



## A Tutorial on the SWEEP Operator

James H. Goodnight

*The American Statistician*, Vol. 33, No. 3. (Aug., 1979), pp. 149-158.

Stable URL:

<http://links.jstor.org/sici?sici=0003-1305%28197908%2933%3A3%3C149%3AATOTSO%3E2.0.CO%3B2-M>

*The American Statistician* is currently published by American Statistical Association.

---

Your use of the JSTOR archive indicates your acceptance of JSTOR's Terms and Conditions of Use, available at <http://www.jstor.org/about/terms.html>. JSTOR's Terms and Conditions of Use provides, in part, that unless you have obtained prior permission, you may not download an entire issue of a journal or multiple copies of articles, and you may use content in the JSTOR archive only for your personal, non-commercial use.

Please contact the publisher regarding any further use of this work. Publisher contact information may be obtained at <http://www.jstor.org/journals/astata.html>.

Each copy of any part of a JSTOR transmission must contain the same copyright notice that appears on the screen or printed page of such transmission.

---

The JSTOR Archive is a trusted digital repository providing for long-term preservation and access to leading academic journals and scholarly literature from around the world. The Archive is supported by libraries, scholarly societies, publishers, and foundations. It is an initiative of JSTOR, a not-for-profit organization with a mission to help the scholarly community take advantage of advances in technology. For more information regarding JSTOR, please contact [support@jstor.org](mailto:support@jstor.org).

## A Tutorial on the SWEEP Operator

JAMES H. GOODNIGHT\*

The importance of the SWEEP operator in statistical computing is not so much that it is an inversion technique, but rather that it is a conceptual tool for understanding the least squares process. The SWEEP operator can be programmed to produce generalized inverses and create, as by-products, such items as the Forward Doolittle matrix, the Cholesky decomposition matrix, the Hermite canonical form matrix, the determinant of the original matrix, Type I sums of squares, the error sum of squares, a solution to the normal equations, and the general form of estimable functions. First, this tutorial describes the use of Gauss-Jordan elimination for least squares and continues with a description of a completely generalized sweep operator that computes and stores  $(X'X)^{-}$ ,  $(X'X)^{-}X'X$ ,  $(X'X)^{-}X'Y$ , and  $Y'Y - Y'X(X'X)^{-}X'Y$ , all in the space of a single upper triangular matrix.

**KEY WORDS:** Statistical computing; Sweep operator; Least squares; Regression analysis; Gaussian elimination.

### 1. INTRODUCTION

The SWEEP operator is perhaps the most versatile of all statistical operators. It can be adapted for use in

- Ordinary least squares (including multiple regression and the general linear model),
- Two-stage and three-stage least squares,
- Nonlinear least squares,
- Multivariate analysis of variance,
- All possible regressions,
- Regression by leaps and bounds,
- Stepwise regression, and
- Partial correlation.

As an instructional tool, the SWEEP operator's most important aspect is that each element of the matrix being operated on is readily identifiable and has statistical meaning. To understand the significance of each element of a matrix being swept and to understand the interrelationship between Gauss-Jordan elimination, the Forward Doolittle, Cholesky decomposition, Hermite canonical forms, and the SWEEP operator, this article starts at the basic level, Gauss-Jordan elimination.

Throughout the article the general linear model

$$Y = X\beta + e \quad (1.1)$$

will be used, where  $Y$  is an  $n \times 1$  vector of individual observations,  $X$  is an  $n \times k$  matrix of zeros and ones and/or continuous variables,  $\beta$  is a  $k \times 1$  vector of constant but unknown parameters, and  $e$  is distributed NID  $(0, \sigma^2)$ .

### 2. GAUSS-JORDAN ELIMINATION

Gauss-Jordan elimination may be used to solve directly the normal equations:

$$X'Xb = X'Y \quad (2.1)$$

that arise from (1.1). Gauss-Jordan elimination involves only two operations, multiplying equations by a constant and adding a multiple of one equation to another. The following simple example illustrates these points.

Given the system:

$$4b_1 + 2b_2 = 6$$

$$2b_1 + 6b_2 = 10$$

Step 1: Multiply the first equation by  $\frac{1}{4}$ :

$$b_1 + \frac{1}{2}b_2 = \frac{3}{2}$$

$$2b_1 + 6b_2 = 10$$

Step 2: Add  $-2$  times the first equation to the second:

$$b_1 + \frac{1}{2}b_2 = \frac{3}{2}$$

$$0b_1 + 5b_2 = 7$$

Step 3: Multiply the second equation by  $\frac{1}{5}$ :

$$b_1 + \frac{1}{2}b_2 = \frac{3}{2}$$

$$0b_1 + b_2 = \frac{7}{5}$$

Step 4: Add  $-\frac{1}{2}$  times the second equation to the first:

$$b_1 + 0b_2 = \frac{4}{5}$$

$$0b_1 + b_2 = \frac{7}{5}$$

This same sequence of operations can be carried out in a simple matrix tableau by using equivalent row operations (multiplying a row by a constant and adding a multiple of one row to another). For example,

Given the tableau:

$$\left[ \begin{array}{cc|c} 4 & 2 & 6 \\ 2 & 6 & 10 \end{array} \right]$$

Step 1: Multiply row 1 by  $\frac{1}{4}$

$$\left[ \begin{array}{cc|c} 1 & \frac{1}{2} & \frac{3}{2} \\ 2 & 6 & 10 \end{array} \right]$$

Step 2: Add  $-2$  times row 1 to row 2:

$$\left[ \begin{array}{cc|c} 1 & \frac{1}{2} & \frac{3}{2} \\ 0 & 5 & 7 \end{array} \right]$$

\* James H. Goodnight, SAS Institute, P.O. Box 10066, Raleigh, NC 27605.

Step 3: Multiply row 2 by  $1/5$ :

$$\left[ \begin{array}{cc|c} 1 & 1/2 & 3/2 \\ 0 & 1 & 7/5 \end{array} \right]$$

Step 4: Add  $-1/2$  times row 2 to row 1:

$$\left[ \begin{array}{cc|c} 1 & 0 & 4/5 \\ 0 & 1 & 7/5 \end{array} \right]$$

Thus, to solve full-rank regression equations, form the augmented matrix

$$[X'X | X'Y] \quad (2.2)$$

and use row operations to convert the left matrix to an identity. Once done, the right matrix will be the solution. In symbols:

$$[X'X | X'Y] \xrightarrow[\text{operations}]{\text{row}} [I | b]. \quad (2.3)$$

Note that  $(X'X)^{-1}$  need not be computed in order to solve the normal equations and that the entire process may be completed in-place on a computer.

An important aspect of performing row operations on a matrix is that it is equivalent to multiplying the matrix on the left by another matrix. Thus, the row operations performed in (2.3) are equivalent to multiplying (2.2) by  $(X'X)^{-1}$ .

