SINGULAR WEIGHING DESIGNS[1]

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1. Summary and introduction. Suppose we are given p objects to be weighed in N weighings with a chemical balance having no bias. Let $X = (x_{ij})$ be the weighing design matrix, where $x_{ij} = +1$ or -1 if the jth object is included in the ith weighing by being placed respectively in the left or right hand pan, and $x_{ij} = 0$ if the jth object is not weighed in the ith weighing. The weighing results may be represented by means of the following matrix equation,

$$y = Xw + \epsilon, \tag{1.1}$$

where y is the column vector of the results recorded in the N weighings, ϵ is the column vector of the errors in these results and w is the column vector of the true weights. Under the assumption that ϵ has mean $0_{N,1}$ and dispersion matrix $\sigma^2 I_N$, where $0_{m \times n}$ is the $m \times n$ null matrix and I_N is the Nth order identity matrix, the normal equations estimating w are given by the equation

$$S\hat{w} = X'y, \tag{1.2}$$

where $S = X'X$ and $\hat{w}$ is the column vector of the estimated weights. The weighing designs problem was studied till now when S is non singular (cf. Hotelling [1], Kishen [2], Mood [3], Raghavarao [4]).

There is no recorded literature dealing with weighing designs whose S is singular. Occasions may arise when the experimenter is faced with weighing designs whose S is singular. We now define

Definition 1.1. A weighing design X is said to be singular if the matrix S is singular.

The word "singular weighing design" in the above definition is somewhat misleading, but is used for the lack of a suitable word. Singular weighing designs may occur in the following cases.

1. *Bad designing*. As there are no best weighing designs tables, an experimenter who desires to use a particular order weighing design, has to construct one for himself before starting the weighing operations. In such circumstances bad designing may result in singular weighing designs.

2. *Laboratory observations*. Many scientists are of the opinion that they can achieve greater precision in their readings by repeating their experiments. The process of repeating weighing operations may also lead to singular weighing designs, when the number of independent linear weighing operations made is less than the number of objects.

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3. *Accidental.* Though optimum or best weighing designs have been selected by the experimenter, accidentally some objects may fall down and break while taking the weighings. In that case, if the experimenter continues his weighing operations, putting $x_{ij} = 0$ for the broken objects, he may finally obtain a singular weighing design. For example, let an experimenter plan to weigh 5 objects in 5 weighings with the design P_5 of [4]. After two weighings, the first two objects fell down and broke. If he continues the weighing operations assuming $x_{ij} = 0$ $(i = 3, 4, 5; j = 1, 2)$, he gets a singular weighing design.

This paper deals with two statistical questions. The first question concerns the estimability of individual weights of the objects and the second question considered is the taking of additional weighings so as to render the problem one of full rank and if possible so as to minimize the resulting generalized variance of the estimates, which is equivalent to Mood's efficiency definition.

In Section 2, results on singular weighing designs together with some matrix lemmas are given, outlining the proofs wherever necessary. Necessary and sufficient conditions for the estimability of individual weights of the objects are given in Section 3 and the problem of taking additional weighings so as to obtain the estimates of all the objects is considered in Section 4.

2. Preliminaries and some matrix lemmas. Let the singular weighing design X, be of rank r. Without loss of generality we assume that the first r columns of X are independent and $X = [X_1 \quad X_2]$, where X_1 is an $N \times r$ matrix of rank r and X_2 is an $N \times (p - r)$ matrix. Let us define $J = (X_1'X_1)^{-1}X_1'X_2$. Then it is easy to see that $X_2 = X_1J$. A solution of the normal equations (1.2) is

$$\hat{w} = \begin{bmatrix} (X_1' X_1)^{-1}X_1' y \\ 0_{p-r,1} \end{bmatrix}. \tag{2.1}$$

We devote the rest of this section for some matrix results, which will be re quired for further development of our problem.

LEMMA 2.1. *Given four matrices A, B, C and D of orders $p \times p$, $p \times q$, $q \times p$ and $q \times q$ respectively, if D is non singular then*

$$\begin{vmatrix} A & B \\ C & D \end{vmatrix} = |D| \, |A - BD^{-1}C|. \tag{2.2}$$

