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A Note on Estimability in Linear Models

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Abstract Estimable functions of the parameters are characterized in terms of generalized inverses. The concept of estimability is applied to data from a designed experiment on varietal trials. We demonstrate in this note that this technique of solving the normal equations is equivalent to the nearest neighbour method for the analysis of unbalanced randomized design.

Keywords BLUE, Estimable Functions, Estimability, Generalized Inverses, Less than Full Rank, Linear Combination, Linear Models

1. Introduction

Linear models are generally of the form

$$y = X\beta + \varepsilon \tag{1}$$

(where y is an $n \times 1$ observation vector, X is an $n \times p$ design matrix of fixed constants having rank r $(r \leq k)$, β is an $p \times 1$ vector of unknown parameters, ε is an $n \times 1$ vector of unknown random errors having zero means) and $E(y) = X\beta$. The Ordinary Least Square (OLS) solution of (1) is $\hat{\beta} = (X'X)^{-1} X'y$, a unique solution.

In practice, not all linear models of the form in (1) are of full rank. When X is not of full rank, then $X'X$ is singular and the normal equations $(X'X)b = X'y$ do not have a unique solution. However, there are various approaches of obtaining the inverse of singular matrices, for which the row echelon form given by Elswick et al (1991), Moore Penrose and the generalized inverse, Searle (1977) are popular in the literature. The generalized inverse is the approach we apply in this paper.

2. Form of Estimability

With X less than full rank and $X'X$ singular, i.e. $r \leq k$, there is an infinite number of solutions of $\hat{\beta}$ to the normal equations. Attention is therefore directed not to the solutions themselves but to linear functions of their elements. Consider a linear function $q'\beta$ of the parameters in β, where q is a known vector. This linear function is defined as being an estimable function if there exists some linear combinations of the observations $y_1, y_2, \ldots, y_n$ whose expected value is $q'\beta$, i.e. if there exists a vector t such that the expected value of $t'y$ is $q'\beta$, then $q'\beta$ is said to be estimable. Consider the following theorem given in Graybill, 1976:

Theorem 1. (Graybill, 1976)

Assuming a linear model in (1), $q'\beta$ is an estimable function if and only if there exist an $n \times 1$ vector t such that $q' = t'X$

***Proof**. If there exist a vector t such that $q' = t'X$, then,*

$$E(t'y) = t'E(y) = t'X\beta = q'\beta.$$

Only if: Conversely, if $q'\beta$ is estimable, then,

$$E(t'y) = q'\beta$$

Thus

$$t'X\beta = q'\beta \Rightarrow t'X = q'$$

In addition, Elswick et al (1991) argues that if X is of full rank, $(X'X)^{-1}$ exists and the rows of $p \times n$ matrix $(X'X)^{-1} X'$ serve as the necessary set of vectors because $\left\{(X'X)^{-1} X'\right\} X\beta = \beta$.

3. Illustration

We demonstrate this discussion by considering the data from a study to compare classical and nearest neighbour methods in the analysis of varietal trials (See, e.g. Nwobi, 2000). In the experiment, nine (9) different varieties of cassava crop were tried, six at a time over a maximum of five years in such a way that these varieties were not replicated

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equally. The model (without interaction) is given by

$$y_{ij} = \mu + \tau_i + \varepsilon_{ij} \quad i = 1, 2, ..., 9; \; j = r_i \qquad (3)$$

where y_{ij} is the yield from the j[th] trial of the i[th] variety, μ is the general mean, τ_i is the effect of the i[th] variety, ε_{ij} is the random error associated with y_{ij}.

Equation (3) is written in matrix form as

$$y = X\beta + \varepsilon. \qquad (4)$$

Based on the model in (2), the parameter vector β is given by

$$\beta' = (\beta_0 \beta_1 \; \beta_2 \; \beta_3 \; \beta_4 \; \beta_5 \; \beta_6 \; \beta_7 \; \beta_8 \; \beta_9)$$
$$\equiv (\mu \, \tau_1 \, \tau_2 \, \tau_3 \, \tau_4 \, \tau_5 \, \tau_6 \, \tau_7 \, \tau_8 \, \tau_9)$$

