A NOTE ON GENERALISED INVERSE MATRICES IN LEAST SQUARES ANALYSIS[1]

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1. Introduction

In least squares estimation, normal equations with a singular coefficient matrix admit an infinite number of estimates of the parameters. The conventional operation to eliminate this indeterminacy is to impose suitable constraints on the parameters or on their estimates such that the estimates are unique under the given constraints (Scheffe, 1959; Graybill, 1961). In the present work, two generally used methods of imposing constraints are discussed and it is shown, by use of generalised inverse matrices sugested by Rao (1962, 1965), that the least squares estimates of all estimable functions of parameters are unique regardless the different forms of the constraints.

2. The Normal Equations

Consider the general linear model

$$E(\boldsymbol{y})=\boldsymbol{X}\beta, \qquad \mathrm{Var}(\boldsymbol{y})=\boldsymbol{I}\sigma^2, \tag{1}$$

where $\boldsymbol{y}$ is an n-vector of observable random variables, $\boldsymbol{X}$ is a non-stochastic $n\times p$ matrix $(p<n)$, β is an p-vector of unknown parameters and σ^2 is an unknown parameter. If rank $\boldsymbol{X}=p$, i.e. $\boldsymbol{X}'\boldsymbol{X}$ is non-singular, the normal equations are solved by inverting the matrix $\boldsymbol{X}'\boldsymbol{X}$. When rank $\boldsymbol{X}=r<p$, $\boldsymbol{X}'\boldsymbol{X}$ does not possess an inverse and the constriants on parameters or on their estimates

$$\boldsymbol{H}\beta=\boldsymbol{0} \quad \text{or} \quad \boldsymbol{Hb}=\boldsymbol{0}$$

are necessary for unique solutions.

When the constraints are $\boldsymbol{H}\beta=\boldsymbol{0}$, the model (1) is augmented to

$$\begin{bmatrix} E(\boldsymbol{y}) \\ \boldsymbol{0} \end{bmatrix}=\begin{bmatrix} \boldsymbol{X} \\ \boldsymbol{H} \end{bmatrix}\beta \tag{2}$$

where $\boldsymbol{H}$ is a matrix of order $(p-r)\times p$ and rank $p-r$ and its rows are inde-

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pendent of the rows of X. Therefore $\begin{bmatrix} X \\ H \end{bmatrix}$ is of rank p and the normal equations

$$(X'X+H'H)b=X'y \tag{3}$$

have a non-singular coefficient matrix. The least squares estimate is then

$$b=(X'X+H'H)^{-1}X'y. \tag{4}$$

When SSE is minimized subject to the constraints $Hb=0$, the least squares estimate is obtained by solving

$$\frac{\partial}{\partial\beta}[(y-Xb)'(y-Xb)+\lambda'Hb]=0$$

and

$$\frac{\partial}{\partial\lambda}[(y-Xb)'(y-Xb)+\lambda'Hb]=0,$$

or

$$\begin{bmatrix} X'X & H' \\ H & 0 \end{bmatrix}\begin{bmatrix} b \\ \frac{1}{2}\lambda \end{bmatrix}=\begin{bmatrix} X'y \\ 0 \end{bmatrix}. \tag{5}$$

where λ is an $(p-r)$-vector of Lagrange multipliers.
Since H is full ranked and its rows are independent of rows of X, the coefficient matrix is non-singular. Let us denote its inverse matrix by

$$\begin{bmatrix} X'X & H' \\ H & 0 \end{bmatrix}^{-1}=\begin{bmatrix} B_{11} & B_{12} \\ B_{12}' & B_{22} \end{bmatrix}.$$

Then the least squares estimate is

$$b=B_{11}X'y \tag{6}$$

3. Generalised Inverse Matrices and uniqueness of estimates

By Rao's definition, a matrix $(X'X)^-$ is a generalised inverse of $X'X$ if $X'X(X'X)^-X'X=X'X$. We shall show that the matrices B_{11} and $(X'X+H'H)^{-1}$ are generalised inverses of $X'X$.

Since X is $n\times p$ of rank r, there exists an $p\times(p-r)$ matrix N of rank $(p-r)$ such that $XN=0$ (note that the columns of N form a basis of the null space of X). Then $N'(X'X+H'H)N$ is non-singular since $(X'X+H'H)$ is non-singular. But

$$N'(X'X+H'H)N=N'H'HN,$$

hence HN is non-singular.

