SOLUTIONS TO SINGULAR NORMAL EQUATIONS

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SUMMARY

A formula for obtaining the solution to the normal equations in the linear model not of full rank subject to a linear constraint is derived and is shown to generalize the results reported previously by Searle (1971,1984) and by Rayner and Pringle (1976,1987). Its practical importance is appraised and illustrated. Numerical solutions to the normal equations can also be obtained by using generalized inverses of the design matrix . The equivalence of this approach to that of imposing linear restrictions is formally demonstrated and the implications are discussed in some detail.

Some key words: Linear model; Linear constraints; Generalized inverses.

1. INTRODUCTION

Consider the linear model not of full rank in the form

$$y = X\beta + \epsilon \tag{1.1}$$

where y is an $nx1$ vector of observations, X is an nxp matrix with non-stochastic elements and rank $r < p$, β is a $px1$ vector of unknown parameters, and ϵ is an $nx1$ vector of errors such that $E(\epsilon) = 0$ and $V(\epsilon) = \sigma^2 I$. The general solution to the normal equations

$$X'Xb = X'y \tag{1.2}$$

is given by

$$b = b^* + C_o'z \tag{1.3}$$

where b^* is a particular solution to (1.2), C_o is an orthogonal complement of X not necessarily of full row rank, and z is an arbitary vector.

Suppose that the linear constraint $Cb = c$, where C is a matrix complementary to X in the sense defined by Chipman (1964) and is not necessarily of full row rank and $c \in \mathbb{C}(C)$, is imposed on the normal equations. Then the resultant solution is unique and is valuable firstly in that it provides a numerical solution to (1.2) and secondly in that it is the solution vector for the constrained model $y = X\beta + \epsilon$ with $C\beta = c$. Searle (1971,1984) and Rayner and Pringle (1976,1987) have derived expressions relating such a solution to certain other solutions to the normal equations. However the equivalence of their results is not obvious and furthermore the formulae derived are somewhat specific. In

Section 2 of the present article therefore a general formula which unifies these earlier results is developed and its usefulness is appraised .

Numerical solutions to the normal equations can also be obtained as $GX'y$ where G is a generalized inverse of $S = X'X$, and this approach is used by many statistical computer packages, e.g. SAS. The relation of such solutions to those obtained by imposing linear constraints on the normal equations is clearly of interest. In particular Searle (1971, 1984), Rayner and Pringle(1976), and Mazumdar, Li ,and Bryce (1980) have characterised certain generalized inverses of S which provide solutions to (1.2) satisfying a given constraint $Cb = 0$ but their approaches are seemingly different. Furthermore no explicit method for identifying the linear constraints with which a given solution $GX'y$ complies has been established. In Section 3 the relationship between solutions to (1.2) of the form $GX'y$ and those subject to $Cb = 0$ is therefore reinvestigated in some detail.

The ideas of Sections 2 and 3 are illustrated and elaborated upon in Section 4 by means of two examples.

For convenience the following notation is introduced. A generalized inverse of a matrix A, say G, which satisfies a particular combination i, where $i \in \{1,12,13,123,124\}$ of the four conditions of Penrose (1955), viz.

$$
\begin{aligned}
&(1) \quad AGA = A \\
&(2) \quad GAG = G \\
&(3) \quad (AG)' = AG \qquad (1.4) \\
&(4) \quad (GA)' = GA
\end{aligned}
$$

is termed a g_i-inverse of A and is denoted A^{g_i}. The unique Moore-Penrose inverse of A which satisfies all four conditions of (1.4) is termed <u>the</u> g-inverse of A and is written A^g.

2. FORMULA FOR OBTAINING THE SOLUTION TO THE NORMAL EQUATIONS SUBJECT TO THE CONSTRAINT $Cb = c$ FROM ANY OTHER SOLUTION VECTOR b^*