The components of the model (4) are

$$\begin{pmatrix} 36.6 \\ 37.9 \\ 21.49 \\ 23.8 \\ 8.0 \\ 0.29 \\ 41.9 \\ 31.6 \\ 17.68 \\ 29.05 \\ 28.33 \\ 31.6 \\ 15.1 \\ 15.13 \\ 33.7 \\ 9.4 \\ 7.07 \\ 20.41 \\ 29.52 \\ 2.8 \\ 12.7 \\ 6.22 \\ 4.41 \\ 2.99 \\ 13.42 \\ 9.84 \\ 19.85 \\ 15.81 \\ 1.1 \\ 20.88 \end{pmatrix} = \begin{pmatrix} 1&1&0&0&0&0&0&0&0&0 \\ 1&1&0&0&0&0&0&0&0&0 \\ 1&1&0&0&0&0&0&0&0&0 \\ 1&0&1&0&0&0&0&0&0&0 \\ 1&0&1&0&0&0&0&0&0&0 \\ 1&0&1&0&0&0&0&0&0&0 \\ 1&0&0&1&0&0&0&0&0&0 \\ 1&0&0&1&0&0&0&0&0&0 \\ 1&0&0&1&0&0&0&0&0&0 \\ 1&0&0&1&0&0&0&0&0&0 \\ 1&0&0&1&0&0&0&0&0&0 \\ 1&0&0&0&1&0&0&0&0&0 \\ 1&0&0&0&1&0&0&0&0&0 \\ 1&0&0&0&1&0&0&0&0&0 \\ 1&0&0&0&0&1&0&0&0&0 \\ 1&0&0&0&0&1&0&0&0&0 \\ 1&0&0&0&0&1&0&0&0&0 \\ 1&0&0&0&0&1&0&0&0&0 \\ 1&0&0&0&0&1&0&0&0&0 \\ 1&0&0&0&0&0&1&0&0&0 \\ 1&0&0&0&0&0&1&0&0&0 \\ 1&0&0&0&0&0&1&0&0&0 \\ 1&0&0&0&0&0&1&0&0&0 \\ 1&0&0&0&0&0&1&0&0&0 \\ 1&0&0&0&0&0&0&1&0&0 \\ 1&0&0&0&0&0&0&1&0&0 \\ 1&0&0&0&0&0&0&0&1&0 \\ 1&0&0&0&0&0&0&0&1&0 \\ 1&0&0&0&0&0&0&0&0&1 \\ 1&0&0&0&0&0&0&0&0&1 \end{pmatrix} \begin{pmatrix} \mu \\ t_1 \\ t_2 \\ t_3 \\ t_4 \\ t_5 \\ t_6 \\ t_7 \\ t_8 \\ t_9 \end{pmatrix} + \begin{pmatrix} e_{11} \\ e_{12} \\ e_{13} \\ e_{21} \\ e_{22} \\ e_{23} \\ e_{31} \\ e_{32} \\ e_{33} \\ e_{34} \\ e_{35} \\ e_{41} \\ e_{42} \\ e_{43} \\ e_{51} \\ e_{52} \\ e_{53} \\ e_{54} \\ e_{55} \\ e_{61} \\ e_{62} \\ e_{63} \\ e_{64} \\ e_{65} \\ e_{71} \\ e_{72} \\ e_{81} \\ e_{82} \\ e_{91} \\ e_{92} \end{pmatrix}$$

from where we obtain

$$X'X = \begin{pmatrix} 30 & 3 & 3 & 5 & 3 & 5 & 5 & 2 & 2 & 2 \\ 3 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 3 & 0 & 3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 5 & 0 & 0 & 5 & 0 & 0 & 0 & 0 & 0 & 0 \\ 3 & 0 & 0 & 0 & 3 & 0 & 0 & 0 & 0 & 0 \\ 5 & 0 & 0 & 0 & 0 & 5 & 0 & 0 & 0 & 0 \\ 5 & 0 & 0 & 0 & 0 & 0 & 5 & 0 & 0 & 0 \\ 2 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 \\ 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 & 0 \\ 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 2 \end{pmatrix}; X'y = \begin{pmatrix} 548.59 \\ 95.99 \\ 32.09 \\ 148.56 \\ 61.83 \\ 100.1 \\ 29.12 \\ 23.26 \\ 35.66 \\ 21.98 \end{pmatrix}$$

A generalized inverse of $X'X$ written as G^- such that $X'XG^{-1}X'X = X'X$ see, e.g. Searle (1977) is

$$G^- = \begin{pmatrix} 0.0310 & 0.0023 & 0.0023 & -0.0110 & 0.0023 & -0.0110 & -0.0110 & 0.0190 & 0.0190 & 0.0190 \\ 0.0023 & 0.2977 & -0.0357 & -0.0223 & -0.0357 & -0.0223 & -0.0223 & -0.0523 & -0.0523 & -0.0523 \\ 0.0023 & -0.0357 & 0.2977 & -0.0223 & -0.0357 & -0.0223 & -0.0223 & -0.0523 & -0.0523 & -0.0523 \\ -0.0110 & 0.0023 & -0.0223 & 0.1910 & -0.0023 & -0.0090 & -0.0090 & -0.0390 & -0.0390 & -0.0390 \\ 0.0023 & -0.0357 & -0.0357 & -0.0223 & 0.2977 & -0.0223 & -0.0223 & -0.0523 & -0.0523 & -0.0523 \\ -0.0110 & 0.0023 & -0.0223 & -0.0090 & -0.0023 & 0.1910 & -0.0090 & -0.0390 & -0.0390 & -0.0390 \\ 0.0110 & -0.0023 & -0.0223 & -0.0090 & -0.0023 & -0.0090 & 0.1910 & -0.0390 & -0.0390 & -0.0390 \\ 0.0190 & -0.0523 & -0.0523 & -0.0390 & -0.0523 & -0.0390 & -0.0390 & 0.4310 & -0.0690 & -0.0690 \\ 0.0190 & -0.0523 & -0.0523 & -0.0390 & -0.0523 & -0.0390 & -0.0390 & -0.0690 & 0.4310 & -0.0690 \\ 0.0190 & -0.0523 & -0.0523 & -0.0390 & -0.0523 & -0.0390 & -0.0390 & -0.0690 & -0.0690 & 0.4310 \end{pmatrix}$$

