Tests of Linear Hypotheses Using a Generalized Inverse Matrix

S. R. Searle

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Abstract

A generalized inverse of the matrix X'X can be defined as any matrix G for which X'XGX'X = X'X. One such matrix can be developed from reducing X'X to diagonal form; in so doing, G is symmetric and satisfies GX'XG = G.

Solutions to normal equations X'Xb = X'y derived for the linear model E(y) = Xb can then be expressed as $\hat{b} = GX'y$. If H = GX'X the hypothesis Q'b = m can be tested provided Q'H = Q'. On the basis of normality assumptions the F-value for testing the hypothesis is $F = (Q'\hat{b} - m)'(Q'GQ)^{-1} (Q'\hat{b} - m)/s\hat{\sigma}^2$, where s is the rank and order of Q' and $\hat{\sigma}^2 = (y'y - \hat{b}X'y)/(n - r)$, n being the number of observations and r the rank of X.

Biometrics Unit, Cornell University, Ithaca, New York.

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"Generalized inverse" and allied expressions are defined in various places (e.g. Penrose, 1955, Greville, 1957, Rao, 1962 and Goldman and Zelen, 1964). The definition chosen here is that G is a generalized inverse of A if

 $AGA = A \qquad ----(1)$

Utilizing this definition, the first part of this paper summarizes results given in Rao (1962).

A generalized inverse of a symmetric matrix

If A is symmetric at least one method of obtaining a matrix G that satisfies (1) also leads to having

$$GAG = G$$
. ----(2)

Such a matrix can be derived from first reducing A to diagonal form. Suppose this reduction is

where D_r is a diagonal matrix of r non-zero elements, r being the rank of A (of order k). Then, in defining

 $\Delta^{-} = \begin{bmatrix} D_{\mathbf{r}}^{-\perp} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \qquad - - - - - - - (\mathbf{4})$

and

$$G = P' \Delta P$$
, -----(5)

Biometrics Unit, Cornell University, Ithaca, New York.

it is clear that G is symmetric and has rank r. Because G satisfies (1) it is, in the context of this paper, a generalized inverse of A. It also satisfies (2); and clearly, by its definition, it is not unique.

The product GA is of interest in subsequent developments. Let it be denoted by H:

H = GA. -----(6)

Then, because G and A have rank r, so does H, and because of (1)

 $H^2 = H$, -----(7) i.e. H is idempotent with rank r.

Solutions to linear equations

If the equations

$$Ax = u$$
 -----(8)

are consistent, then

$$\tilde{\mathbf{x}} = \mathbf{G}\mathbf{u} + (\mathbf{H} - \mathbf{I})\mathbf{z}$$

is a solution of (8) for z being any arbitrary vector of order k. In particular, when z is taken as a null vector

 $\tilde{\mathbf{x}} = \mathbf{G}\mathbf{u}$ -----(9)

is a solution. Furthermore, if

q'H = q' ----(10)

then q' \tilde{x} is unique, no matter what solution \tilde{x} given by (9) is used.

The linear model

1

The general linear model can be written as

y = Xb + e -----(11)

where y is a vector of n observations, b is a vector of the k parameters of the model, X is the "design" matrix and e is a vector of random error terms having variance-covariance matrix $\sigma^2 I$.¹ The normal equations resulting from

Note: b is a vector of parameters, and \hat{b} an estimate of it.

the least squares procedure are

$$X'X\hat{b} = X'y$$
 -----(12)

where \hat{b} is the solution corresponding to the parameter vector b.

Equations (12) are exactly analogous to (8). Let G now be a generalized inverse of X'X, defined in the manner of (5). Then, corresponding to (9), a solution of (12) is

Estimable functions

As in (6), define H as H = GX'X. Then if, as in (10), q'H = q', the function $q'\hat{b}$ of the solution (13) is unique. Furthermore, the expected value of this function is

$$E(q'\hat{b}) = q'GX'E(y)$$

= q'Hb
= q'b - - - - - - - - - - (14)

Hence $q'\hat{b}$ is an unbiased estimator of q'b: and because $q'\hat{b}$ is unique it is the unbiased estimator of the estimable function q'b.