2.1 Main Result

Let b be the solution to (1.2) subject to the constraint $Cb = c$. Then b can be written in terms of b^* using expression (1.3) with z satisfying the equations

$$CC_o'z = c - Cb^*. \tag{2.1}$$

Since $C = MX + NC_o$ for some matrices M and N with $r(C) = r(NC_o) = p-r$ (Rayner and Pringle, 1987), $r(CC_o') = r(NC_oC_o') = r(NC_o) = p-r = r(C_o)$, and it follows that

$$\mathbb{C}(C) = \mathbb{C}(CC_o') \tag{2.2a}$$

$$\mathbb{R}(C_o') = \mathbb{R}(CC_o') \tag{2.2b}$$

and that the equations (2.1) are consistent. Hence $C_o'z = C_o'(CC_o')^{g_1}(c-Cb^*)$ and substituting this into (1.3) gives the main result

$$b = b^* - C_o'(CC_o')^{g_1}(Cb^* - c). \tag{2.3}$$

The validity of (2.3) is readily demonstrated as follows. By (2.2a) $CC_o'(CC_o')^{g_1}C = C$, and premultiplication of this equation by C' gives $C'CC_o'(CC_o')^{g_1}C = C'C$, i.e. $(K - S)C_o'(CC_o')^{g_1}C = C'C$ where $K= S + C'C$ is nonsingular. Hence

$$C_o'(CC_o')^{g_1}C = K^{-1}C'C \tag{2.4}$$

and, since $c \in \mathbb{C}(C)$ and $Sb^* = X'y$, (2.3) can be written as

$$b = b^* - K^{-1}C'(Cb^* - c)$$

$$= K^{-1}X'y + K^{-1}C'c \qquad (2.5)$$

which is the explicit solution to the normal equations subject to $Cb = c$ as given by Pringle and Rayner (1971, p.91).

Note that formula (2.3) is necessarily invariant to choice of orthogonal complement C_o, of g_1-inverse of CC_o', and of solution vector b^*. Also observe that if C has full row rank, then it follows from (2.4) that $C_o'(CC_o')^{g_1} = K^{-1}C'$ is unique. If in addition C_o has full row rank, then (2.3) becomes

$$b = b^* - C_o'(CC_o')^{-1}(Cb^* - c). \qquad (2.6)$$

a result which can in fact be written down directly from (1.3) and (2.1).

2.2 Special Cases of (2.3)

The formulae reported previously by other authors for expressing b in terms of certain solutions to the normal equations are now readily seen to be special cases of the main result (2.3) involving particular choices of C_o.

Consider firstly $C_o' = (I - GS)$ where G is a generalized inverse of S. Then (2.3) becomes

$$b = b^* - (I - GS)[C(I - GS)]^{g_1}(Cb^* - c) \qquad (2.7)$$

and for $c = 0$, C of full row rank, and $b^* = GX'y$ this expression reduces to that presented by Searle (1971,1984).

Consider also $C_o' = K_1^{-1}C_1'$ where C_1 is a matrix complementary to X and different to C and $K_1 = S + C_1'C_1$. Then (2.3) can be written as

$$b = b^* - K_1^{-1}C_1'(CK_1^{-1}C_1')^{g_1}(Cb^* - c). \qquad (2.8)$$

Rayner and Pringle (1976, 1987) derived this result for the case of b^* such that $C_1b^* = c_1$ where $c_1 \in \mathbb{C}(C_1)$ and in addition attempted to relate their work to that of Searle (1971) in the following way. Suppose C and C_1 both have full row rank and $b^* = GX'y$ is such that $C_1b^* = C_1GX'y = 0$. Then $(I - GS)C_1'(C_1C_1')^{-1} = K_1^{-1}C_1$ and (2.8) becomes

$$b = b^* - (I - GS)C_1'[C(I - GS)C_1']^{g_1}(Cb^* - c),$$

an expression similar to but not the same as (2.7).

2.3 An Alternative Approach

A more general approach to finding b in terms of b^* than that of Section 2.1 can be developed as follows. For $b = b^* - A(Cb^* - c)$ to be a solution to the normal equations subject to $Cb = c$, it is sufficient for A to satisfy the conditions

$$\begin{aligned} XAC &= 0 \\ CAC &= C \quad \text{i.e. } A = C^{g_1} . \end{aligned} \qquad (2.9)$$

Clearly A can be taken to be the matrix $C_o'(CC_o')^{g_1}$ of expression (2.3), but a more general form can be derived by observing that the conditions (2.9) are equivalent to $AC = K^{-1}C'C$ or from (2.4) to $AC = C_o'(CC_o')^{g_1}C$, and hence to

$$A = K^{-1}C'CC^{g_1} + Z(I - CC^{g_1}) \qquad (2.10a)$$

or equivalently to

$$A = C_o'(CC_o')^{g_1}CC^{g_1} + Z(I - CC^{g_1}) \tag{2.10b}$$

where Z is arbitary. For C of full row rank the conditions (2.9) become $\begin{matrix} XA = 0 \\ CA = I \end{matrix}$, and A is uniquely $K^{-1}C' = C_o'(CC_o')^{g_1}$ as noted earlier.