In addition to computing the  $b$  values, the error sum of squares may also be simultaneously computed by augmenting (2.2) as follows:

$$\left[ \begin{array}{cc|c} X'X & X'Y \\ Y'X & Y'Y \end{array} \right]. \quad (2.4)$$

If (2.4) is multiplied on the left by

$$\left[ \begin{array}{cc|c} (X'X)^{-1} & 0 \\ -Y'X(X'X)^{-1} & I \end{array} \right], \quad (2.5)$$

then the resulting product is

$$\left[ \begin{array}{cc|c} I & (X'X)^{-1}X'Y \\ 0 & Y'Y - Y'X(X'X)^{-1}X'Y \end{array} \right]. \quad (2.6)$$

Because (2.6) was achieved by multiplying (2.4) on the left by matrix (2.5), (2.6) may also be achieved by performing row operations on (2.4). That is,

$$\left[ \begin{array}{cc|c} X'X & X'Y \\ Y'X & Y'Y \end{array} \right] \xrightarrow[\text{operations}]{\text{row}} \left[ \begin{array}{cc|c} I & (X'X)^{-1}X'Y \\ 0 & Y'Y - Y'X(X'X)^{-1}X'Y \end{array} \right]. \quad (2.7)$$

Because  $X'X$  is positive definite, the row operations used in (2.3) and (2.7) (see Wilkinson 1961) need consist of only a sequence of pivots on the diagonal elements of  $X'X$ . In fact, by restricting the row operations to pivots on the diagonal elements of  $X'X$ , much valuable statistical information may be obtained and an easily programmed algorithm is achieved. Since pivoting on a diagonal element "adjusts" the remaining matrix elements for the variable associated with the

diagonal element, it is helpful to define this operation as an operator called the ADJUST operator.

*Definition:* ADJUST( $K$ ) operator

The ADJUST( $K$ ) operator performs a pivot on element  $a_{kk}$  of a matrix  $A$  as follows:

Step 1: Set  $B = a_{kk}$ .

Step 2: Divide row  $k$  by  $B$ .

Step 3: For each other row  $i \neq k$ , set  $B = a_{ik}$  and subtract  $B$  times row  $k$  from row  $i$ .

Using the ADJUST operator on a simple example shows the amount of statistical information available through its use. For the regression model

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + e,$$

the augmented normal equations (2.4) are

$$A = \begin{bmatrix} N & \sum X_1 & \sum X_2 & \sum Y \\ \sum X_1 & \sum X_1^2 & \sum X_1 X_2 & \sum X_1 Y \\ \sum X_2 & \sum X_1 X_2 & \sum X_2^2 & \sum X_2 Y \\ \sum Y & \sum X_1 Y & \sum X_2 Y & \sum Y^2 \end{bmatrix}.$$

If an ADJUST(1) operation is performed on  $A$ , then

$$A_1 = \left[ \begin{array}{ccc|ccc} 1 & \bar{X}_1 & \bar{X}_2 & \bar{Y} & & \\ \hline 0 & \sum x_1^2 & \sum x_1 x_2 & \sum x_1 y & & \\ 0 & \sum x_1 x_2 & \sum x_2^2 & \sum x_2 y & & \\ 0 & \sum x_1 y & \sum x_2 y & \sum y^2 & & \end{array} \right].$$

The lower-right  $3 \times 3$  in  $A_1$  is the corrected sum of squares and cross-product (SS&CP) matrix. The upper-right  $1 \times 3$  matrix consists of  $b$  values for the submodels:  $X_1 = \beta'_0 + e'$ ,  $X_2 = \beta''_0 + e''$  and  $Y = \beta'''_0 + e'''$ . The diagonals in the lower-right  $3 \times 3$  correspond to the error sum of squares for these submodels. If an ADJUST(2) operation is performed on  $A_1$ , the following matrix results:

$$A_2 = \left[ \begin{array}{cc|cc} 1 & 0 & b'_0 & b''_0 \\ 0 & 1 & b'_1 & b''_1 \\ \hline 0 & 0 & \sum x_2^2.1 & \sum x_2 y.1 \\ 0 & 0 & \sum x_2 y.1 & \sum y^2.1 \end{array} \right].$$

In  $A_2$  the upper-right  $2 \times 2$  matrix contains the  $b$  values for the submodels:  $X_2 = \beta'_0 + \beta'_1 X_1 + e'$  and  $Y = \beta''_0 + \beta''_1 X_1 + e''$ . The lower-right  $2 \times 2$  matrix is the error SS&CP matrix for these two models. If an ADJUST(3) operation is performed on  $A_2$ , the following matrix results:

$$A_3 = \left[ \begin{array}{ccc|c} 1 & 0 & 0 & b_0 \\ 0 & 1 & 0 & b_1 \\ 0 & 0 & 1 & b_2 \\ \hline 0 & 0 & 0 & \sum y^2.1, 2 \end{array} \right].$$

This last adjustment completes the solution of the normal equations and yields the error sum of squares in the bottom-right position.

The Type I SS for each variable (see Barr, Goodnight, Sall, and Helwig 1976) is an important by-product of the ADJUST operator. If the augmented matrix

$A$  is  $p \times p$ , as in (2.4), then whenever ADJUST( $K$ ) is made, the  $Y'Y$  element  $a_{pp}$  is reduced by  $(a_{kp})^2/a_{kk}$ . Thus,  $R(X_k | \text{the other variables adjusted for})$  equals  $(a_{kp})^2/a_{kk}$ . An auxiliary vector can be used to store the Type I SS before each use of ADJUST.

As noted before, after each use of ADJUST, the diagonals not yet adjusted represent error sums of squares for submodels among the independent variables. Suppose that a matrix  $A$ , as in (2.4), has been adjusted for 1, 2, . . . ,  $K - 1$ . Then  $a_{kk}$  is the error SS (ESS) for the model

$$X_k = \beta_0 + \beta_1 X_1 + \dots + \beta_{k-1} X_{k-1} + e.$$

The  $R^2$  value for this model is

$$R_k^2 = (CSS_k - a_{kk})/CSS_k$$

where  $CSS_k$  is the corrected SS for  $X_k$ .

The  $R_k^2$  value, or the tolerance value defined to be  $1 - R_k^2$ , provides an invaluable singularity check. For instance, if  $R_k^2 > .9999$ , then  $X_k$  is "statistically," at least, a linear combination of the preceding  $X$ 's, and the elements in column  $k$  associated with previously adjusted variables define the linear combination. The interested reader is referred to Hemmerle (1967) for additional discussion and numerical examples of Gauss-Jordan elimination and to Frane (1977) and Berk (1977) for additional discussion on the use of the tolerance value for checking for singularities. Section 10 of this article also discusses the tolerance check in greater detail.

In the past few years, numerous articles have been written on the numerical accuracy and stability of regression solutions obtained by using Gaussian elimination. Beaton, Rubin, and Barone (1976, 1977) reference some of the more important articles and conclude that, in many cases, the attempt to estimate regression coefficients in highly collinear problems cannot be justified statistically. When data are highly collinear, then the lab technician recording the data may have more effect on the solution than does the technique used to achieve it. One of the most obvious, yet overlooked, facts about accuracy is that when Gauss-Jordan elimination is used, the mantissa length on the machine must at least be able to contain the largest element of  $X'X$  (see Golub and Klema 1978). Any program written in single precision is obviously headed for trouble when more than four significant digits appear in the input data. No least squares programs should be written in single precision when Gauss-Jordan elimination is used. For the very large class of least squares problems that involve only  $X$ 's with zeros and ones and whose largest  $X'X$  element is equal to the number of observations, Gauss-Jordan elimination programmed in double precision is more than adequate with respect to accuracy.

### 3. OTHER ADJUST USES

For multivariate linear models in which several dependent variables have the same set of independent

variables, the  $b$  values and the error SS&CP matrix may be obtained simultaneously. That is,

$$\left[ \begin{array}{c|c} X'X & X'Y \\ \hline Y'X & Y'Y \end{array} \right] \xrightarrow[\text{columns of } X'X]{\text{ADJUST on}} \left[ \begin{array}{c|c} I & (X'X)^{-1}X'Y \\ \hline 0 & Y'Y - Y'X(X'X)^{-1}X'Y \end{array} \right]. \quad (3.1)$$

This is equivalent to the univariate case, except that  $Y$  has dimensions  $N \times p$  instead of  $N \times 1$ .