The variance of \hat{b} is $var(\hat{b}) = GX'E(ee')XG$ $= G\sigma^2$

and the variance of $q'\hat{b}$ is

. .

$$var(q'\hat{b}) = q'Gqo^2$$
. - - - - - - - - - (15)

As shown by Rao (1962), this variance is less than that of any other linear unbiased estimator of q'b. Hence q' \hat{b} is the unique, minimum variance, linear, unbiased estimator of the estimable function q'b.

The above results are equivalent to those given in Rao (1962). We now turn to additional topics.

What functions are estimable?

Results (14) and (15) are true for any q' for which (10) is true; i.e. for which q'H = q'. The question of whether or not a particular function q'b is estimable can therefore be answered by ascertaining if q' satisfies q'H = q'. If it does, the function is estimable, otherwise it is not estimable. By this means the estimability of any linear function of the parameters can be investigated.

There is however, a second question of interest, namely "what functions are estimable?", i.e. what values of q' do satisfy q'H = q'? Utilizing (7) the answer is simple. For any arbitrary vector w' (of order k, the number of parameters in b) the vector

satisfies q'H = q'. Furthermore, because the rank of H is the same as the rank of X'X, r say, the number of linearly independent vectors q' given by (16) is r; i.e. there are only r linearly independent estimable functions.

Use of (16) leads to an explicit expression for the estimable function q'b in terms of the elements of the arbitrary vector w':

$$q'b = (w'H)b$$
$$= (\sum_{i=1}^{k} w_ih_{i1})b_1 + (\sum_{i=1}^{k} w_ih_{i2})b_2 + \dots + (\sum_{i=1}^{k} w_ih_{ik})b_k - -(17)$$

The coefficient of each parameter b_i in this expression is a linear function of the elements w_i of w', namely the i'th element of w'H.

The estimator of the estimable function (17) is, for q' satisfying (16),

In using a generalized inverse that satisfies (2), which is equivalent to HG = G, the form of q'b therefore reduces to

$$q'\hat{b} = w'GX'y$$

= w'\hat{b}
= w_1\hat{b}_1 + w_2\hat{b}_2 + \dots + w_k\hat{b}_k \cdot - - - - - - - - (18)

Equations (17) and (18) now provide opportunity for developing a whole series of estimable functions and the estimator of each. For any arbitrary set of values used for the w_i 's in (17), q'b as there defined will be an estimable function, and using the same values of the w_i 's in (18) gives the estimator of the estimable function. The \hat{b}_i 's in (18) are, of course, the numerical values obtained in the solution $\hat{b} = GX$ 'y given in (13).

As in (15)

$$var(q'\hat{b}) = q'Gq\sigma^2$$
$$= w'HGH'w\sigma^2$$
$$= w'GX'XGX'XG'w\sigma^2$$

and because of results like (1) and (2) this reduces to

$$var(q'\hat{b}) = w'Gw\sigma^2$$
. -----(19)

Similarly the covariance between two estimators $q_1'\hat{b}$ and $q_2'\hat{b}$ for which $q_1' = w_1'H$ and $q_2' = w_2'H$ is

Residual variance

For the solution $\hat{b} = GX'y$, the vector of predicted y-values is

 $\hat{\mathbf{y}} = \mathbf{X}\hat{\mathbf{b}} = \mathbf{X}\mathbf{G}\mathbf{X}^{\dagger}\mathbf{y}$

and hence the residual sum of squares is

$$SSR = (y - \hat{y})'(y - \hat{y})$$

= (y - X\u00fc)'(y - X\u00fc)
= y'(I - XGX')y - - - - - - - - (21)

Since it can be shown that XGX' is unique no matter what generalized inverse of X'X is used for G, SSR is, as one would expect, unique. The form given in (22)

is the most suitable computationally, namely the total uncorrected sum of squares y'y after subtracting from it the sum of products of the elements in \hat{b} each multiplied by the corresponding right-hand side of the equation $X'X\hat{b} = X'y$. On the other hand, the form given in (21) is suitable for finding the expected value of SSR. Thus, substituting (11) in (21) gives

$$SSR = e'(I - XGX')e$$
.