Expression (2.10a) also emerges by considering a set of necessary and sufficient conditions for $b = b^* + w$ to be a solution to (1.2) subject to $Cb = c$, viz.

$$\begin{bmatrix} X \\ C \end{bmatrix} w = \begin{bmatrix} 0 \\ -(Cb^* - c) \end{bmatrix}. \tag{2.11}$$

Following Rayner and Pringle (1976),the general form for a left inverse of $\begin{bmatrix} X \\ C \end{bmatrix}$ is given, by

$$[\ U \quad V\ ] = [K^{-1}SX^{g_1} + W(I - XX^{g_1}) \qquad K^{-1}C'CC^{g_1} + Z(I - CC^{g_1})]$$

where W and Z are arbitary, so that solving for w in (2.11) gives $w = -V(Cb^* - c)$ where V coincides with (2.10a).

It is interesting and important to observe that the conditions (2.9) are not strictly necessary. In particular if $b = b^* - A(Cb^* - c)$ is the solution to the normal equations subject to $Cb = c$ for <u>all</u> consistent c, then $\begin{bmatrix} X \\ C \end{bmatrix} ACz = \begin{bmatrix} 0 \\ Cz \end{bmatrix}$ for arbitary z, and hence (2.9) holds. However for some specific vector c, where c is not a scalar, it is always possible to find a matrix A not satisfying (2.9) but such that $b = b^* - A(Cb^* - c)$ is the required solution.

3. RELATIONSHIP BETWEEN SOLUTIONS TO THE NORMAL EQUATIONS OF THE FORM $GX'y$ WHERE G IS A GENERALIZED INVERSE OF X'X AND THOSE OBTAINED BY IMPOSING CONSTRAINTS OF THE TYPE $Cb = 0$

3.1 g_1-inverses of X'X

Let G be a generalized inverse of S such that $b = GX'y$ is the solution to the normal equations subject to the constraint $Cb = 0$ where C is complementary to X. Then G must satisfy

$$CGX' = 0 \tag{3.1}$$

or, equivalently,

$$GX' = K^{-1}X'. \tag{3.2}$$

Now using an approach similar to that of Rayner and Pringle (1976) it is readily seen that the subset of g_1-inverses of S which satisfy (3.1) for some matrix C is characterized by

$$G_1 = K^{-1}SG^{*} + ZC_o \tag{3.3}$$

or, equivalently, by

$$G_1 = K^{-1} + ZC_o$$

where G^{*} is a particular g_1-inverse of S and Z is arbitary. Note that this result is more general than that originally established by Rayner and Pringle (1976).

Consider now <u>all</u> the subsets of the g_1-inverses of S of the form (3.3) which can be generated from <u>all</u> possible choices of the matrix C in (3.1). Let the equivalence classes formed by partitioning the set of matrices complementary to X into subsets consisting of matrices having the same row space as C be denoted by [C] and note the following result.

Lemma 3.1 Let C_1 and C_2 be two matrices complementary to X. Then $K_1^{-1}X' = K_2^{-1}X'$ if and only if $\mathbb{R}(C_1) = \mathbb{R}(C_2)$, i.e. solutions to the normal equations b_1 and b_2, obtained by imposing the constraints $C_1b_1 = 0$ and $C_2b_2 = 0$ respectively, are the same if and only if $\mathbb{R}(C_1) = \mathbb{R}(C_2)$.

Proof: If $K_1^{-1}X' = K_2^{-1}X'$, then $C_1K_2^{-1}X' = 0$ and, since C_2 is an orthogonal complement of $K_2^{-1}X'$ and $r(C_1) = r(C_2)$, it follows that $\mathbb{R}(C_1) = \mathbb{R}(C_2)$. The converse is given in Silvey (1978).

Then it follows from Lemma 3.1 and from equation (3.2) that all distinct subsets of the form (3.3) can be generated by using a representative element from each of the equivalence classes [C], and also from Lemma 3.1 that these subsets are in fact disjoint. Furthermore any g_1-inverse of S, say G, belongs to one of these subsets. This follows by constructing the matrix

$$C = C_o(I - GS)$$

which is complementary to X (Rayner and Pringle, 1987) and is such that $CGX' = C_o(I - GS)GX' = 0$. Thus the set of g_1-inverses of S can be partitioned into equivalence classes based on the form (3.3) and denoted by $[K^{-1}SG^* + ZC_o]$.