LEMMA 2.2. *If*

$$Z = \begin{bmatrix} Z_1 & Z_2 \\ Z_2' & Z_3 \end{bmatrix} \tag{2.3}$$

is a partitioned symmetric matrix such that Z and Z_1 are non singular, then

$$Z^{-1} = \begin{bmatrix} Z_1^{-1}\{I + Z_2 F^{-1}Z_2' Z_1^{-1}\} & -Z_1^{-1}Z_2 F^{-1} \\ -F^{-1}Z_2' Z_1^{-1} & F^{-1} \end{bmatrix}, \tag{2.4}$$

where

$$F = Z_3 - Z_2'Z_1^{-1}Z_2. \tag{2.5}$$

LEMMA 2.3. *If Z is a non singular $n \times n$ matrix, and U and V are $n \times m$ and $m \times n$ matrices respectively, then*

$$(Z + UV)^{-1} = Z^{-1} - Z^{-1}U\{I_m + VZ^{-1}U\}^{-1}VZ^{-1}. \tag{2.6}$$

The result can be proved by multiplying the members of the above relation in either direction by $Z + UV$, yielding the identity matrix.

LEMMA 2.4. *For the matrices Z, U and V as defined in Lemma 2.3, we have*

$$|Z + UV| = |Z|\,|I_m + VZ^{-1}U|. \tag{2.7}$$

PROOF. Taking the determinants on both sides of (2.6),

$$|(Z + UV)^{-1}| = |Z^{-1}|\,|I_n - U\{I_m + VZ^{-1}U\}^{-1}VZ^{-1}|. \tag{2.8}$$

Let $c_1, c_2, \cdots, c_n$ be the characteristic roots of $U\{I_m + VZ^{-1}U\}^{-1}VZ^{-1}$, out of which $c_1, c_2, \cdots, c_s$ are non zero. Then, it is well known that $VZ^{-1}U\{I_m + VZ^{-1}U\}^{-1}$ has $c_1, c_2, \cdots, c_s$ as the only non zero characteristic roots. Now,

$$\begin{aligned} |I_n - U\{I_m + VZ^{-1}U\}^{-1}VZ^{-1}| &= (1 - c_1)(1 - c_2) \cdots (1 - c_n) \\ &= (1 - c_1)(1 - c_2) \cdots (1 - c_s) = |I_m - VZ^{-1}U\{I_m + VZ^{-1}U\}^{-1}| \\ &= |\{I_m + VZ^{-1}U\} - VZ^{-1}U|\,|\{I_m + VZ^{-1}U\}^{-1}| \\ &= |\{I_m + VZ^{-1}U\}^{-1}|. \end{aligned} \tag{2.9}$$

Substituting the above value in (2.8) and taking the reciprocals, we get the required result.

3. Estimability of individual weights of the objects for singular weighing designs.

If b is any column vector of order p, $b'w$ is said to be a linear parametric function of the weights. The linear parametric function $b'w$ of the weights is said to be estimable, if there exists a column vector a of order N such $E(a'y) = b'w$, where E stands for the mathematical expectation of the random variable. It easily follows that the linear parametric function $b'w$ of the weights is estimable for a singular weighing design, if, and only if

$$\text{rank }(X') = \text{rank }(X' \mid b). \tag{3.1}$$

In weighing designs, we will be interested in finding the estimates of the individual weights of the objects. Hence, we try to find necessary and sufficient conditions for the estimability of the parametric function $\rho_i'w$ of the weights, where $\rho_i (i = 1, 2, \cdots, p)$ is the ith column vector of I_p. Let $x_1, x_2, \cdots, x_p$ be the column vectors of X. We now have

THEOREM 3.1. *A necessary and sufficient condition that the parametric function $\rho_i'w$ of the weights is estimable, is that*

$$\text{rank }\{x_1, x_2, \cdots, x_{i-1}, x_{i+1}, \cdots, x_p\} = r - 1. \tag{3.2}$$

By noting that rank $(X' \mid \rho_i) = 1 + \text{rank }(x_1, x_2, \cdots, x_{i-1}, x_{i+1}, \cdots, x_p)$, the above theorem follows easily from the necessary and sufficient Condition (3.1) for the estimability of the parametric function $\rho_i' w$ of the weights.

An interesting corollary to the above theorem is

COROLLARY 3.1.1. *The parametric functions* $\rho_{r+j}' w$ *of the weights are not estimable* $(j = 1, 2, \cdots, p - r)$.

Let $\xi_1, \xi_2, \cdots, \xi_r$ be the r column vectors of order $p - r$ of J'. If the individual weight of the i_1th object $(i_1 = 1, 2, \cdots, r)$ is estimable, then from Theorem 3.1 we should have rank $(x_1, x_2, \cdots, x_{i_1-1}, x_{i_1+1}, \cdots, x_r, X_2) = r - 1$, which is possible if and only if $\xi_{i_1} = 0_{p-r,1}$. Hence we have

THEOREM 3.2. *The individual weight of the* i_1th $(i_1 = 1, 2, \cdots, r)$ *object is estimable if and only if* $\xi_{i_1} = 0_{p-r,1}$.