Then, because E(e) = 0, $var(e) = \sigma^2 I$ and I - XGX' is idempotent with rank n - r, a theorem from Graybill (1961) may be invoked to give

$$E(SSR) = (n - r)\sigma^2$$

Hence, an unbiased estimator of σ^2 is

$$\hat{\sigma}^2 = SSR/(n - r)$$
. - - - - - - - - - - (23)

Tests of hypotheses

1

Consider the general linear hypothesis Q'b = m, where Q'b consists of s linearly independent estimable functions q_i^{tb} for i = 1, 2, ..., s. The vector m is a vector of s arbitrary constants. We consider cases in which $s \le k - r$, k being the order of b and r the rank of X.

It has just been shown that after fitting the model (11) the residual sum of squares is as given in (21), and the corresponding estimator of the residual variance is $\hat{\sigma}^2$ shown in (23). Now consider the residual sum of squares after fitting the reduced model, namely y = Xb + e restricted by the hypothesis Q'b = m. Were this model to be written as $y = X_1b + \epsilon$, the normal equations would be $X_1^!X\tilde{b} = X_1^!y$ and, corresponding to (21), the residual sum of squares after fitting the model would be $SSR_1 = y'(I - X_1G_1X_1^!)y$, where G_1 is a generalized inverse of $X_1^!X$. Then, based on normality assumptions, the F-test of the hypothesis would depend on

which has the F-distribution with s and n - r degrees of freedom.

To avoid the necessity of deriving the normal equations $X_1'X_1\tilde{b} = X_1'y$, their

-6-

14

solution $G_1 X_1' y$, and thence SSR_1 for every hypothesis that one wants to test, we develop an expression for SSR_1 in terms of X and the hypothesis Q'b = m. It is contained in the following theorem.

Theorem. When fitting the linear model y = Xb + e, the numerator sum of squares of the F-value used for testing the (testable) general linear hypothesis Q'b = m, for Q' consisting of s linearly independent rows, is $(Q'\hat{b} - m)'(Q'GQ)^{-1}(Q'\hat{b} - m)$ where $\hat{b} = GX'y$ is a solution to the normal equations $X'X\hat{b} = X'y$ and G is a symmetric generalized inverse of X'X.

The following lemma is used in proving the theorem.

Lemma. Q'GQ is non-singular.

<u>Proof of lemma</u>. Because Q'b = m is a testable hypothesis the rows of Q'b are estimable functions and therefore Q'H = Q' where H = GX'X. Hence

Q'GQ = Q'HGQ = Q'GX'XGQ = Q'GX'(Q'GX')',

so that r(Q'GQ) = r(Q'GX'). But Q' = Q'H = Q'GX'X; therefore, by the rule for the rank of a product, $r(Q') = s \le r(Q'GX')$, and also $r(Q'GX') \le r(Q') = s$. Hence r(Q'GX') = s, and so therefore does the rank of Q'GQ. But s is the order of Q'GQ. Therefore Q'GQ is non-singular.

<u>Proof of theorem</u>. Fitting the reduced model is equivalent to fitting the full model y = Xb + e subject to the condition Q'b = m. The appropriate normal equations are derived by minimizing $(y - Xb)'(y - Xb) + 2\lambda'(Q'b - m)$ where λ' is a vector of Lagrange multipliers. The resulting equations are

$$X'X\tilde{b} + Q\lambda = X'y$$
 -----(25)
 $Q'\tilde{b} = m$ -----(26)

and

$$4,0-m$$
.