Overall therefore there is a one-to-one correspondence between (i)solutions to the normal equations of the form $b = K^{-1}X'y$, i.e. solutions satisfying the linear constraint $Cb = 0$,

(ii)equivalence classes of g_1-inverses of S of the type $[\ K^{-1}SG^* + ZC_o]$, and

(iii)equivalence classes of matrices complementary to X of the type [C].

This correspondence is particularly important in understanding the nature of numerical solutions to the normal equations. It has undoubtedly been recognized at least implicitly by other authors but has not been formally demonstrated in the literature.

3.2 g_{12}- and g_{123}-inverses of X'X

The general form of a g_{12}-inverse of S satisfying (3.1) for some matrix C complementary to X is given by

$$\begin{aligned} G_{12} &= (\ K^{-1}SG^* + ZC_o)S(\ K^{-1}SG^* + ZC_o) \\ &= K^{-1}SG^* + K^{-1}SZC_o \end{aligned} \qquad (3.4)$$

where G^* is a particular g_1-inverse of S and Z is arbitary. Further there is only one such g_{12}-inverse which is symmetric, viz. $K^{-1}SK^{-1}$. Note that these results follow closely those of Rayner and Pringle (1976).

It is relevant at this point to examine the approach adopted by Searle (1984) to finding a generalized inverse of S satisfying (3.1) for some matrix C. Consider the result (2.3) in the form

$$b = Rb^{*} + C_o'(CC_o')^{g_1}c$$

where $R = I - C_o'(CC_o')^{g_1}C$, and observe from (2.2b) that $RC_o' = 0$ and thus that $\mathbb{R}(R) \subseteq \mathbb{R}(S)$. Then for b^{*} having the general form $GX'y + (I - GS)z$, where G is a g_1-inverse of S and z is an arbitary vector, and for c = 0 it follows that $b = Rb^{*} = RGX'y$. Now KR = S, i.e. $R = K^{-1}S$, so that $RG = K^{-1}SG$ has the form (3.4) and is thus a g_{12}-inverse of S satisfying (3.1). Searle (1984) derived the matrix RG for the specific case $C_o' = I - GS$, and further constructed a g_{12}-inverse of S from RG as (RG)S(RG), a step which is clearly unnecessary. In addition he formed the symmetric g_{12}-inverse (RG)S(RG)', which can be more simply expressed as $K^{-1}SK^{-1}$.

It should also be noted that Mazumdar, Li, and Bryce (1980) derived a g_{12}-inverse of S satisfying (3.1) in partitioned form. Their result cannot be readily related to those presented here but in any case would seem to be less tractible.

Consider now characterizing the g_{123}-inverses of S which satisfy (3.1) for some matrix C. Any such inverse, say G_{123}, must have the form (3.4) and must in addition satisfy condition (3) of (1.4). Then $SG_{123} = SK^{-1}SG^{*} + SK^{-1}SZC_o = SG^{*} + SZC_o$, and for this matrix to be symmetric, SZC_o must be 0 since Z is arbitary and G^{*} must be a g_{13}-inverse of S. Thus the required characterization is

$$G_{123} = K^{-1}SS^{g_{13}}. \tag{3.5}$$

Now for G_1 and G_2 two g_{13}-inverses of S, $SG_1S = G_1'S^2 = SG_2S = G_2'S^2$, so that $G_1'S = G_2'S$ and hence $SG_1 = SG_2$. Thus $SS^{g_{13}}$ is unique and there is precisely one g_{123}-inverse of S satisfying (3.1) for a given matrix C.

An interesting and appropriate choice of $S^{g_{13}}$ in (3.5) can be made from the following lemma:

Lemma 3.2 A g_1-inverse of S of the form K^{-1} where $K = S + C'C$ is a commuting g_1-inverse if and only if C is an orthogonal complement of X.
Proof: Assume $K^{-1}S = SK^{-1}$. Then $K^{-1}SC' = SK^{-1}C' = 0$, so that C is an orthogonal complement of X. Conversely suppose $K_o = S + C_o'C_o$. Then $K_oS = S^2 = SK_o$ and hence $K_o^{-1}S = SK_o^{-1}$.

Thus (3.5) can be written as

$$G_{123} = K^{-1}SK_o^{-1}. \tag{3.6}$$

Note that Rayner and Pringle (1976, p.452) used a different approach to the one above to derive the g_{123}-inverse of S satisfying (3.1) as $(S^2 + C'C)^{-1}S^2$,a result which is in fact wrong. The correct formulation should be $(S^2 + C'C)^{-1}S$, which is then seen to be equivalent to (3.6) since $K(S^2 + C'C)^{-1}SK_o = S$.

