

PSEUDO-INVERSES IN THE ANALYSIS OF VARIANCE

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1. Summary. The normal equations in the analysis of variance with suitable side conditions give a unique set of estimates, $\tilde{\beta}_i$, of the parameters β_i . These estimates are unique linear forms in the actual observations. In the solutions to the normal equations they appear as linear forms in the treatment and block totals; these totals are not independent and so the forms in them are not unique. Thus the normal equations, while giving a unique solution vector, admit an infinite number of pseudo-inverses of the matrix $X'X$. In this paper the relationship between the two most common pseudo-inverses is discussed.

2. The general case. Let X be the design matrix. X has n rows and p columns with rank $(p - m)$. There exists a matrix D of order $p \times m$ with rank m such that $XD = 0$. The normal equations $X'X\tilde{\beta} = X'Y$ are consistent. If $\tilde{\beta} = PX'Y$ is any solution vector, the matrix P is called a pseudo-inverse or generalized inverse (g -inverse) of $X'X$ (Rao, 1962). When the normal equations are solved subject to the set of linear constraints $H\tilde{\beta} = 0$, where H is a matrix of order $m \times p$ such that HD has rank m , the solution vector $\tilde{\beta}$ is unique, but the g -inverse P is not. The relationship $D'X'Y = 0$ allows different estimates of the same parameter β_i to be identical numerically but to differ in form by some linear combination of the rows of $D'X'Y$. Thus, if P^* is any other g -inverse of $X'X$, subject to $H\tilde{\beta} = 0$,

$$(1) \quad P^* = P + ED',$$

where E is a matrix of order $p \times m$. If only symmetric g -inverses are considered, (1) becomes $P^* = P + DCD'$, where C is a symmetric matrix of order m .

There are two standard methods of obtaining a g -inverse of $X'X$. In one method (Graybill [1], p. 292, and Kempthorne [2], p. 79), the matrix $X'X$ is augmented to

$$\begin{pmatrix} X'X & H' \\ H & 0 \end{pmatrix} = B^{-1} = \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix}^{-1}$$

Then B_{11} is a g -inverse of $X'X$.

In the second method (Plackett [3], p. 41, and Scheffé [5], p. 19), the g -inverse is $(X'X + H'H)^{-1}$. These two g -inverses are not identical. Plackett has shown that

$$\text{cov}(\tilde{\beta}) = (I - D(HD)^{-1}H)(X'X + H'H)^{-1}\sigma^2.$$

With this result, B_{11} can be obtained from $(X'X + H'H)^{-1}$, but

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$(\mathbf{I} - \mathbf{D}(\mathbf{H}\mathbf{D})^{-1}\mathbf{H})^{-1}$ does not exist, since $\mathbf{I} - \mathbf{D}(\mathbf{H}\mathbf{D})^{-1}\mathbf{H}$ is idempotent and thus not of full rank.

In this note a different relationship (2) between these g -inverses is derived by which each may be obtained from the other. Multiplying out $\mathbf{B}\mathbf{B}^{-1} = \mathbf{I}$ gives the four equations

$$\begin{aligned} \mathbf{X}'\mathbf{X}\mathbf{B}_{11} + \mathbf{H}'\mathbf{B}_{21} &= \mathbf{I}_p, & \mathbf{X}'\mathbf{X}\mathbf{B}_{12} + \mathbf{H}'\mathbf{B}_{22} &= \mathbf{0}, \\ \mathbf{H}\mathbf{B}_{11} &= \mathbf{0}, & \mathbf{H}\mathbf{B}_{12} &= \mathbf{I}_m. \end{aligned}$$

After multiplying the first two equations on the left by \mathbf{D}' and simplifying, we have $\mathbf{B}_{22} = \mathbf{0}$, $\mathbf{B}_{12} = \mathbf{D}(\mathbf{H}\mathbf{D})^{-1}$ and

$$\mathbf{X}'\mathbf{X}\mathbf{B}_{11} = \mathbf{I} - \mathbf{H}'\mathbf{B}_{21} = \mathbf{I} - \mathbf{H}'(\mathbf{D}'\mathbf{H}')^{-1}\mathbf{D}'.$$

