Section 10.4.

10.4. EXPECTED VALUE OF EXTRA SUM OF SQUARES

Write

$$\begin{aligned}
\mathbf{Y} &= \mathbf{X}_1\boldsymbol{\beta}_1 + \mathbf{X}_2\boldsymbol{\beta}_2 + \boldsymbol{\epsilon}, \quad &&\text{for model 1,} \\
\mathbf{Y} &= \mathbf{X}_1\boldsymbol{\beta}_1 \qquad\quad\; + \boldsymbol{\epsilon}, \quad &&\text{for model 2,}
\end{aligned}$$

where $\mathbf{X}_1$ is $n \times q$, and $\mathbf{X}_2$ is $n \times (p - q)$. Note that the $n \times (p - q)$ matrix

$$\begin{aligned}
\mathbf{X}_{2\cdot 1} &= \mathbf{X}_2 - \mathbf{X}_1(\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{X}_1'\mathbf{X}_2 \\
&= \{\mathbf{I} - \mathbf{X}_1(\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{X}_1'\}\mathbf{X}_2,
\end{aligned}$$

which is the matrix of "residuals of $\mathbf{X}_2$ regressed on $\mathbf{X}_1$," is orthogonal to $\mathbf{X}_1$. [*Proof.* $\mathbf{X}_1'\mathbf{X}_{2\cdot 1} = \{\mathbf{X}_1' - \mathbf{X}_1'\mathbf{X}_1(\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{X}_1'\}\mathbf{X}_2 = \{\mathbf{0}\}\mathbf{X}_2 = \mathbf{0}$.] If we define $\mathbf{A} = (\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{X}_1'\mathbf{X}_2$ as the alias or bias matrix, we can also rewrite $\mathbf{X}_{2\cdot 1}$ as

$$\mathbf{X}_{2\cdot 1} = \mathbf{X}_2 - \mathbf{X}_1\mathbf{A},$$

whereupon model 1 can be rewritten in the form

$$\mathbf{Y} = \mathbf{X}_1(\boldsymbol{\beta}_1 + \mathbf{A}\boldsymbol{\beta}_2) + \mathbf{X}_{2\cdot 1}\boldsymbol{\beta}_2 + \boldsymbol{\epsilon},$$

where we have simply added and subtracted $\mathbf{X}_1\mathbf{A}\boldsymbol{\beta}_2$ and regrouped. We can set $\boldsymbol{\alpha}_1 = \boldsymbol{\beta}_1 + \mathbf{A}\boldsymbol{\beta}_2$ and thus rewrite model 1 as

$$\mathbf{Y} = \mathbf{X}_1\boldsymbol{\alpha}_1 + \mathbf{X}_{2\cdot 1}\boldsymbol{\beta}_2 + \boldsymbol{\epsilon},$$

where the two parts of the model are orthogonal to each other because $\mathbf{X}_1'\mathbf{X}_{2\cdot 1} = \mathbf{0}$. Let $\mathbf{a}_1$, $\mathbf{b}_2$ be the least squares estimates of $\boldsymbol{\alpha}_1$, $\boldsymbol{\beta}_2$ in model 1. Then the regression sum of squares S_1 for model 1 is the appropriate "$\mathbf{b}'\mathbf{X}'\mathbf{Y}$," that is,

$$\begin{aligned} S_1 &= (\mathbf{a}_1, \mathbf{b}_2)'[\mathbf{X}_1, \mathbf{X}_{2\cdot 1}]'\mathbf{Y} \\ &= \mathbf{Y}'[\mathbf{X}_1, \mathbf{X}_{2\cdot 1}]\begin{bmatrix} \mathbf{X}_1'\mathbf{X}_1 & \mathbf{X}_1'\mathbf{X}_{2\cdot 1} \\ \mathbf{X}_{2\cdot 1}'\mathbf{X}_1 & \mathbf{X}_{2\cdot 1}'\mathbf{X}_{2\cdot 1} \end{bmatrix}^{-1}\begin{bmatrix} \mathbf{X}_1' \\ \mathbf{X}_{2\cdot 1}' \end{bmatrix}\mathbf{Y}. \end{aligned}$$

Because of the orthogonality of $\mathbf{X}_1$ and $\mathbf{X}_{2\cdot 1}$, the off-diagonal terms of the inverse matrix vanish, and we can invert the diagonal terms individually to get

$$\begin{aligned} S_1 &= \mathbf{Y}'\mathbf{X}_1(\mathbf{X}_1'\mathbf{X}_1)^{-1}\mathbf{X}_1'\mathbf{Y} + \mathbf{Y}'\mathbf{X}_{2\cdot 1}(\mathbf{X}_{2\cdot 1}'\mathbf{X}_{2\cdot 1})^{-1}\mathbf{X}_{2\cdot 1}'\mathbf{Y} \\ &= S_2 + \mathbf{Y}'\mathbf{Q}\mathbf{Y}, \end{aligned}$$

say, where S_2 is clearly the appropriate regression sum of squares for model 2, and $\mathbf{Q}$ is defined as implied above. We can thus write the "extra sum of squares for b_2 given b_1" as

$$S_1 - S_2 = \mathbf{Y}'\mathbf{Q}\mathbf{Y}.$$

To get the expectation of this, we apply the general formula

$$E(\mathbf{Y}'\mathbf{Q}\mathbf{Y}) = \{E(\mathbf{Y})\}'\mathbf{Q}\{E(\mathbf{Y})\} + \text{trace}\{\mathbf{Q}\boldsymbol{\Sigma}\},$$