Partial correlation coefficients for two sets of variables,  $X_1(N \times p)$  and  $X_2(N \times q)$ , may be obtained by using the ADJUST operator. If the correlations among the  $X_2$ 's are needed after their adjustment for  $X_1$ , then proceed as follows (assume  $X_1$  contains a column of ones):

$$\left[ \begin{array}{c|c} X_1'X_1 & X_1'X_2 \\ \hline X_2'X_1 & X_2'X_2 \end{array} \right] \xrightarrow[\text{columns of } X_1'X_1]{\text{ADJUST for}} \left[ \begin{array}{c|c} I & (X_1'X_1)^{-1}X_1'X_2 \\ \hline 0 & X_2'X_2 - X_2'X_1(X_1'X_1)^{-1}X_1'X_2 \end{array} \right]. \quad (3.2)$$

Next, divide each element of  $X_2'X_2 - X_2'X_1(X_1'X_1)^{-1}X_1'X_2$  by the square root of the two associated diagonals. The partial correlation matrix is now complete.

### 4. THE FORWARD DOOLITTLE

The basic Doolittle method (see Steel and Torrie 1960) was introduced in 1878 while Doolittle was an engineer with the U.S. Coast and Geodetic Survey. Doolittle popularized and slightly restructured Gaussian elimination to fit the statistician's needs. The method is now referred to as the abbreviated Doolittle and consists of two parts. The first part, the Forward Doolittle, maps the sum of squares and cross-products matrix into an upper triangular matrix. The second part, the Backward solution, computes the regression coefficients and the inverse matrix.

Symbolically, the Forward Doolittle is used to map any symmetric positive definite matrix  $C$  into an upper triangular matrix  $A$ :

$$C = \begin{bmatrix} C_{11} & C_{12} & C_{13} \\ C_{21} & C_{22} & C_{23} \\ C_{31} & C_{32} & C_{33} \end{bmatrix} \xrightarrow[\text{operations}]{\text{row}} \begin{bmatrix} C_{11} & C_{12} & C_{13} \\ 0 & C_{22.1} & C_{23.1} \\ 0 & 0 & C_{33.12} \end{bmatrix} = A.$$

The Forward Doolittle matrix is constructed by adding multiples of the first row of the matrix to all following rows such that zeros are introduced below the diagonal in column 1. Multiples of row 2 are then added to all following rows to introduce zeros below the diagonal in column 2, and so on. The tolerance check discussed in Section 3 should be used to check for rank deficiency. Note that if the ADJUST operator had been applied to the  $C$  matrix and if the adjustments were made se-

quentially ( $k = 1, 2, 3, \dots$ ), then before the adjustment for row  $k$ , row  $k$  of  $C$  is equal to row  $k$  of  $A$ .

When only the adjusted SS&CP matrix is needed, as in (3.1) and (3.2), the Forward Doolittle affords a faster method of computing than the ADJUST operator. An example is the computation of

$$SS(HO: L\beta = 0) = (Lb)'(L(X'X)^{-1}L')^{-1}(Lb)$$

where  $L\beta$  is estimable and  $b$  is any solution to (1.1). If the following matrix is formed

$$\left[ \begin{array}{c|c} L(X'X)^{-1}L' & Lb \\ \hline (Lb)' & 0 \end{array} \right]$$

and a Forward Doolittle is performed on the diagonals of the upper-left matrix, then the lower-right matrix is transformed into

$$0 - (Lb)'(L(X'X)^{-1}L')^{-1}(Lb),$$

the negative of which is  $SS(HO: L\beta = 0)$ .

## 5. FACTORING A SYMMETRIC POSITIVE DEFINITE MATRIX

If the symmetric positive definite matrix  $C$  has been mapped as follows:

$$C \xrightarrow[\text{Doolittle}]{\text{Forward}} A$$

and if each row of  $A$  is divided by its diagonal to produce a matrix  $B$ , then

$$B'A = C.$$

Furthermore, if each row of  $A$  is divided by the square root of its diagonal to produce a matrix  $U$ , then

$$U'U = C.$$

The matrix  $U$  is called the Cholesky decomposition of  $C$  (see Isaacson and Keller 1966).

## 6. THE DETERMINANT OF A SYMMETRIC POSITIVE DEFINITE MATRIX

Having mapped  $C$  into  $A$  by the Forward Doolittle and created  $B$  by dividing each row of  $A$  by its diagonal, then

$$\begin{bmatrix} C_{11} & C_{12} & C_{13} \\ C_{21} & C_{22} & C_{23} \\ C_{31} & C_{32} & C_{33} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ b_{12} & 1 & 0 \\ b_{13} & b_{23} & 1 \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ 0 & a_{22} & a_{23} \\ 0 & 0 & a_{33} \end{bmatrix}$$

That is,  $C = B'A$ . Therefore,

$$\begin{aligned} |C| &= |B'| |A| \\ &= 1 \cdot \prod_i a_{ii}. \end{aligned}$$

By the basic permuted products-summation definition, the determinant of an upper or lower triangular matrix is always the product of its diagonal elements.

Therefore, the determinant is easily a by-product of both the Forward Doolittle and the ADJUST operator.

## 7. FINDING THE INVERSE

The inverse of a symmetric positive definite matrix  $A$  may be found by augmenting an identity matrix to the right of  $A$  and then using the ADJUST operator on the diagonals of  $A$ . Symbolically,

$$[A | I] \xrightarrow[\text{diagonals}]{\text{ADJUST } A} [I | A^{-1}]. \quad (7.1)$$

Because repetitive use of the ADJUST operator is equivalent to multiplication on the left by some matrix, (7.1) is equivalent to (7.2)

$$A^{-1}[A | I] = [I | A^{-1}]. \quad (7.2)$$

Because the original identity matrix keeps count of the row operations being performed, this technique has been referred to as the method of counters.

This process is also reversible because

$$A[I | A^{-1}] = [A | I].$$

Thus,

$$[I | A^{-1}] \xrightarrow[\text{diagonals}]{\text{ADJUST } A^{-1}} [A | I].$$

## 8. OBTAINING $b$ VALUES, ERROR SS, AND INVERSE

By forming the following augmented matrix and adjusting the columns associated with  $X'X$ , the regression coefficients, ESS, and inverse may be computed simultaneously. For example,

$$\left[ \begin{array}{c|c|c} X'X & X'Y & I \\ \hline Y'X & Y'Y & 0 \end{array} \right] \xrightarrow[X'X \text{ columns}]{\text{ADJUST}} \left[ \begin{array}{c|c|c} I & b & (X'X)^{-1} \\ \hline 0 & \text{ESS} & -b' \end{array} \right].$$

This is equivalent to the matrix multiplication,

$$\begin{bmatrix} (X'X)^{-1} & 0 \\ -Y'X(X'X)^{-1} & I \end{bmatrix} \begin{bmatrix} X'X & X'Y & I \\ Y'X & Y'Y & 0 \end{bmatrix} = \begin{bmatrix} I & b & (X'X)^{-1} \\ 0 & \text{ESS} & -b' \end{bmatrix}.$$