If the individual weights of the first r objects are estimable, then from Theorem 3.2, we have $\xi_1 = \xi_2 = \cdots = \xi_r = 0_{p-r,1}$. Thus $X_2 = 0_{N,p-r}$. If we agree to call a weighing design to be real if each object is weighed at least once, then, for a real design, $X_2 \neq 0$ and we have

COROLLARY 3.2.1. *In a real singular weighing design of rank* r, *at most* $r - 1$ *objects have estimable weights.*

If the parametric function $\rho_i' w$ of the weights is estimable, its best unbiased estimate can be obtained, from Gauss Markoff theorem, as $\rho_i^{*\prime}(X_1'X_1)^{-1}X_1'y$, where ρ_i^* is the ith column vector of I_r. The variance of $\rho_i^{*\prime}(X_1'X_1)^{-1}X_1'y$ can easily be seen to be equal to the ith diagonal element of $(X_1'X_1)^{-1}$ times σ^2. These results may be summarized in

THEOREM 3.3. *If the parametric function* $\rho_i' w$ *of the weights is estimable for a singular weighing design, its best unbiased estimate is* $\rho_i^{*\prime}(X_1'X_1)^{-1}X_1'y$, *with a variance equal to the* ith *diagonal element of* $(X_1'X_1)^{-1}$ *times* σ^2.

4. Problem of taking additional weighings. Given a singular weighing design, it is easy to see that by taking $p - r$ independent additional weighings, we can make the problem one of full rank and obtain the estimates of all the weights. Let $p - r$ additional weighings be taken, on the same balance on which the first N weighings are made according as the design matrix $B = [B_1\ B_2]$, where B_1 is a $(p - r) \times r$ matrix and B_2 is a $(p - r)$th order square matrix. Let z be the column vector of the results recorded in these additional weighings and ω be the column vector of errors in these results.

The results of the additional weighings can be written as

$$z = Bw + \omega. \tag{4.1}$$

Letting

$$Z_1 = X_1'X_1 + B_1'B_1, \qquad Z_2 = X_1'X_2 + B_1'B_2, \qquad Z_3 = X_2'X_2 + B_2'B_2, \tag{4.2}$$

from (1.1) and (4.1), we obtain the normal equations

$$\begin{bmatrix} Z_1 & Z_2 \\ Z_2' & Z_3 \end{bmatrix} \hat{w} = \begin{bmatrix} X_1' & B_1' \\ X_2' & B_2' \end{bmatrix} \begin{bmatrix} y \\ z \end{bmatrix} \text{ i. e. } S_1\hat{w} = \begin{bmatrix} X_1'y + B_1'z \\ X_2'y + B_2'z \end{bmatrix}. \tag{4.3}$$

If we define F to be equal to $Z_3 - Z_2'Z_1^{-1}Z_2$, its value is given by the following

LEMMA 4.1.

$$F = (B_2 - B_1J)'D(B_2 - B_1J), \tag{4.4}$$

where

$$D = \{I_{p-r} + B_1(X_1'X_1)^{-1}B_1'\}^{-1}. \tag{4.5}$$

PROOF.

$$\begin{aligned} F &= Z_3 - Z_2'Z_1^{-1}Z_2 = (X_2'X_2 + B_2'B_2) - (X_2'X_1 + B_2'B_1) \\ &\cdot\{(X_1'X_1)^{-1} - (X_1'X_1)^{-1}B_1'DB_1(X_1'X_1)^{-1}\}(X_1'X_2 + B_1'B_2) \\ &= J'B_1'DB_1J - J'B_1'DB_2 - B_2'DB_1J + B_2'DB_2 = (B_2 - B_1J)'D(B_2 - B_1J). \end{aligned}$$

We now prove

LEMMA 4.2.

$$|S_1| = |X_1'X_1|\,|B_2 - B_1J|^2, \tag{4.6}$$

PROOF.

$$|S_1| = |Z_1|\,|F| = |Z_1|\,|D|\,|B_2 - B_1J|^2 = |X_1'X_1|\,|B_2 - B_1J|^2,$$

from Lemmas 2.4 and 4.1.