Clearly the arguements invoked in Section 3.1 for partitioning the set of g_1-inverses of S apply here. In particular observe that the set of g_{12}-inverse of S can be partitioned into equivalence classes of the form $[K^{-1}SG^* + K^{-1}SZC_o]$ which are in one-to-one correspondence with the equivalence classes [C] ,and also that the individual elements of the set of symmetric g_{12}- and of the set of g_{123}-inverses of S ,viz. $K^{-1}SK^{-1}$ and $K^{-1}SK_o^{-1}$ respectively, are in one-to-one correspondence with [C]. These and certain other relationships are summarized in Table 1.

3.3 <u>g_{124}-inverses and the g-inverse of X'X</u>

A g_{124}-inverse of S which satisfies (3.1) for some matrix C complementary to X, say G_{124}, must have the form (3.4) and must in addition satisfy condition (4) of (1.4). Now it follows from Lemma 3.2 that for $G_{124}S = K^{-1}S$ to be symmetric, K must be taken to be $K_o = S + C_o'C_o$. Thus the required characterization is given by

$$G_{124} = K_o^{-1}SG^* + K_o^{-1}SZC_o \qquad (3.7)$$

where G^* is a particular g_1-inverse of S and Z is arbitary. Furthermore it is clear from the partitioning of the set of g_1-inverses of S derived in Section 3.1 that (3.7) is a general form for <u>all</u> g_{124}-inverses of S and as such provides an interesting variant on the usual form $S(S^2)^{g_1}$ (Pringle and Rayner, 1971, p.27).

The Moore-Penrose inverse of S can be readily derived from (3.6) or from (3.7) by using Lemma 3.2 as

$$S^g = K_o^{-1}SK_o^{-1}.$$

This expression is considerably more simple than the partitioned form of S^g given by Mazumdar, Li, and Bryce (1980), and is clearly equivalent to the form $(S^2 + C_o'C_o)^{-1}S$ <u>implied</u> by Rayner and Pringle (1976).

Thus the solution to the normal equations of the form $GX'y$ with G a g_{124}- or the g-inverse of S is uniquely $b = K_o^{-1}X'y$ and satisfies constraints of the type $C_o b = 0$. It should be noted that Rayner and Pringle (1976) observed the solution $b = S^g X'y$ to satisfy $C_o b = 0$ and that Mazumdar, Li, and Bryce (1980) identified the constraints to which such a solution complies for two specific examples but without recognizing these constraints as involving orthogonal complements of X. For completeness the relationships between all generalized inverses of S which satisfy (3.1) for C an orthogonal complement of X are summarized in Table 2.

4. EXAMPLES

4.1 One-way Classification

Searle (1971,1984) gave an example of the single classification model $y_{ij} = \mu + \tau_i + \epsilon_{ij}$ (i=1,2,3) for which

$\beta = \begin{bmatrix} \mu \\ \tau_1 \\ \tau_2 \\ \tau_3 \end{bmatrix}$ and $X = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix}$ in (1.1). The solution $b^* = \begin{bmatrix} 0 \\ 100 \\ 86 \\ 32 \end{bmatrix}$

obtained either implicitly or explicitly by imposing the constraint m = 0 is to be converted to the solution for the restricted model with $\tau_1 + \tau_2 + \tau_3 = 0$. The calculations using (2.3) with C_o taken to be $[-1 \ 1 \ 1 \ 1]$ are straightforward; thus $C = [\ 0 \ 1 \ 1 \ 1\ ]$ and $Cb^* - c = 218$ so that $b = b^* - \frac{218}{3}C_o' = \frac{1}{3}\begin{bmatrix} 218 \\ 82 \\ 40 \\ -122 \end{bmatrix}$.

Note that in this example, and indeed in many experimental design models, an orthogonal complement of X of full row rank is readily obtained by inspection. Note also that the calculations involved in using alternative formulations of (2.3) can be cumbersome; in particular (2.7) requires a generalized inverse of S which may or may not be available and (2.8) requires that K^{-1} be computed.

This example leads naturally to the following more general result. Suppose that $r(X) = p - 1$ and that C and C_o have full row rank of 1;

then CC_o' and $Cb^* - c$ are scalars and the difference vector $b - b^*$ is a multiple of C_o'. In fact the numerical examples of Searle (1971, p.219) and Mazumdar, Li, and Bryce (1980) illustrate this point but were offered at the time without explanation.