Using G and GX'y = \hat{b} , equation (25) can be solved as

$$\tilde{b} = \hat{b} - GQ\lambda$$
. -----(27)

Pre-multiplying (27) by Q', substituting from (26) and using the lemma gives

$$u = (Q^{*}GQ)^{-1}(Q^{*}\hat{b} - m) , - - - - - - - (28)$$

and substitution back into (27) yields

$$\tilde{b} = \hat{b} - GQ(Q'GQ)^{-1}(Q'\hat{b} - m) \cdot - - - - - - - (29)$$

For
$$\tilde{y} = X\tilde{b}$$
 the residual sum of squares after fitting the reduced model is
 $SSR_1 = (y - X\tilde{b})'(y - X\tilde{b})$.
Substituting for \tilde{b} from (27) this leads, after a little reduction to
 $SSR_1 = (y - X\hat{b})'(y - X\hat{b}) + \lambda'Q'GQ\lambda$
 $= SSR + \lambda'Q'GQ\lambda$ -----(30)
so that expression (24) for F becomes
 $F = \lambda'Q'GQ\lambda/s\sigma^2$

$$F = (Q'\hat{b} - m)'(Q'GQ)^{-1}(Q'\hat{b} - m)/s\hat{\sigma}^2 - - - - (31)^{-1}$$

Hence the theorem is proved. With $Q'\hat{b}$ being the estimator of the estimable functions Q'b in the full model it is apparent that once b = GX'y has been calculated, F is readily obtainable.

A by-product of the theorem is the solution of the normal equations in the reduced model, given in (30), for which the variance-covariance matrix is

In situations where m is a null vector the expressions for F and $\tilde{\mathbf{b}}$ reduce to the simpler forms

$$F = \hat{b}' Q (Q' G Q)^{-1} Q' \hat{b} / s \hat{\sigma}^{2} - - - - - - (33)$$

and $\tilde{b} = \hat{b} - G Q (Q' G Q)^{-1} Q' \hat{b} \cdot - - - - - - - (34)$

This is the theorem given in Searle (1965a).

Example

The above expressions can be demonstrated by considering the simple, nointeraction, two-way, model

$$Y_{ijk} = \mu + \alpha_i + \beta_j + e_{ijk},$$

for which one might have the following unbalanced data.

~ F	A sample	of 6 observations	3
Row		Column	Total
	1	2	
l	4,7	3	14
2	5	2	7
3	1	no observation	1
Total	17	5	22

The normal equations (12), namely

(29)----

$$X'X\hat{b} = X'y$$

are

$$\begin{bmatrix} 6 & 3 & 2 & 1 & 4 & 2 \\ 3 & 3 & 0 & 0 & 2 & 1 \\ 2 & 0 & 2 & 0 & 1 & 1 \\ 1 & 0 & 0 & 1 & 1 & 0 \\ 4 & 2 & 1 & 1 & 4 & 0 \\ 2 & 1 & 1 & 0 & 0 & 2 \end{bmatrix} \begin{bmatrix} \mu \\ \alpha_1 \\ \alpha_2 \\ \alpha_3 \\ \beta_1 \\ \beta_2 \end{bmatrix} = \begin{bmatrix} 22 \\ 14 \\ 7 \\ 1 \\ 17 \\ 5 \end{bmatrix},$$

where b is the vector of parameters b' = $(\mu \alpha_1 \alpha_2 \alpha_3 \beta_1 \beta_2)$ and X'y is the vector on the right-hand side of equation (35). By following the procedures suggested in (3), (4) and (5) it is found that a generalized inverse of X'X is