For Z_1, Z_2, Z_3 and F as defined by (4.2) and (4.4), by making use of Lemma 2.3, we get

$$-Z_1^{-1}Z_2F^{-1} = -\{J + (X_1'X_1)^{-1}B_1'D(B_2 - B_1J)\}F^{-1},$$

$$\begin{aligned} Z_1^{-1}\{I + Z_2F^{-1}Z_2'Z_1^{-1}\} &= (X_1'X_1)^{-1} + JF^{-1}J' \\ &+ JF^{-1}(B_2 - B_1J)'DB_1(X_1'X_1)^{-1} \\ &+ (X_1'X_1)^{-1}B_1'D(B_2 - B_1J)F^{-1}J'. \end{aligned} \tag{4.7}$$

If we choose B_1 and B_2, such that $|B_2 - B_1J| \neq 0$, from Lemma 2.2, we get

(4.8) S_1^{-1}

$$= \begin{bmatrix} (X_1'X_1)^{-1} + JF^{-1}J' + JF^{-1}(B_2 - B_1J)'DB_1(X_1'X_1)^{-1} & -\{J + (X_1'X_1)^{-1} \\ \quad + (X_1'X_1)^{-1}B_1'D(B_2 - B_1J)F^{-1}J' & \cdot B_1'D(B_2 - B_1J)\}F^{-1} \\ -F^{-1}\{J' + (B_2 - B_1J)'DB_1(X_1'X_1)^{-1}\} & F^{-1} \end{bmatrix}.$$

Now, on simplifying we get the solution of the normal equations (4.3)

(4.9)

$$\hat{w} = \begin{bmatrix} (X_1'X_1)^{-1}X_1'y + J(B_2 - B_1J)^{-1}B_1(X_1'X_1)^{-1}X_1'y - J(B_2 - B_1J)^{-1}z \\ (B_2 - B_1J)^{-1}z - (B_2 - B_1J)^{-1}B_1(X_1'X_1)^{-1}X_1'y \end{bmatrix}.$$

The dispersion matrix of the estimates (4.9) is $\sigma^2S_1^{-1}$. The above results can be summarized in the following

THEOREM 4.1. *Given a singular weighing design, unbiased estimates of all the weights can be determined by taking $p - r$ additional weighings with the design matrix $B = [B_1 \quad B_2]$ such that $|B_2 - B_1 J| \neq 0$. The estimates thus obtained are given by the Equation* (4.9) *with the dispersion matrix $\sigma^2 S_1^{-1}$.*

The estimated weights (4.9) will be efficiently determined, for Mood's efficiency definition, if the determinant of S_1 is maximum. When $r = p - 1$, $|S_1|$ can be maximized, independent of the choice of X_1, whereas when $r < p - 1$, it is possible to maximize $|S_1|$ only for a particular choice of X_1. In this paper we shall consider the case $r = p - 1$ in detail. Maximizing $|S_1|$ for a particular choice of X_1 and some connected results are given in the author's unpublished thesis [5].

Now let $[A_1 \, A_2]$, where A_1 is a $(p - 1)$th order row vector and A_2 is a scalar, denote the pattern of taking the additional weighing. The normal equations in this case are

$$\begin{bmatrix} X_1'X_1 + A_1'A_1 & X_1'X_2 + A_1'A_2 \\ X_2'X_1 + A_2'A_1 & X_2'X_2 + A_2'A_2 \end{bmatrix} \hat{w} = \begin{bmatrix} X_1' & A_1' \\ X_2' & A_2' \end{bmatrix} \begin{bmatrix} y \\ z \end{bmatrix} \tag{4.10}$$

$$\text{i. e., } S_2 \hat{w} = \begin{bmatrix} X_1'y + A_1'z_1 \\ X_2'y + A_2'z \end{bmatrix}.$$

$|S_2|$ can be obtained from Lemma 4.2 to be equal to $|X_1'X_1| \, (A_2 - A_1 J)^2$. In order to make S_2 nonsingular, we choose A_1 and A_2 such that $(A_2 - A_1 J) \neq 0$. The value of the determinant of S_2 can be maximized for a given X_1, by choosing A_1' to be the column vector obtained from J where the non null elements are replaced by $+1$ or -1 according as the element is positive or negative and finally taking $A_2 = -1$. Thus

LEMMA 4.3. *$|S_2|$ is maximum for a given X_1, subject to the choice of the elements $+1$, -1 and 0 for A_1 and A_2, by taking A_1' to be the column vector obtained from J where the non null elements are replaced by $+1$ or -1 according as the element is positive or negative and $A_2 = -1$.*

Let the column vectors of $[X_1 \, X_2]$ be reshuffled, so that another set of $p - 1$ independent column vectors occupy the first $p - 1$ positions. Let the newly obtained matrix be $[Y_1 \, Y_2]$ and let $L = (Y_1'Y_1)^{-1} Y_1'Y_2$. Let $[H_1 \, H_2]$, be a row vector, where H_1' is the column vector obtained from L where the non null elements are replaced by $+1$ or -1 according as the element is positive or negative and $H_2 = -1$. We now prove