Also note that

$$\left[ \begin{array}{c|c|c} I & b & (X'X)^{-1} \\ \hline 0 & \text{ESS} & -b' \end{array} \right] \xrightarrow[(X'X)^{-1} \text{ columns}]{\text{readjust}} \left[ \begin{array}{c|c|c} X'X & X'Y & I \\ \hline Y'X & Y'Y & 0 \end{array} \right].$$

The reversibility of adjustments allows you to adjust any of the original columns of  $X'X$  and thus "enter" that variable into the model and also to readjust any column in the  $(X'X)^{-1}$  area and thus "remove" that variable from the model. For example, consider the following data:

$X_0$	$X_1$	$X_2$	$Y$
1	1	1	1
1	2	1	3
1	3	1	3
1	1	-1	2
1	2	-1	2
1	3	-1	1

$$\text{Form} \left[ \begin{array}{c|c|c} X'X & X'Y & I \\ \hline Y'X & Y'Y & 0 \end{array} \right]$$

$$\begin{array}{l} \text{Step 0} \\ \text{Form} \\ \text{Matrix} \end{array} \begin{array}{c} \begin{array}{c} X_0 \quad X_1 \quad X_2 \quad b \end{array} \\ \begin{array}{c} X_0 \quad X_1 \quad X_2 \end{array} \end{array} \begin{bmatrix} 6 & 12 & 0 & 12 & 1 & 0 & 0 \\ 12 & 28 & 0 & 25 & 0 & 1 & 0 \\ 0 & 0 & 6 & 1 & 0 & 0 & 1 \\ 12 & 25 & 2 & 28 & 0 & 0 & 0 \end{bmatrix} \quad (8.1)$$

$$\begin{array}{l} \text{Step 1} \\ \text{Enter } X_0 \end{array} \begin{array}{c} \begin{array}{c} X_0 \quad X_1 \quad X_2 \quad b \end{array} \\ \begin{array}{c} X_0 \quad X_1 \quad X_2 \end{array} \end{array} \begin{bmatrix} 1 & 2 & 0 & 2 & 1/6 & 0 & 0 \\ 0 & 4 & 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 6 & 2 & 0 & 0 & 1 \\ 0 & 1 & 2 & 4 & -2 & 0 & 0 \end{bmatrix} \quad (8.2)$$

$$\begin{array}{l} \text{Step 2} \\ \text{Enter } X_1 \end{array} \begin{array}{c} \begin{array}{c} X_0 \quad X_1 \quad X_2 \quad b \end{array} \\ \begin{array}{c} X_0 \quad X_1 \quad X_2 \end{array} \end{array} \begin{bmatrix} 1 & 0 & 0 & 3/2 & 7/6 & -1/2 & 0 \\ 0 & 1 & 0 & 1/4 & -1/2 & 1/4 & 0 \\ 0 & 0 & 6 & 2 & 0 & 0 & 1 \\ 0 & 0 & 2 & 15/4 & -3/2 & -1/4 & 0 \end{bmatrix} \quad (8.3)$$

$$\begin{array}{l} \text{Step 3} \\ \text{Enter } X_2 \end{array} \begin{array}{c} \begin{array}{c} X_0 \quad X_1 \quad X_2 \quad b \end{array} \\ \begin{array}{c} X_0 \quad X_1 \quad X_2 \end{array} \end{array} \begin{bmatrix} 1 & 0 & 0 & 3/2 & 7/6 & -1/2 & 0 \\ 0 & 1 & 0 & 1/4 & -1/2 & 1/4 & 0 \\ 0 & 0 & 1 & 1/3 & 0 & 0 & 1/6 \\ 0 & 0 & 0 & 37/12 & -3/2 & -1/4 & -1/3 \end{bmatrix} \quad (8.4)$$

$$\begin{array}{l} \text{Step 4} \\ \text{Remove } X_1 \end{array} \begin{array}{c} \begin{array}{c} X_0 \quad X_1 \quad X_2 \quad b \end{array} \\ \begin{array}{c} X_0 \quad X_1 \quad X_2 \end{array} \end{array} \begin{bmatrix} 1 & 2 & 0 & 2 & 1/6 & 0 & 0 \\ 0 & 4 & 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & 1/3 & 0 & 0 & 1/6 \\ 0 & 1 & 0 & 10/3 & -2 & 0 & -1/3 \end{bmatrix} \quad (8.5)$$

$$\begin{array}{l} \text{Step 5} \\ \text{Remove } X_2 \end{array} \begin{array}{c} \begin{array}{c} X_0 \quad X_1 \quad X_2 \quad b \end{array} \\ \begin{array}{c} X_0 \quad X_1 \quad X_2 \end{array} \end{array} \begin{bmatrix} 1 & 2 & 0 & 2 & 1/6 & 0 & 0 \\ 0 & 4 & 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 6 & 2 & 0 & 0 & 1 \\ 0 & 1 & 2 & 4 & -2 & 0 & 0 \end{bmatrix} \quad (8.6)$$

$$\begin{array}{l} \text{Step 6} \\ \text{Remove } X_0 \end{array} \begin{array}{c} \begin{array}{c} X_0 \quad X_1 \quad X_2 \quad b \end{array} \\ \begin{array}{c} X_0 \quad X_1 \quad X_2 \end{array} \end{array} \begin{bmatrix} 6 & 12 & 0 & 12 & 1 & 0 & 0 \\ 12 & 28 & 0 & 25 & 0 & 1 & 0 \\ 0 & 0 & 6 & 2 & 0 & 0 & 1 \\ 12 & 25 & 2 & 28 & 0 & 0 & 0 \end{bmatrix} \quad (8.7)$$

These tableaux represent the following models with respect to  $Y$ :

Step	Model	$b$ Values	ESS
0	$Y = 0$		28
1	$Y = b_0$	2	4
2	$Y = b_0 + b_1X_1$	$3/2, 1/4$	$15/4$
3	$Y = b_0 + b_1X_1 + b_2X_2$	$3/2, 1/4, 1/3$	$37/12$
4	$Y = b_0 + b_2X_2$	$2, 1/3$	$10/3$
5	$Y = b_0$	2	4
6	$Y = 0$		28

Observing the tableau at Step 3 (the full model), note that if  $X_1$  is removed, the ESS will increase by  $(1/4 \times 1/4)/1/4 = 1/4 = \text{Type II SS due to } X_1$ . If  $X_2$  is removed from

the full model, the ESS will increase by  $(1/3 \times 1/3)/1/6 = 2/3 = \text{Type II SS due to } X_2$ . The Type II SS due to  $X_i$  (given the full model) is always  $(b_i)^2/C_{ii}$ , where  $C_{ii}$  is  $i$ th diagonal element of  $(X'X)^{-1}$ . The Type II SS corresponds to the SS due to the hypothesis that  $\beta_i = 0$ . The reversibility of adjustments demonstrated forms the basis for stepwise regression.

## 9. THE SWEEP OPERATOR

The SWEEP operator is a modification of the ADJUST operator that reduces the amount of core needed

to compute the  $b$  values, ESS, and  $(X'X)^{-1}$ . Whereas the ADJUST operator performs the in-place mapping,

$$\left[ \begin{array}{c|c|c} X'X & X'Y & I \\ \hline Y'X & Y'Y & 0 \end{array} \right] \xrightarrow[\text{X'X columns}]{\text{ADJUST}} \left[ \begin{array}{c|c|c} I & b & (X'X)^{-1} \\ \hline 0 & \text{ESS} & -b' \end{array} \right],$$

the SWEEP operator performs the in-place mapping,

$$\left[ \begin{array}{c|c} X'X & X'Y \\ \hline Y'X & Y'Y \end{array} \right] \xrightarrow[\text{X'X columns}]{\text{SWEEP}} \left[ \begin{array}{c|c} (X'X)^{-1} & b \\ \hline -b' & \text{ESS} \end{array} \right].$$

One of the first references to sweep operations may be found in Ralston (1960), but the term *sweep operator* was coined by Beaton (1964).