G	= (1/7)	Γο	0	0	0	0	0	,
		0	5	2	4	- 4	0	
		0	2	5	3	-3	0	
		0	4	3	13	-6	0	
		0	-4	- 3	-6	6	0	
		0	0	0	0	0	0	

and corresponding to (13) a solution of the normal equations is

$$\hat{b} = GX' y = (1/7) \begin{bmatrix} 0 \\ 20 \\ 15 \\ -12 \\ 19 \\ 0 \end{bmatrix}$$

The matrix H is

H =	GX'X	=	0	0	0	0	0	0	
			1	1	0	0	0	l	
			1	0	1	0	0	l	
			1	0	0	1	0	l	
			0	0	0	0	l	-1	
			lo	0	0	0	0	0	

and, using

as the arbitrary vector in equation (17), the estimable functions are

$$q'b = w'Hb$$

$$= (w_{2} + w_{3} + w_{4})\mu + w_{2}\alpha_{1} + w_{3}\alpha_{2} + w_{4}\alpha_{3} + w_{5}\beta_{1}$$

$$+ (w_{2} + w_{3} + w_{4} - w_{5})\beta_{2} \cdot - -(38)$$

From (18), (36) and (37) their estimators are

$$q^{\dagger}\hat{b} = w^{\dagger}\hat{b} = (1/7)(20w_2 + 15w_3 - 12w_4 + 19w_5) - - - - (39)$$

From (38) it is seen at once that $\alpha_1 - \alpha_2$, for example, is estimable because, with $w_2 = 1$, $w_3 = -1$, $w_4 = 0$ and $w_5 = 0$, q'b reduces to $\alpha_1 - \alpha_2$; and with the same values of the w's in (39) the estimate of $\alpha_1 - \alpha_2$ is

$$\alpha_1 - \alpha_2 = (1/7)(20 - 15) = 5/7$$
.

Likewise, with $w_2 = w_3 = w_4 = 0$ and $w_5 = 1$ it is clear from (38) that $\beta_1 - \beta_2$ is estimable and from (39) its estimate is

$$\beta_1 - \beta_2 = 19/7$$
.

Equation (19) gives the variance of an estimator as w'Gwo² and from (37) and the computed value of G this is

$$w' Gw \sigma^{2} = (1/7)(5w_{2}^{2} + 5w_{3}^{2} + 13w_{4}^{2} + 6w_{5}^{2} + 4w_{2}w_{3} + 8w_{2}w_{4}$$
$$- 8w_{2}w_{5} + 6w_{3}w_{4} - 6w_{3}w_{5} - 12w_{4}w_{5})\sigma^{2}.$$

Hence the variances of $\alpha_1 - \alpha_2$ and $\beta_1 - \beta_2$ are $\operatorname{var}(\alpha_1 - \alpha_2) = (1/7)(5 + 5 - 4) = 6\sigma^2/7$ $var(\beta_1 - \beta_2) = (1/7)(6)\sigma^2 = 6\sigma^2/7$,

and

coincidentally the same.

The estimate of σ^2 is obtained through using (22) and (23):

SSR =
$$y'y - \hat{b}'X'y$$

= 104 - (1/7)[20(14) + 15(7) - 12(1) + 19(17)]
= 104 - 696/7
= 32/7 .

The rank of X'X is clearly 4 and there are 6 observations, so the estimated variance is

$$\delta^2 = 32/7(6 - 4) = 32/14$$
. - - - - - - - - - (40)

The hypothesis $\alpha_1 = \alpha_2$ can be written as $\alpha_1 - \alpha_2 = 0$ and we have seen that α_1 - α_2 is estimable. Therefore the hypothesis can be tested. Writing it in the form Q'b = 0 with

$$Q' = (0 \ 1 \ -1 \ 0 \ 0 \ 0)$$

we have

$$Q^{\dagger}\hat{b} = 5/7$$

and

$$Q'GQ = (1/7)(5 + 5 - 4) = 6/7$$
.

Therefore, from (33) and (40), the F-value for testing the hypothesis is F = (5/7)(7/6)(5/7)/1(32/14)= 25/96.