Now consider the identity

$$(X'X+H'H)(X'X+H'H)^{-1}=I,$$

or

$$X'X(X'X+H'H)^{-1}+H'H(X'X+H'H)^{-1}=I,$$

Multiplying by N' to the left and by X' to the right, we get

$$N'H'H(X'X+H'H)^{-1}X'=0.$$

Therefore

$$H(X'X+H'H)^{-1}X'=0, \tag{7}$$

since HN is non-singular. Then

$$X'X(X'X+H'H)^{-1}X'X=(X'X+H'H)(X'X+H'H)^{-1}X'X=X'X.$$

Next, from the identity

$$\begin{pmatrix} X'X & H' \\ H & 0 \end{pmatrix}\begin{pmatrix} B_{11} & B_{12} \\ B'_{12} & B_{22} \end{pmatrix}=I,$$

we get

$$X'XB_{11}+H'B'_{12}=I.$$

Premultiply both sides of this equation by N', get

$$N'H'B'_{12}=N'$$

or

$$B_{12}=N(HN)^{-1}. \tag{8}$$

Therefore

$$X'XB_{11}X'X=(X'XB_{11}+H'B'_{12})X'X=X'X,$$

since

$$B'_{12}X'=[(HN)^{-1}]'N'X'=0.$$

The Lagrange multiplier λ in (5) is then

$$\lambda=B'_{12}X'y=0. \tag{9}$$

By definition that $X'X(X'X)^{-}X'X=X'X$ for $(X'X)^{-}$ a generalised inverse of $X'X$, it is straightforward to show that

$$[X-X(X'X)^{-}X'X]'[X-X(X'X)^{-}X'X[=0,$$

or

$$X=X(X'X)^{-}X'X. \tag{10}$$

Therefore the general form of the solutions to normal equations is

$$b=(X'X)^{-}X'y. \tag{11}$$

It is seen that b and $(X'X)^{-}$ are not unique. We shall show that for $L\beta$ an estimable function of the parameters β, i.e., $L=CX$ for some C, the estimate Lb is unique. First, consider any two generalised inverses $(XX)_1^{-}$ and $(XX)_2^{-}$ we can see that

$$[X(X'X)_1^-X'-X(X'X)_2^-X']'[X(X'X)_1^-X'-X(X'X)_2^-X']=0$$

and hence

$$X(X'X)_1^-X'=X(X'X)_2^-X'. \tag{12}$$

This means that $X(X'X)^-X'$ is unique. Therefore

$$Xb=X(X'X)^-X'y \tag{13}$$

is unique and is an unbiased estimate of $X\beta$. Consequently the estimate Lb of $L\beta$ is also unique regardless the different forms of the generalised inverse matrices.

The SSE is then

$$\text{SSE}=(y-Xb)'(y-Xb)=y'(I-X(X'X)^-X')y. \tag{14}$$

By the fact that

$$X'[I-X(X'X)^-X']=0 \tag{15}$$

it is obvious that Lb and the sum of squares associated with it are independent of SSE. Therefore the hypothesis concerning $L\beta$ can be tested in analysis of variance.

4. Remarks

A general procedure of computing a generalised inverse of $X'X$ is given blow.

1. Find an orthogonal matrix T such that

   $$TX'XT'=D \quad \text{or} \quad X'X=T'DT$$

   where D is a diagonal matrix.
2. Define D^- to be a generalised inverse of D by replacing the non-zero elements d_{ii} in D by $1/d_{ii}$. Then $DD^-D=D$.
3. The matrix $T'D^-T$ is then a generalised inverse of $X'X$ since

   $$X'XT'D^-TX'X=T'DTT'D^-TT'DT=T'DT=X'X.$$

This procedure is equivalent to that of inverting a symmetric matrix when it is non-singular. With this argument, we can use the abbreviated Doolittle's method (Rohde and Harvey, 1965) as a computing technique in the least squares estimation for models of less than full rank as well as for models of full rank.

5. Summary

It is shown that, in the analysis of a general linear model of less than full rank, a generalised inverse matrix of the coefficient matrix of normal

equations can be obtained by imposing a set of independent and unestimable constraints on the parameters or on their estimates. The estimate is not unique since the generalised invese matrix is not unique. But as far as the estimable functions of the parameters are concerned, their estimates are unique.

Generalised Inverse Matrices 在最小二乘分析中的應用

袁 宸 宣

本文旨在說明 Generalised inverse matrices 在最小二乘估算法及變方分析中的應用，考慮一般情況，卽假設模式(1)中行列X非全階(Full rank)，而以全階模式爲一特殊情形。並說明簡化 Doolittle 氏方法應用於此情況的理論依據。

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