By observing tableaus (8.1) through (8.7), note that whenever a variable is in the model, its associated  $X'X$  column is an identity column; whenever a variable is not in the model, its associated column in the original identity matrix remains unchanged. The SWEEP operator takes advantage of these features: After adjusting the tableau for a particular variable, the SWEEP operator replaces the identity column just created by the associated column in the original identity matrix, which has now been modified. By observing what happens to the  $i$ th identity column when variable  $X_i$  is entered, the ADJUST operator can be modified to a SWEEP operator. When variable  $X_k$  is entered, row  $k$  is multiplied by  $1/a_{kk}$ . Therefore, its identity column will have  $1/a_{kk}$  in the  $k$ th row.

To zero out the remaining elements in column  $k$ ,  $-a_{ik} \cdot \text{row } k$  is added to all other rows ( $i \neq k$ ). Since the identity column has zeros in all positions other than row  $k$ , the  $i$ th row of the identity column becomes

$-a_{ik}/a_{kk}$  ( $i \neq k$ ). With this in mind, the SWEEP operator is defined as follows:

*Definition: SWEEP ( $k$ ) operator*

Given an originally symmetric positive definite matrix  $A$ , SWEEP( $k$ ) modifies the current matrix  $A$  as follows:

Step 1: Let  $D = a_{kk}$ .

Step 2: Divide row  $k$  by  $D$ .

Step 3: For every other row  $i \neq k$ , let  $B = a_{ik}$ . Subtract  $B \times \text{row } k$  from row  $i$ . Set  $a_{ik} = -B/D$ .

Step 4: Set  $a_{kk} = 1/D$ .

The reversibility of the SWEEP operator is apparent because it is only a modification of the ADJUST operator. A useful exercise is to use the SWEEP operator on the left-most  $4 \times 4$  matrix in tableau (8.1) to compute the equivalent sweep tableaus associated with (8.2) through (8.7).

Although the amount of core needed to compute the  $b$  values, SS, and  $(X'X)^{-1}$  has been reduced by using SWEEP, none of the by-product information has been lost; the Types I and II SS and the determinant of  $X'X$  may still be computed; the singularity check is still available; and all submodel information is present. For example, let

$$A = \left[ \begin{array}{c|c|c} X'_1X_1 & X'_1X_2 & X'_1Y \\ \hline X'_2X_1 & X'_2X_2 & X'_2Y \\ \hline Y'X_1 & Y'X_2 & Y'Y \end{array} \right]$$

Sweeping  $A$  on the columns associated with  $X'_1X_1$  yields

$$\left[ \begin{array}{c|c|c} (X'_1X_1)^{-1} & (X'_1X_1)^{-1}X'_1X_2 & (X'_1X_1)^{-1}X'_1Y \\ \hline -X'_2X_1(X'_1X_1)^{-1} & X'_2M_1X_2 & X'_2M_1Y \\ \hline -Y'X_1(X'_1X_1)^{-1} & Y'M_1X_2 & Y'M_1Y \end{array} \right], \quad (9.1)$$

where  $M_1 = I - X_1(X'_1X_1)^{-1}X'_1$ . The regression coefficients for the submodels Model  $X_2 = X_1$  and Model  $Y = X_1$  are clearly available.  $X'_2M_1X_2$  is the error SSCP for the first model, and  $Y'M_1Y$  is the error SSCP for the second model.

By observing their symmetry properties, the ADJUST operator and the Forward Doolittle operator are easily programmed to operate only on the upper triangular matrix. The SWEEP operator is also easily modified to operate on just the upper triangular portion of the matrix.

The amount of time it takes to compute  $(X'X)^{-1}$ ,  $b$  values, and ESS using the SWEEP operator is generally only a fraction of the time it takes to form the sum of squares and cross-product matrix. If only the upper triangular portion of the sum of squares and cross-product matrix is formed as the data are read, then one SWEEP operation (modified to operate on the upper triangle) takes about the same amount of CPU time as does the reading and accumulation of two observations. This can be verified by counting the

number of multiplications and additions that are performed. Thus, the approximate CPU time ratio of inversion to building the  $X'X$  is approximately  $2k/N$ , where  $k$  is the total number of independent variables and  $N$  is the number of observations. Because  $N$  is usually much larger than  $k$ , inversion represents only a fraction of the cost of regression analysis. Additional references to the SWEEP operator may be found in Seber (1977).

## 10. COMPUTING GENERALIZED INVERSES

A large family of models, characterized by (1.1), is overparameterized. Linear dependencies are known to exist among the columns of the  $X$  matrix. For some models, the dependencies are easily predictable. For others, the interchanging of effects (putting interactions before main effects), the absence of a cell, or the inclusion of a covariable may bring about un-

expected dependencies. Through use of the tolerance check, the ADJUST operator, the Forward Doolittle, and the SWEEP operator can detect dependencies among the columns of the  $X$  matrix. In this section, the SWEEP operator is modified to produce a generalized inverse and the corresponding particular solution whenever a dependency is encountered. Additional references to generalized inverses may be found in Pringle and Rayner (1971) and Ben-Israel and Greville (1974).

Initially, assume that the  $X$  matrix can be partitioned—for example,  $X = [X_1 | X_2]$ —such that the columns of  $X_1$  are linearly independent, and each column of  $X_2$  is a linear combination of the columns of  $X_1$ . This implies that

$$\begin{aligned} X_2 &= X_1 L && \text{(by definition)} \\ L &= (X_1' X_1)^{-1} X_1' X_2 && \text{(regress } X_2 \text{ on } X_1) \\ X_2' X_2 - X_2' X_1 (X_1' X_1)^{-1} X_1' X_2 &= 0 && \text{(error SS\&CP).} \end{aligned}$$

The  $X'X$  matrix

$$\begin{bmatrix} X_1' X_1 & X_1' X_2 \\ X_2' X_1 & X_2' X_2 \end{bmatrix}$$

has two particular generalized inverses that are easily constructed through use of the SWEEP operator. The first, a  $g_1$  inverse ( $AA^{g_1}A = A$ ) for  $X'X$ , is

$$\left[ \begin{array}{c|c} (X_1' X_1)^{-1} & (X_1' X_1)^{-1} X_1' X_2 \\ \hline -X_2' X_1 (X_1' X_1)^{-1} & 0 \end{array} \right].$$

This matrix results from SWEEPing  $X'X$  on the columns associated with  $X_1' X_1$ . If the full augmented tableau

$$\left[ \begin{array}{cc|c} X_1' X_1 & X_1' X_2 & X_1' Y \\ X_2' X_1 & X_2' X_2 & X_2' Y \\ \hline Y' X_1 & Y' X_2 & Y' Y \end{array} \right] \quad (10.1)$$

is swept on the columns associated with  $X_1' X_1$ , the result is

$$\left[ \begin{array}{cc|c} (X_1' X_1)^{-1} & (X_1' X_1)^{-1} X_1' X_2 & (X_1' X_1)^{-1} X_1' Y \\ -X_2' X_1 (X_1' X_1)^{-1} & 0 & 0 \\ \hline -Y' X_1 (X_1' X_1)^{-1} & 0 & Y' Y - Y' X_1 (X_1' X_1)^{-1} X_1' Y \end{array} \right]. \quad (10.2)$$