where $\boldsymbol{\Sigma} = \mathbf{V}(\mathbf{Y})$. For our situation, $\boldsymbol{\Sigma} = \mathbf{I}\sigma^2$ and $E(\mathbf{Y}) = \mathbf{X}_1\boldsymbol{\beta}_1 + \mathbf{X}_2\boldsymbol{\beta}_2$, so that

$$\begin{aligned} E(S_1 - S_2) = {} & (\boldsymbol{\beta}_1'\mathbf{X}_1' + \boldsymbol{\beta}_2'\mathbf{X}_2')\{\mathbf{X}_{2\cdot 1}(\mathbf{X}_{2\cdot 1}'\mathbf{X}_{2\cdot 1})^{-1}\mathbf{X}_{2\cdot 1}'\}(\mathbf{X}_1\boldsymbol{\beta}_1 + \mathbf{X}_2\boldsymbol{\beta}_2) \\ & + \text{trace}\{\mathbf{X}_{2\cdot 1}(\mathbf{X}_{2\cdot 1}'\mathbf{X}_{2\cdot 1})^{-1}\mathbf{X}_{2\cdot 1}'\mathbf{I}\sigma^2\}. \end{aligned}$$

Now $\mathbf{X}_1'\mathbf{X}_{2\cdot 1} = 0$, from above. Write $\mathbf{U} = \mathbf{X}_2'\mathbf{X}_{2\cdot 1}(\mathbf{X}_{2\cdot 1}'\mathbf{X}_{2\cdot 1})^{-1}\mathbf{X}_{2\cdot 1}'\mathbf{X}_2$. The trace term can be reduced using the fact that trace($\mathbf{ST}$) = trace($\mathbf{TS}$) for two matrices $\mathbf{S}$ and $\mathbf{T}$ that are conformable for both products; with $\mathbf{S} = \mathbf{X}_{2\cdot 1}$ and $\mathbf{T} = (\mathbf{X}_{2\cdot 1}'\mathbf{X}_{2\cdot 1})^{-1}\mathbf{X}_{2\cdot 1}'$, the trace term becomes σ^2 trace$(\mathbf{I}_{p-q}) = (p - q)\sigma^2$. Thus overall we obtain

$$E(S_1 - S_2) = \boldsymbol{\beta}_2'\mathbf{U}\boldsymbol{\beta}_2 + (p - q)\sigma^2.$$

It follows then that, *under the null hypothesis* $H_0: \boldsymbol{\beta}_2 = \mathbf{0}$, $E\{(S_1 - S_2)/(p - q)\} = \sigma^2$.

EXERCISES FOR CHAPTER 10

A. Eight experiments are to be done at the coded levels $(\pm 1, \pm 1)$ of two predictor variables X_1 and X_2. Two experimenters A and B suggest the following designs.

A: Take one observation at each of $(X_1, X_2) = (-1, -1)$ and $(1, 1)$ and take three observations at each of $(-1, 1)$ and $(1 - 1)$.

B: Take two observations at each of the four sites.

1. If a model $Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \epsilon$ is to be fitted by least squares but it is feared there may be some additional quadratic curvature expressed by the extra terms $\beta_{11}X_1^2 + \beta_{22}X_2^2 + \beta_{12}X_1X_2$, evaluate the anticipated biases in the estimated coefficients b_0, b_1, and b_2 for each design.
2. Suppose n_0 center points were added to each design. Would that affect your results? If yes, how?

Which design is better from the point of view of the variances of the estimated coefficients, $V(b_i)$?

B. Consider again the data of Exercise A. Suppose both experimenters agree that quadratic bias is unlikely and so can be ignored. However, one experimenter wants to omit X_1 from the model and fit only $Y = \beta_0 + \beta_2 X_2 + \epsilon$. What biases would the omission of β_1 cause in the estimates b_0, b_2 for designs A and B?

C. Values of a response Y are observed at six locations of a predictor variable X coded as -5, -3, -1, 1, 3 and 5. A model $Y = \beta_0 + \beta_1 X + \epsilon$ is to be fitted but there is fear that bias in the data, arising from a second-order (quadratic) effect $\beta_2 X^2$, might occur. How would the presence of β_2 bias the estimates b_0 and b_1?

D. Using the data in Exercise C, evaluate all the mean squares shown in the table of Section 10.2.

E. As in Exercises C and D, suppose values of $X = -5, -3, -1, 1, 3$, and 5 were to be employed to fit a straight line $Y = \alpha_0 + \alpha_1 X + \epsilon$. Consider the quadratic alternative $Y = \alpha_0 + \alpha_1 X + \alpha_2\{0.375(X^2 - 35/3)\} + \epsilon$. Are the estimates α_0 and α_1 from the straight line fit biased by α_2? (No.) What is the difference between adding the quadratic term above and the quadratic term $\beta_2 X^2$ in Exercise C?

F. In Section 10.2, show that:

1. E (lack of fit mean square) is as given.

2. E (residual mean square) $= \sigma^2$ *if* the model is correct, that is, *if* $\boldsymbol{\beta}_2 = 0$.

(Use the result in Section 10.3.)

G. Suppose we fit, by least squares, the model $E(Y) = \beta_0 + \beta_1 X$, but the model $E(Y) = \beta_0 + \beta_1 X + \beta/X$ is actually the true response function, for $X \geq 1$. If we use five observations of Y at X-values $X = 5, 8, 10, 20, 40$ to estimate β_0 and β_1 in the model actually fitted, what biases will be introduced into the estimates?