And from (3^{4}) and (3^{6}) the solution for b when the hypothesis is true is \cdots

$$\widetilde{b} = (1/7) \begin{bmatrix} 0 \\ 20 \\ 15 \\ -12 \\ 19 \\ 0 \end{bmatrix} - (1/7) \begin{bmatrix} 0 \\ 3 \\ -3 \\ 1 \\ -1 \\ 1 \end{bmatrix}$$
(7/6)(5/7)

which reduces to

$\tilde{b} = (1/6)^{2}$		•
	15	
	15	
	-11	
	17	
	0	

5 1 2 3

The hypothesis that the rows are all equal can also be tested; it can be written as

with	ୡୄ୲	= [0	1	-1	0	0	0]	•
		L	0	1	0	-1	0	0	

Q'b = 0

For this

$$Q'\hat{b} = \begin{bmatrix} 5/7 \\ 32/7 \end{bmatrix}$$

and
$$Q'GQ = (1/7)\begin{bmatrix} 6 & 2 \\ 2 & 10 \end{bmatrix}$$

with
$$(Q'GQ)^{-1} = (1/8)\begin{bmatrix} 10 & -2 \\ -2 & 6 \end{bmatrix}$$

Hence the F-value for testing this hypothesis is

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$$F = \frac{(5/7 \ 32/7)(1/8) \left[\begin{array}{c} 10 \ -2 \\ -2 \ 6 \end{array} \right] \left[\begin{array}{c} 5/7 \\ 32/7 \end{array} \right]}{2(32/14)}$$
$$= \frac{(1/56)(5 \ 32) \left[\begin{array}{c} -2 \\ 26 \end{array} \right]}{32/7}$$
$$= \frac{411/28}{32/7}$$

The solution for b under the null hypothesis of equality of the rows is, from (34) and (36)

$$\tilde{b} = (1/7) \begin{bmatrix} 0 \\ 20 \\ 15 \\ -12 \\ 19 \\ 0 \end{bmatrix} - (1/7) \begin{bmatrix} 0 & 0 \\ 3 & 1 \\ -3 & -1 \\ 1 & -9 \\ -1 & 2 \\ 0 & 0 \end{bmatrix}$$
 (1/8)
$$\begin{bmatrix} 10 & -2 \\ -2 & 6 \end{bmatrix} \begin{bmatrix} 5/7 \\ 32/7 \end{bmatrix}$$

which reduces to

.

$$\tilde{b} = (1/4) \begin{bmatrix} 0 \\ 10 \\ 10 \\ 10 \\ 7 \\ 0 \end{bmatrix}$$

A check can be made on these calculations by noting that the hypothesis of equality of the rows is equivalent to the model

$$y_{ijk} = \mu + \beta_j + e_{ijk}$$
.

The normal equations for this are

$$\begin{bmatrix} 6 & 4 & 2 \\ 4 & 4 & 0 \\ 2 & 0 & 2 \end{bmatrix} \begin{bmatrix} \mu \\ \beta_1 \\ \beta_2 \end{bmatrix} = \begin{bmatrix} 22 \\ 17 \\ 5 \end{bmatrix}$$

for which one solution is

$$\begin{bmatrix} \tilde{\mu} \\ \tilde{\beta}_1 \\ \tilde{\beta}_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 17/4 \\ 5/2 \end{bmatrix}$$

The corresponding residual sum of squares is

$$SSR_{1} = 104 - 17^{2}/4 - 5^{2}/2$$
$$= (416 - 289 - 50)/4$$
$$= 77/4 .$$

Hence the F-value for testing the hypothesis is

$$(SSR_{1} - SSR)/2\hat{\sigma}^{2}$$

$$= \frac{77/4 - 32/7}{2(32/14)}$$

$$= \frac{(539 - 128)/28}{32/7}$$

$$= 411/128$$

as before. Further examples are to be found in Searle (1965b).

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