Thus, sweeping on the columns of  $X_1' X_1$  yields a  $g_1$  inverse and the appropriate adjusted  $Y'Y$ . The  $b$  values,  $b_1 = (X_1' X_1)^{-1} X_1' Y$  and  $b_2 = 0$ , however, do not correspond to the  $b$  values computed by using the  $g_1$  inverse. For example,

$$\begin{aligned} \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} &= \begin{bmatrix} (X_1' X_1)^{-1} & (X_1' X_1)^{-1} X_1' X_2 \\ -X_2' X_1 (X_1' X_1)^{-1} & 0 \end{bmatrix} \begin{bmatrix} X_1' Y \\ X_2' Y \end{bmatrix} \\ b_1 &= (X_1' X_1)^{-1} X_1' Y + (X_1' X_1)^{-1} X_1' X_2 X_2' Y \\ &= (X_1' X_1)^{-1} X_1' Y + L X_2' Y \\ b_2 &= -X_2' X_1 (X_1' X_1)^{-1} X_1' Y \\ &= -L' X_1' Y \\ &= -X_2' Y. \end{aligned}$$

Although  $b_1 = (X_1' X_1)^{-1} X_1' Y$  and  $b_2 = 0$  is a solution to the normal equations, this particular solution does not equal  $(X'X)^{g_1} X'Y$ . Another disadvantage of com-

puting a  $g_1$  inverse is that additional work is necessary to compute the variance of the particular solution because

$$\text{var}((X'X)^{g_1} X'Y) = (X'X)^{g_1} X'X (X'X)^{g_1} \sigma^2.$$

On the other hand, a  $g_2$  inverse ( $AA^{g_2}A = A$ , and  $A^{g_2}AA^{g_2} = A^{g_2}$ ) of  $X'X$  has the property that

$$\text{var}((X'X)^{g_2} X'Y) = (X'X)^{g_2} \sigma^2.$$

It is easily verified that

$$\begin{bmatrix} (X_1' X_1)^{-1} & 0 \\ 0 & 0 \end{bmatrix}$$

is a  $g_2$  inverse of  $X'X$ . If the full augmented tableau (10.1) is swept on the columns associated with  $X_1' X_1$ , then the resulting tableau is (10.2).

Introducing zeros in the two submatrices adjoining  $(X_1' X_1)^{-1}$  in (10.2) yields

$$\left[ \begin{array}{cc|c} (X_1' X_1)^{-1} & 0 & (X_1' X_1)^{-1} X_1' Y \\ 0 & 0 & 0 \\ \hline -Y' X_1 (X_1' X_1)^{-1} & 0 & Y' Y - Y' X_1 (X_1' X_1)^{-1} X_1' Y \end{array} \right]. \quad (10.3)$$

This tableau contains  $(X'X)^{g_2}$  and the adjusted  $Y'Y$ . The  $b$  values  $b_1 = (X_1' X_1)^{-1} X_1' Y$  and  $b_2 = 0$  are equivalent to  $(X'X)^{g_2} X'Y$ , and therefore  $\text{var}(b) = (X'X)^{g_2} \sigma^2$ . If the  $g_2$  inverse of (10.3) is employed, then the expected values of  $b_1$  and  $b_2$  are

$$E(b_1) = E((X_1' X_1)^{-1} X_1' Y) = \beta_1 + (X_1' X_1)^{-1} X_1' X_2 \beta_2$$

and

$$E(b_2) = 0.$$

If the submatrix containing  $(X_1' X_1)^{-1} X_1' X_2$  is saved after sweeping on the columns of  $X_1' X_1$ , this matrix may be used to compute all possible solutions to the normal equations because (for  $Z$  arbitrary)



$$\begin{aligned}
b^* &= (X'X)^{g_2}X'Y + (I - (X'X)^{g_2}X'X)Z \\
&= \begin{bmatrix} (X'_1X_1)^{-1}X'_1Y \\ 0 \end{bmatrix} \\
&\quad + \begin{bmatrix} 0 & -(X'_1X_1)^{-1}X'_1X_2 \\ 0 & I \end{bmatrix} \begin{bmatrix} Z_1 \\ Z_2 \end{bmatrix}. \quad (10.4)
\end{aligned}$$

Therefore,

$$b_1^* = (X'_1X_1)^{-1}X'_1Y - (X'_1X_1)^{-1}X'_1X_2Z_2 = b_1 - LZ_2$$

and

$$b_2^* = Z_2.$$

The foregoing discussion was simplified by assuming that the  $X$ 's were grouped, that  $X_1$  is of full-column rank, and that  $X_2 = X_1L$ . Naturally, this seldom happens. As it turns out, however, the SWEEP operator can be modified to handle the situation in which the linearly independent columns of  $X$  are not all grouped.

For model (1.1), if you know which columns of  $X$  form a linearly independent basis, then an index matrix  $M$  (an identity matrix with columns permuted) can be formed to rearrange the  $X$ 's, and  $M'$  can be used to rearrange the  $\beta$ 's. In other words, since  $MM' = I$ ,

$$\begin{aligned}
Y &= X\beta + e \\
&= XI\beta + e \\
&= XMM'\beta + e.
\end{aligned}$$

Let  $Z = XM$  and  $\gamma = M'\beta$ , then

$$Y = Z\gamma + e$$

where  $Z = [Z_1|Z_2]$ , with the columns of  $Z_1$  linearly independent and  $Z_2 = Z_1L$ . Thus,

$$(Z'Z)^{g_2} = \begin{bmatrix} (Z'_1Z_1)^{-1} & 0 \\ 0 & 0 \end{bmatrix}$$

and  $\hat{\gamma} = (Z'Z)^{g_2}Z'Y$ .

Because

$$(Z'Z)^{g_2} = (M'X'XM)^{g_2} = M'(X'X)^{g_2}M,$$

then

$$(X'X)^{g_2} = M(Z'Z)^{g_2}M' \quad \text{and} \quad \hat{\beta} = M\hat{\gamma}. \quad (10.5)$$

In essence, this rearranging process selects a maximum rank subset of elements from  $X'X$ , inverts the resulting matrix, puts the inverted subset of elements back into their original positions, and zeros out the remaining elements to form  $(X'X)^{g_2}$ . The SWEEP operator can achieve the same results without rearranging rows and columns. When a dependency is encountered, say for variable  $K$ , the SWEEP operator should set the  $K$ th row and column to zero and proceed. A  $g_2$  inverse and corresponding solution will result. Once a row and column have been zeroed, however, the generalized SWEEP is no longer reversible. The critical information that defines that variable's dependency has been set to zero. With these points in mind, the G2SWEEP operator is defined as follows:

*Definition:* G2SWEEP operator

Given an originally symmetric positive definite or symmetric positive semidefinite matrix  $A$ , as in (10.1),

which has not been SWEPT on column  $K$ , G2SWEEP ( $K$ ) modifies the current matrix  $A$  as follows:

Step 1: Let  $D = a_{kk}$ . If  $D$  is less than  $D \text{ MIN}_k$ , then set row and column  $k$  to zero and stop at this step. Otherwise proceed.

Step 2: Divide row  $k$  by  $D$ .