with

$$H = G^- X'X = \begin{pmatrix} 0.9 & 0.1 & 0.1 & 0.1 & 0.1 & 0.1 & 0.1 & 0.1 & 0.1 & 0.1 \\ 0.1 & 0.9 & -0.1 & -0.1 & -0.1 & -0.1 & -0.1 & -0.1 & -0.1 & -0.1 \\ 0.1 & -0.1 & 0.9 & -0.1 & -0.1 & -0.1 & -0.1 & -0.1 & -0.1 & -0.1 \\ 0.1 & -0.1 & -0.1 & 0.9 & -0.1 & -0.1 & -0.1 & -0.1 & -0.1 & -0.1 \\ 0.1 & -0.1 & -0.1 & -0.1 & 0.9 & -0.1 & -0.1 & -0.1 & -0.1 & -0.1 \\ 0.1 & -0.1 & -0.1 & -0.1 & -0.1 & 0.9 & -0.1 & -0.1 & -0.1 & -0.1 \\ 0.8 & 0 & 0 & 0 & 0 & 0 & 1 & -0.1 & -0.1 & -0.1 \\ 0.1 & -0.1 & -0.1 & -0.1 & -0.1 & -0.1 & -0.1 & 0.9 & -0.1 & -0.1 \\ 0.1 & -0.1 & -0.1 & -0.1 & -0.1 & -0.1 & -0.1 & -0.1 & 0.9 & -0.1 \\ 0.1 & -0.1 & -0.1 & -0.1 & -0.1 & -0.1 & -0.1 & -0.1 & -0.1 & 0.9 \end{pmatrix}$$

and $w' = \begin{pmatrix} w_0 & w_1 & w_2 & w_3 & w_4 & w_5 & w_6 & w_7 & w_8 & w_9 \end{pmatrix}$.

The function $q'b = w'Hb = \left(w_1 + w_2 + w_3 + ... + w_8 + w_9\right)\mu + w_1t_1 + w_2t_2 + ... + w_8t_8 + w_9t_9$

is estimable for any given values to the $w's$.
With this we obtain the solution to the normal equation as

$$\hat{b} = G^- X'y = \begin{pmatrix} 15.9 & 16.1 & -5.2 & 13.8 & 4.7 & 4.1 & 2.0 & -4.3 & 1.9 & -4.9 \end{pmatrix}'$$

Therefore, the Best Linear Unbiased Estimator (BLUE) of $q'b$ is

$$q'\hat{b} = w'\hat{b}_0 = 15.9w_0 + 16.1w_1 - 5.2w_2 + 13.8w_3 + 4.7w_4 + 4.1w_5 + 2.0w_6 - 4.3w_7 + 1.9w_8 - 4.9w_9$$

To see if β_i where $i = 0,1,2,3,...,9$ is estimable, we write the parameter as $\beta_i = t'\beta$ where, in this case, we define $T = \left(\underline{t}'_0, \underline{t}'_1, \ldots, \underline{t}'_9\right)$, a $p \times p$ matrix; $\underline{t}'_i$ is of dimension $1 \times p$, so that

$$T' = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

and

$$T'G\left(X'X\right) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

Since $T'G\left(X'X\right) \neq T'$, β_i is not estimable. However, considering $\beta_i - \beta_{i'}$, $i < i'$, this function may be written for $i = 1$ and $i' = 2$ as $\beta_1 - \beta_2 = T'\beta$ where $T' = \left[01{-}10000000\right]$ so that $T'G^{-}\left(X'X\right) = \left(0 \;\; 1 \;\; -1 \;\; 0 \;\; 0 \;\; 0 \;\; 0 \;\; 0 \;\; 0 \;\; 0\right) = T'$. This implies that $\beta_1 - \beta_2$ is estimable.

Similarly, since there are 9 (nine) parameters, taking two (contrast) at a time gives ${}^9C_2 = 36$ estimable functions

$$T' = \begin{pmatrix} 0 & 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & -1 \end{pmatrix}$$

Therefore, $T'G^{-}\left(X'X\right) = T'$. Thus, we can say that a linear combination of estimable functions is estimable.

4. Conclusions

We have shown that for any arbitrary vector w, $q'b = w'Hb$ is estimable with BLUE $q'\hat{b} = w'\hat{b}_0$. The solution of the normal equation, $\hat{b}$, confirms that this approach is equivalent to the Nearest Neighbour method of analysis of designed experiments. Both methods agree on the selection of varieties though the value of these estimates are not unique due to the application of generalized inverses. Furthermore, we verified that the linear combination of estimable functions is estimable.

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