The results of Section 3 are also illustrated using the present example with C = [0 1 1 1] and C_o = [-1 1 1 1]. It is straightforward to calculate K^{-1} and K_o^{-1} and hence the generalized inverses of X'X shown in Table 3. Note that the g_1-, g_{12}-, and g_{123}-inverses displayed there provide solutions to the normal equations which satisfy the constraint $t_1 + t_2 + t_3 = 0$, and that the g_{124}- and g-inverses provide solutions satisfying $-m + t_1 + t_2 + t_3 = 0$.

4.2 A Cheese-making Experiment

a) Data from a cheese-making experiment were described by the model

$$y_{ijk} = \mu + \delta_i + \tau_j + \alpha_k + (\tau\alpha)_{jk} + \epsilon_{ijk} \qquad (4.1)$$

for i=1,...,5 and j,k=1,2,3 where μ represents a common component, δ_i the effect of the ith day, τ_j that of the jth treatment, α_k that of the kth operator , and $(\tau\alpha)_{jk}$ represents a treatments x operators interaction. 15 observations were taken and the data were unbalanced due to mishap with

β' = [μ δ_1 δ_2 δ_3 δ_4 δ_6 τ_1 τ_2 τ_3 α_1 α_2 α_3 $(\tau\alpha)_{11}$ $(\tau\alpha)_{12}$ $(\tau\alpha)_{13}$ $(\tau\alpha)_{21}$ $(\tau\alpha)_{22}$ $(\tau\alpha)_{23}$ $(\tau\alpha)_{31}$ $(\tau\alpha)_{32}$ $(\tau\alpha)_{33}$]

$$X = \begin{bmatrix} 1&1&0&0&0&0&0&1&0&0&0&1&0&0&0&0&0&1&0&0&0 \\ 1&1&0&0&0&0&1&0&0&0&1&0&0&1&0&0&0&0&0&0&0 \\ 1&1&0&0&0&0&0&0&1&1&0&0&0&0&0&0&0&0&0&0&0 \\ 1&0&1&0&0&0&0&0&1&0&0&1&0&0&0&0&0&0&0&0&1 \\ 1&0&1&0&0&0&1&0&0&0&1&0&0&1&0&0&0&0&0&0&0 \\ 1&0&1&0&0&0&0&1&0&1&0&0&0&0&0&1&0&0&0&0&0 \\ 1&0&0&1&0&0&1&0&0&0&0&1&0&0&1&0&0&0&0&0&0 \\ 1&0&0&1&0&0&0&1&0&0&1&0&0&0&0&0&1&0&0&0&0 \\ 1&0&0&1&0&0&0&0&1&1&0&0&0&0&0&0&0&0&1&0&0 \\ 1&0&0&0&1&0&0&0&1&0&1&0&0&0&0&0&0&0&0&1&0 \\ 1&0&0&0&1&0&1&0&0&1&0&0&1&0&0&0&0&0&0&0&0 \\ 1&0&0&0&1&0&0&1&0&0&0&1&0&0&0&0&0&1&0&0&0 \\ 1&0&0&0&0&1&1&0&0&1&0&0&1&0&0&0&0&0&0&0&0 \\ 1&0&0&0&0&1&0&1&0&0&1&0&0&0&0&0&1&0&0&0&0 \\ 1&0&0&0&0&1&0&0&1&0&0&1&0&0&0&0&0&0&0&0&1 \end{bmatrix} \text{ and } y = \begin{bmatrix} 26.9 \\ 27.6 \\ 28.1 \\ 25.6 \\ 25.8 \\ 26.1 \\ 26.8 \\ 27.1 \\ 27.3 \\ 27.5 \\ 26.5 \\ 26.8 \\ 27.1 \\ 26.9 \\ 26.9 \end{bmatrix}$$

in (1.1).