Step 3: For every other row  $i \neq k$ , let  $B = a_{ik}$ . Subtract  $B \times \text{row } k$  from row  $i$ . Set  $a_{ik} = -B/D$ .

Step 4: Set  $a_{kk} = 1/D$ .

As stated before, the G2SWEEP operator should be applied only once to any given column of  $A$  (although the order is unimportant), since information needed may have been set to zero. In addition,  $a_{kk}$  once swept may be legitimately less than  $D \text{ MIN}_k$ .

The  $D \text{ MIN}_k$  values used in the G2SWEEP operator are functions of the TOLERANCE value and either the corrected SS (CSS) or uncorrected SS (USS) for variable  $k$ . If no intercept is used in the model then,

$$\begin{aligned}
D \text{ MIN}_k &= \text{Tolerance if USS} = 0, \\
&= \text{Tolerance} * \text{USS otherwise.}
\end{aligned}$$

If an intercept is used in the model then,

$$\begin{aligned}
D \text{ MIN}_k &= \text{Tolerance if } X_k \text{ does not vary or has} \\
&\quad \text{a computed CSS} < = 0. \\
&= \text{Tolerance} * \text{CSS otherwise.}
\end{aligned}$$

While one is checking to see if  $X_k$  varies (has more than two distinct values), if the smallest and largest nonzero absolute values of  $X_k$  are saved, the ratio of the largest to smallest nonzero absolute values of  $X_k$  can be computed. If the ratio is greater than  $1E7$  (or  $1E8$ ), then the computed  $X'X$  matrix in double precision is probably incorrect.

Establishing the value to use for tolerance is not a simple task because it involves (as does the comparison of two means) compromising between a Type I and Type II error. The major difference between choosing a tolerance and an  $\alpha$  level is the lack of distributional theory. Too large a tolerance may declare variables dependent on others when they in fact are not. Too small a tolerance may let dependencies go unchecked. For variables that take on only zero or one values,  $(1 - R^2)$  values in the range  $1E-12$  to  $1E-14$  are quite common when dependencies occur. Fifth- and sixth-degree polynomials may exhibit  $(1 - R^2)$  values as small as  $1E-8$  even when they are linearly independent. Thus, tolerance values in the range of  $1E-8$  to  $1E-12$  seem appropriate when one is looking for dependencies.

## 11. THE UPPER TRIANGULAR G2SWEEP

The time it takes to perform a sweep operation may be reduced by approximately one-half by taking into account the symmetry properties of the sweep tableau (Schatzoff, Tsao, and Fienberg 1968). The amount of core needed may also be reduced by almost one-half

by saving and operating on only the upper triangular portion of the tableau. Because operating on the upper triangular tableau, stored in a one-dimensional array, is an extension of what is to be discussed here, the tableau is assumed to be stored in a rectangular array, but reference will be made only to elements on or above the diagonal.

Starting with the following tableau:

$$\begin{bmatrix} X'_1 X_1 & X'_1 X_2 & X'_1 Y \\ X'_2 X_1 & X'_2 X_2 & X'_2 Y \\ Y' X_1 & Y' X_2 & Y' Y \end{bmatrix} \quad (11.1)$$

perform a G2SWEEP on the  $X'_1 X_1$  columns. This results in

$$\left[ \begin{array}{c|c|c} (X'_1 X_1)^- & (X'_1 X_1)^- X'_1 X_2 & (X'_1 X_1)^- X'_1 Y \\ \hline -X'_2 X_1 (X'_1 X_1)^- & X'_2 M_1 X_2 & X'_2 M_1 Y \\ \hline -Y' X_1 (X'_1 X_1)^- & Y' M_1 X_2 & Y' M_1 Y \end{array} \right] \quad (11.2)$$

where  $(X'_1 X_1)^-$  is a symmetric  $g_2$  inverse and  $M_1 = I - X_1(X'_1 X_1)^- X'_1$ . Note that (11.2) is symmetric, except for the sign of the submatrices below  $(X'_1 X_1)^-$ . Letting  $a_{ij}$  denote the elements of (11.2), the elements below the diagonal  $a_{ij}$  (with  $i > j$ ) may be constructed from the elements above the diagonal as follows:

$$\begin{aligned} a_{ij} &= a_{ji} && \text{if } i \text{ and } j \text{ have been swept,} \\ &= a_{ji} && \text{if neither } i \text{ nor } j \text{ has been swept,} \\ &= -a_{ji} && \text{if } i \text{ or } j \text{ (but not both) has been swept.} \end{aligned}$$

By keeping track of which columns have been swept, the lower triangular portion of the tableau can be constructed from the upper.

Using an auxiliary vector  $V$  is the easiest way to keep track of what has and has not been swept. The elements of  $V$  are initially set to one; then, after sweeping on column  $k$ ,  $V_k$  is set to  $-V_k$ . If this vector  $V$  is used, then elements below the diagonal may be constructed from the upper triangular portion as follows:

$$a_{ij} = a_{ji} * V_i * V_j \quad (\text{for } i > j).$$

Note that the upper triangular elements are always correct as they are. Only when an element is not in the upper triangular portion of the tableau is multiplying  $a_{ji}$  by  $V_i * V_j$  necessary.

The upper triangular G2SWEEP makes the same assumptions about the matrix  $A$  as does the G2SWEEP operator. Until a dependency is declared, reversibility is possible. The vector  $V$  is assumed to have been set to one before any sweeps. UTG2SWEEP( $K$ ) modifies the upper triangular portion of the matrix  $A$  as follows:

**Definition:** UTG2SWEEP( $K$ )

Step 1: Let  $D = a_{kk}$ . If  $V_k = 1$  and  $D < = D \text{ MIN}_k$ , zero elements above and to the right of  $a_{kk}$ , including  $a_{kk}$ . Then terminate. Otherwise proceed.

Step 2: For each value of  $i$ :  $i = 1, 2, \dots, \text{NROWS}$  except for  $i = k$ , perform Step 3. Then go to Step 5.

Step 3: If  $i < k$  then  $B = a_{ik}/D$ . Otherwise,  $B = V_i \times V_k \times a_{ki}/D$ . Then for each value  $j$ :  $j = i, i + 1, \dots, \text{NCOLS}$  except for  $j = k$  perform Step 4.

Step 4: If  $k < j$ , then  $c = a_{kj}$ . Otherwise,  $c = V_j \times V_k \times a_{jk}$ . Set  $a_{ij} = a_{ij} - B \times c$ .

Step 5: For each value of  $i$ :  $i = 1, \dots, k$  set  $a_{ij} = -a_{ij}/D$ . For each value of  $j$ :  $j = k, \dots, \text{NCOLS}$  set  $a_{kj} = a_{kj}/D$ . Then set  $a_{kk} = 1/D$  and  $V_k = -V_k$ .