Then $\mathbf{X}'\mathbf{X}\mathbf{B}_{11}\mathbf{X}'\mathbf{Y} = \mathbf{X}'\mathbf{Y} - \mathbf{H}'(\mathbf{D}'\mathbf{H}')^{-1}\mathbf{D}'\mathbf{X}'\mathbf{Y} = \mathbf{X}'\mathbf{Y}$ and $\tilde{\beta} = \mathbf{B}_{11}\mathbf{X}'\mathbf{Y}$ is a solution. The variance covariance matrix of the estimates is $\text{cov}(\tilde{\beta}) = \mathbf{B}_{11}\mathbf{X}'\mathbf{X}\mathbf{B}_{11}\sigma^2 = \mathbf{B}_{11}\sigma^2$. If $\lambda'\tilde{\beta}$ is estimable, $\lambda'\mathbf{D} = \mathbf{0}$ and $\text{var}(\lambda'\tilde{\beta}) = \lambda'\mathbf{B}_{11}\lambda = \lambda'\mathbf{P}^*\lambda$ so that, for computing the variance of any estimable function, any pseudo-inverse may be used as the variance covariance matrix.

Writing $(\mathbf{X}'\mathbf{X} + \mathbf{H}'\mathbf{H})^{-1} = \mathbf{B}_{11} + \mathbf{D}\mathbf{C}\mathbf{D}'$, we have

$$\begin{aligned} \mathbf{I} &= (\mathbf{X}'\mathbf{X} + \mathbf{H}'\mathbf{H})(\mathbf{B}_{11} + \mathbf{D}\mathbf{C}\mathbf{D}') = \mathbf{X}'\mathbf{X}\mathbf{B}_{11} + \mathbf{H}'\mathbf{H}\mathbf{D}\mathbf{C}\mathbf{D}' \\ &= \mathbf{I} - \mathbf{H}'(\mathbf{D}'\mathbf{H}')^{-1}\mathbf{D}' + \mathbf{H}'\mathbf{H}\mathbf{D}\mathbf{C}\mathbf{D}'. \end{aligned}$$

Then $\mathbf{H}'(\mathbf{D}'\mathbf{H}')^{-1}\mathbf{D}' = \mathbf{H}'\mathbf{H}\mathbf{D}\mathbf{C}\mathbf{D}'$, and multiplying both sides on the left by $(\mathbf{D}'\mathbf{H}')^{-1}\mathbf{D}'$ and on the right by $\mathbf{H}'(\mathbf{D}'\mathbf{H}')^{-1}$ gives $(\mathbf{D}'\mathbf{H}')^{-1} = \mathbf{H}\mathbf{D}\mathbf{C}$, whence

$$\mathbf{C} = (\mathbf{H}\mathbf{D})^{-1}(\mathbf{D}'\mathbf{H}')^{-1} = (\mathbf{D}'\mathbf{H}'\mathbf{H}\mathbf{D})^{-1},$$

so that the desired relationship is

$$(2) \quad (\mathbf{X}'\mathbf{X} + \mathbf{H}'\mathbf{H})^{-1} = \mathbf{B}_{11} + \mathbf{D}(\mathbf{D}'\mathbf{H}'\mathbf{H}\mathbf{D})^{-1}\mathbf{D}'.$$

3. Application to incomplete block designs. Let $\mathbf{A}\hat{\epsilon} = \mathbf{Q}$ be the adjusted intrablock normal equations for an incomplete block design, where \mathbf{Q} is the vector of adjusted treatment totals, $\hat{\epsilon}$ the vector of the estimates of the v treatment effects, and \mathbf{A} is a symmetric matrix of order v and rank $(v - 1)$. Then $\mathbf{A}\mathbf{1} = \mathbf{0}$ and $\mathbf{1}'\mathbf{Q} = 0$ where $\mathbf{1}$ is a vector with each element unity. We solve the equations subject to the single side condition $\mathbf{H}\hat{\epsilon} = \sum_i h_i \hat{\epsilon}_i = 0$. Substituting \mathbf{A} for $\mathbf{X}'\mathbf{X}$ and $\mathbf{1}$ for \mathbf{D} in (2) above gives

$$(\mathbf{A} + \mathbf{H}'\mathbf{H})^{-1} = \mathbf{B}_{11} + \mathbf{1}(\mathbf{1}'\mathbf{H}'\mathbf{H}\mathbf{1})^{-1}\mathbf{1}' = \mathbf{B}_{11} + \mathbf{1}\mathbf{1}' / \left(\sum_i h_i \right)^2.$$

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