The solution to the normal equations provided by the statistical computer package SAS ,which implicitly sets the estimates of δ_5, τ_3, α_3, $(\tau\alpha)_{13}$, $(\tau\alpha)_{23}$, $(\tau\alpha)_{31}$, $(\tau\alpha)_{32}$, and $(\tau\alpha)_{33}$ equal to zero, was available as $b^{*'} = [\ 26.941\dot{6}\ 0.\dot{3}\ -1.38\dot{3}\ -0.1\dot{3}\ -0.18\dot{3}\ 0\ -0.008\dot{3}\ -0.1\dot{6}\ 0\ 0.658\dot{3}\ 0.741\dot{6}\ 0\ -0.7\ -0.45\ 0\ 0.05\ -0.45\ 0\ 0\ 0\ 0\ ]$. In order to obtain the solution to model (4.1) subject to the 'usual constraints'

$$\Sigma\delta_i = \Sigma\tau_j = \Sigma\alpha_k = \sum_j(\tau\alpha)_{jk} = \sum_k(\tau\alpha)_{jk} = 0,$$

formula (2.6) was applied with

$$C = \begin{bmatrix} 0&1&1&1&1&1&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&1&1&1&0&0&0&0&0&0&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0&0&1&1&1&0&0&0&0&0&0&0&0.0 \\ 0&0&0&0&0&0&0&0&0&0&0&0&1&1&1&0&0&0&0&0&0 \\ 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&1&1&0&0&0 \\ 0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&0&1&1&1 \\ 0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&1&0&0&1&0&0 \\ 0&0&0&0&0&0&0&0&0&0&0&0&0&1&0&0&1&0&0&1&0 \end{bmatrix} \qquad (4.2)$$

and

$$C_o = \begin{bmatrix} -1 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \end{bmatrix} \tag{4.3}$$

where C_o was found by inspection and C and C_o have been contrived to have full row rank. The required solution is $b' = [26.90\dot{4}\ 0.60\dot{6}\ -1.11\ 0.14\ 0.09\ 0.27\dot{3}\ -0.16\dot{1}\ -0.069\dot{4}\ 0.230\dot{5}\ 0.147\dot{2}\ 0.147\dot{2}\ -0.29\dot{4}\ -0.27\dot{2}\ 0.06\dot{1}\ 0.2\dot{1}\ 0.22\dot{7}\ -0.1\dot{8}\ -0.03\dot{8}\ 0.0\dot{4}\ 0.12\dot{7}\ -0.17\dot{2}]$.

The matrix operations involved in this example can be performed using packages such as SAS/IML or MINITAB. However such calculations are tedious and attention should turn to the feasibility of using the explicit solution (2.5) *ab initio*. Most statistical computer packages do not handle a constrained model $y = X\beta + \epsilon$ such that $C\beta = c$ directly. However it is usually possible to analyse the augmented model $\begin{bmatrix} y \\ c \end{bmatrix} = \begin{bmatrix} X \\ C \end{bmatrix}\beta + \epsilon$ with attendant normal equations $Kb = X'y + C'c$, thereby obtaining a solution which coincides with the required constrained solution.

b) Suppose that the interaction term is dropped from model (4.1) and that one is interested in obtaining the solution to the normal equations subject to the 'usual constraints' from some other solution $b^{*'} = [m^* \ d_1^* \ d_2^* \ d_3^* \ d_4^* \ d_5^* \ t_1^* \ t_2^* \ t_3^* \ a_1^* \ a_2^* \ a_3^* \ ]$. Then C and C_o can be taken as the leading 3 x 12 submatrices of (4.2) and (4.3) respectively, $CC_o' = \text{diag}\ \{5,3,3\}$, and b^* can be adjusted to give the required solution b as :

$$
\begin{aligned}
m &= m^* + \Sigma d_i^* + \Sigma t_j^* + \Sigma a_k^* \\
d_i &= m^* - \Sigma d_i^* \qquad i=1,\ldots,5 \\
t_j &= m^* - \Sigma t_j^* \qquad j=1,2,3 \\
a_k &= m^* - \Sigma a_k^* \qquad k=1,2,3
\end{aligned}
$$

adjustments which seem natural and may well be familiar. Note that the numerical solution *b* has no meaning *per se*, but is nevertheless attractive in that it provides estimated treatment means which coincide with the observed treatment means.

This example suggests the following more general result. Consider an experimental design model (Graybill, 1976, p.506) written as (1.1) with X partitionable as $[\ 1_n\ X_1\ X_2 \ldots X_g\ ]$ and β conformably partitioned as $\beta' = [\ \beta_o\ \beta_1'\ \beta_2'\ \ldots\ \beta_g'\ ]$. The vectors $\beta_1, \beta_2, \ldots, \beta_g$ with $p_1, p_2, \ldots, p_g$ elements respectively represent g groups of parameters corresponding to the classifications of the design and each submatrix X_i, $i=1,\ldots,g$, is such that it has full column rank, p_i, and every row has one element equal to 1 and all others zero. Assume that $r(X) = p - g$ and observe that $X_i 1_{p_i} = 1_n$ for all i. Then an orthogonal complement of X can taken as

$$C_o = \begin{bmatrix} -1 & 1_{p_1} & 0 & \dots & 0 \\ -1 & 0 & 1_{p_2} & \dots & 0 \\ \cdot & \cdot & \cdot & & \cdot \\ -1 & 0 & 0 & & 1_{p_g} \end{bmatrix}$$

If C corresponds to g linear constraints which involve each group separately, then CC_o' is diagonal, and it is trivial to obtain a g_1-inverse of CC_o'.