## 12. THE REVERSIBLE UPPER TRIANGULAR G2SWEEP

Reversibility may be achieved by modifying the UTG2SWEEP so that it does not zero the  $k$ th row and column when a dependency occurs. In addition, the resulting tableau will contain both  $(X'X)^{g_2}$  and  $(X'X)^{g_2} X'X$ , which are easily separated, along with  $(X'X)^{g_2} X'Y$  and  $Y'Y - Y'X(X'X)^{g_2} X'Y$ . To demonstrate these properties, reconsider the case in which  $X$  was partitioned into  $[X_1|X_2]$  with  $X_1$  of full-column rank and  $X_2 = X_1 L$ . Sweeping the initial tableau,

$$\begin{bmatrix} X'_1 X_1 & X'_1 X_2 & X'_1 Y \\ X'_2 X_1 & X'_2 X_2 & X'_2 Y \\ Y' X_1 & Y' X_2 & Y' Y \end{bmatrix} \quad (12.1)$$

on the columns of  $X'_1 X_1$  yields

$$\left[ \begin{array}{c|c|c} (X'_1 X_1)^- & (X'_1 X_1)^- X'_1 X_2 & (X'_1 X_1)^- X'_1 Y \\ \hline -X'_2 X_1 (X'_1 X_1)^- & 0 & 0 \\ \hline -Y' X_1 (X'_1 X_1)^- & 0 & Y' M_1 Y \end{array} \right] \quad (12.2)$$

where  $M_1 = I - X_1(X'_1 X_1)^- X'_1$ . Sweeping (12.2) on the columns of  $(X'_1 X_1)^-$  yields (12.1). Therefore, reversibility is achieved. Note in (12.1) and (12.2) that the same symmetry properties discussed for the UTG2SWEEP also hold.

The  $(X'X)^{g_2}$  matrix can be obtained from the final tableau (in which no columns are left to sweep) by use of the  $V$  vector described earlier. Letting  $G$  represent the  $g_2$  inverse and  $A$  the final tableau, then

$$\begin{aligned} g_{ij} &= 0 && \text{if } V_i + V_j > 0; \text{ otherwise,} \\ &= a_{ij} && \text{if } i < = j \text{ or } a_{ji} \text{ if } i > j. \end{aligned}$$

Using the  $g_2$  inverse described previously,

$$(X'X)^{g_2} X'X = \begin{bmatrix} I & (X'_1 X_1)^- X'_1 X_2 \\ 0 & 0 \end{bmatrix}.$$

Letting  $H$  represent  $(X'X)^{g_2} X'X$ , and  $A$  the final tableau, then

$$\begin{aligned} h_{ii} &= 0 && \text{if } V_i = 1, \\ &= 1 && \text{otherwise.} \\ h_{ij} &= 0 && \text{if } V_i + V_j \neq 0; \text{ otherwise,} \\ &= a_{ij} && \text{if } i < = j \text{ or } -a_{ji} \text{ if } i > j. \end{aligned}$$

As discussed with the G2SWEEP operator, it is unnecessary for the columns of  $X$  to be grouped, since the tolerance check can be used to determine which variables are linearly dependent on the ones previously swept. In defining the reversible UTG2SWEEP,

the same initial tableau and  $V$  vector used in the UTG2SWEEP is assumed.

The RUTG2SWEEP( $K$ ) modifies the upper triangular portion of the matrix  $A$  as follows:

*Definition:* RUTG2SWEEP( $K$ )

Step 1: Let  $D = a_{kk}$ . If  $V_k = 1$  and  $D < = D \text{ MIN}_k$  then terminate. Column  $K$  cannot be swept at this time. Otherwise proceed.

Steps 2 through 5 are the same as for UTG2SWEEP.

If one is using the RUTG2SWEEP, the Type II SS for any effect may be computed by starting with the tableau at any stage and making the appropriate sweeps.

### 13. USING RUTG2SWEEP SEQUENTIALLY

If one uses the RUTG2SWEEP sequentially ( $K = 1, 2, \dots, NX$ ), all the statistics described previously are available. Before any sweep, row  $k$ 's diagonal and elements to the right of the diagonal correspond to the  $k$ th row of the Forward Doolittle; thus,  $(a_{ku})^2/a_{kk}$  (provided  $a_{kk} > D \text{ MIN}_k$ ) is the Type I SS for variable  $k$ . Also, the product of each diagonal (just before sweeping) equals the determinant of  $X'X$ . When sweeping is done sequentially,  $(X'X)^{-1}X'X$  is the Hermite canonical form  $H$ . The  $H$  is upper triangular, and the elements of  $H$  (except for some zeros and ones) are already in place in the final tableau. The  $H$  can also be computed by sequentially pivoting on each nonzero row of  $X'X$ . Because the expected value of the solution achieved by using RUTG2SWEEP equals  $H\beta$ , the nature of the bias in the solution is at hand. The  $H$  matrix is also one of many matrices whose rows can be used as a generating set to compute any estimable function. In other words, any linear combination of the rows of  $H$  produces a matrix  $L$  such that  $L\beta$  is estimable (Goodnight 1976).

### 14. SUMMARY

The SWEEP operator and its extensions are versatile tools that not only afford solutions to the normal equations and a gamut of additional statistics but also allow complete insight into the nature of least squares. Once mastered, the general concepts of the SWEEP operator

allow the whole least squares process to be visualized. Without this conceptual tool, it is extremely difficult to explain concepts such as absorption and what the  $R$  notation is testing in terms of the parameters of the model. With the SWEEP tool in mind, these concepts can be readily grasped.

[Received March 1978. Revised January 1979.]

### REFERENCES

- Barr, A.J., Goodnight, J.H., Sall, J.P., and Helwig, J.T. (1976), *A User's Guide to SAS 76*, Raleigh, N.C.: SAS Institute.
- Beaton, A.E. (1964), "The Use of Special Matrix Operators in Statistical Calculus," Educational Testing Service, RB-64-51.
- , Rubin, D.B., and Barone, J.L. (1976), "The Acceptability of Regression Solutions: Another Look at Computational Accuracy," *Journal of the American Statistical Association*, 71, 158-168.
- (1977), "Comment on 'More on Computational Accuracy in Regression,'" *Journal of the American Statistical Association*, 72, 600.
- Ben-Israel, Adi, and Greville, T.N.E. (1974), *Generalized Inverses Theory and Application*, New York: John Wiley & Sons.
- Berk, K.N. (1977), "Tolerance and Condition in Regression Computations," *Journal of the American Statistical Association*, 72, 863-866.
- Frane, J.W. (1977), "A Note on Checking Tolerance in Matrix Inversion and Regression," *Technometrics*, 19, 513-514.
- Golub, Gene, and Klema, Virginia (1978), "Software for Rank Degeneracy," *Proceedings of the Computer Science and Statistics: Eleventh Annual Symposium on the Interface*, Raleigh: Institute of Statistics, North Carolina State University, 79-83.
- Goodnight, J.H. (1976), "Computational Methods in General Linear Models," *Proceedings of the American Statistical Association*, Statistical Computing Section, 68-72.
- Hemmerle, William J. (1967), *Statistical Computations on a Digital Computer*, Waltham, Mass.: Blaisdell Publishing Co.
- Isaacson, E., and Keller, H.B. (1966), *Analysis of Numerical Methods*, New York: John Wiley & Sons.
- Pringle, R.M., and Rayner, A.A. (1971), *Generalized Inverse Matrices With Applications to Statistics*, New York: Hafner Press.
- Ralston, Anthony (1960), *Mathematical Methods for Digital Computers*, New York: John Wiley & Sons.
- Schatzoff, M., Tsao, R., and Fienberg, S. (1968), "Efficient Calculation of All Possible Regressions," *Technometrics*, 10, 769-779.
- Seber, G.A.F. (1977), *Linear Regression Analysis*, New York: John Wiley & Sons.
- Steel, R.G.D., and Torrie, J.H. (1960), *Principles and Procedures of Statistics*, New York: McGraw-Hill Book Co.
- Wilkinson, J.H. (1961), "Error Analysis of Direct Methods of Matrix Inversion," *Journal of the Association of Computing Machinery*, 8, 281-330.