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Table 3. Generalized inverses of X'X satisfying (3.1) for Example 4.1

Inverse	Formulation	Example
g_1	$K^{-1}SG^{*}+ZC_0$ [a]	$\frac{1}{18}\begin{bmatrix}0 & 2 & 3 & 9\\ 0 & 4 & -3 & -9\\ 0 & -2 & 6 & -9\\ 0 & -2 & -3 & 18\end{bmatrix} + \begin{bmatrix}z_1\\ z_2\\ z_3\\ z_4\end{bmatrix}[-1\ \ 1\ \ 1\ \ 1]$ [b]
g_{12}	$K^{-1}SG^{*}+K^{-1}SZC_0$ [a]	$\frac{1}{18}\begin{bmatrix}0 & 2 & 3 & 9\\ 0 & 4 & -3 & -9\\ 0 & -2 & 6 & -9\\ 0 & -2 & 6 & 18\end{bmatrix} + \begin{bmatrix}z_1\\ z_2\\ z_3\\ -z_2+z_3\end{bmatrix}[-1\ \ 1\ \ 1\ \ 1]$ [b]
symmetric g_{12}	$K^{-1}SK^{-1}$	$\frac{1}{54}\begin{bmatrix}11 & -5 & -2 & 7\\ -5 & 17 & -4 & -13\\ -2 & -4 & 20 & -16\\ 7 & -13 & -16 & 29\end{bmatrix}$ [c]
g_{123}	$K^{-1}SK_0^{-1}$	$\frac{1}{72}\begin{bmatrix}11 & -3 & 1 & 13\\ -5 & 21 & -7 & -19\\ -2 & -6 & 26 & -22\\ 7 & -15 & -19 & 41\end{bmatrix}$
g_{124}	$K_0^{-1}SG^{*}+K_0^{-1}SZC_0$ [a]	$\frac{1}{24}\begin{bmatrix}0 & 2 & 3 & 6\\ 0 & 6 & -3 & -6\\ 0 & -2 & 9 & -6\\ 0 & -2 & -3 & 18\end{bmatrix} + \begin{bmatrix}z_1\\ z_2\\ z_3\\ z_1-z_2-z_3\end{bmatrix}[-1\ \ 1\ \ 1\ \ 1]$ [b]
unique g	$K_0^{-1}SK_0^{-1}$	$\frac{1}{96}\begin{bmatrix}11 & -3 & 1 & 13\\ -3 & 27 & -9 & -21\\ 1 & -9 & 35 & -25\\ 13 & -21 & -25 & 29\end{bmatrix}$

[a] $G^{*} = \begin{bmatrix}0 & & & \\ & \frac{1}{3} & & \\ & & \frac{1}{2} & \\ & & & 1\end{bmatrix}$

[b] z_i arbitrary, $i = 1,\dots,4$

[c] Also obtained by Searle (1971)

Table 1. Equivalence classes of the generalized inverses of X'X

[C]

$\left[K^{-1}SG^{*}+ZC_0\right]$	$\left[K^{-1}SG^{*}+K^{-1}SZC_0\right]$	$\left[K^{-1}SK_0^{-1}\right]^{+}$
$\left[K^{-1}+ZC_0\right]$		g_{123} - inverses
g_1 - inverses	$\left[K^{-1}SK^{-1}\right]^{+}$ symmetric	
	g_{12} - inverses	

+One element in each equivalence class

Table 2. Generalized inverses of X'X satisfying (3.1) for C an orthogonal complement of X

$\left[G:G = K_0^{-1}SG^{*}+ZC_0\right]$	$\left[G:G = K_0^{-1}SG^{*}+K_0^{-1}SZC_0\right]$	$K_0^{-1}SK_0^{-1}$
	g_{12} - inverses	symmetric g_{12} - inverse
$\left[G:G = K^{-1}+ZC_0\right]$	g_{124} - inverses+	g_{123} - inverse
g_1 - inverses		the g - inverse

+<u>All</u> g_{124} - inverses of X'X