LEMMA 4.4.

$$|X_1'X_1|(A_2 - A_1 J)^2 = |Y_1'Y_1|(H_2 - H_1 L)^2. \tag{4.11}$$

PROOF. Let $x_1, x_2, \cdots, x_p$ be the columns of $[X_1 \; X_2]$. Without loss of generality, we assume that Y_1 consists of the columns $x_1, x_2, \cdots, x_{t-1}, x_p, x_{t+1}, \cdots, x_{p-1}$. Let J' be the row vector $(a_1, a_2, \cdots, a_{p-1})$. Then

$$x_p = a_1 x_1 + a_2 x_2 + \cdots + a_{p-1} x_{p-1}. \tag{4.12}$$

We can easily see that L' is the row vector $-a_t^{-1}(a_1, a_2, \cdots, a_{t-1}, -1, a_{t+1}, \cdots, a_{p-1})$. Now

$$(4.13)\quad |Y_1'Y_1| = \begin{vmatrix} x_1'x_1 & x_1'x_2 & \cdots & x_1'x_{t-1} & x_1'x_p & x_1'x_{t+1} & \cdots & x_1'x_{p-1} \\ x_2'x_1 & x_2'x_2 & \cdots & x_2'x_{t-1} & x_2'x_p & x_2'x_{t+1} & \cdots & x_2'x_{p-1} \\ \vdots & \vdots & & \vdots & \vdots & \vdots & & \vdots \\ x_{t-1}'x_1 & x_{t-1}'x_2 & \cdots & x_{t-1}'x_{t-1} & x_{t-1}'x_p & x_{t-1}'x_{t+1} & \cdots & x_{t-1}'x_{p-1} \\ x_p'x_1 & x_p'x_2 & \cdots & x_p'x_{t-1} & x_p'x_p & x_p'x_{t+1} & \cdots & x_p'x_{p-1} \\ x_{t+1}'x_1 & x_{t+1}'x_2 & \cdots & x_{t+1}'x_{t-1} & x_{t+1}'x_p & x_{t+1}'x_{t+1} & \cdots & x_{t+1}'x_{p-1} \\ \vdots & \vdots & & \vdots & \vdots & \vdots & & \vdots \\ x_{p-1}'x_1 & x_p'x_2 & \cdots & x_{p-1}'x_{t-1} & x_p'\ x_p & x_{p-1}'x_{t+1} & \cdots & x_{p-1}'x_{p-1} \end{vmatrix}.$$

On substituting the value of x_p from (4.12) and simplifying the above determinant, we get

$$(4.14)\qquad |Y_1'Y_1| = |X_1'X_1|a_t^2.$$

Now

$$|X_1'X_1|(A_2 - A_1J)^2 = |X_1'X_1| \left\{\sum_{i=1}^{p-1} |a_i| + 1\right\}^2$$

$$(4.15)\qquad = a_t^{-2}\,|Y_1'Y_1| \left\{\sum_{i=1}^{p-1} |a_i| + 1\right\}^2 = |Y_1'Y_1| \left\{\sum_{i=1}^{p-1} |a_i|\, a_t^{-1} + a_t^{-1}\right\}^2$$

$$= |Y_1'Y_1| \left\{\sum_{\substack{i=1 \\ i\neq t}}^{p-1} |a_i|\, a_t^{-1} + 1 + a_t^{-1}\right\}^2 = |Y_1'Y_1|(H_2 - H_1L)^2.$$

Hence the lemma is proved.

The solution of the normal equations can be obtained as

(4.16)

$$\hat{w} = (A_2 - A_1J)^{-1}\begin{bmatrix} (A_2 - A_1J)(X_1'X_1)^{-1}X_1'y + JA_1(X_1'X_1)^{-1}X_1'y - Jz \\ z - A_1(X_1'X_1)^{-1}X'y \end{bmatrix}.$$

The dispersion matrix of the above estimates is

$$(4.17)\qquad \sigma^2 S_2^{-1}.$$

The estimates (4.16) will be efficiently determined, for Mood's efficiency definition, if $|S_2|$ is maximum. $|S_2|$ is maximum when A_1 and A_2 are chosen according to Lemma 4.3. Lemma 4.4 insures that the maximum value of $|S_2|$ will be obtained by selecting A_1 and A_2 as in Lemma 4.3, whatever $p - 1$ independent columns we choose for X_1. These results are summarized in

THEOREM 4.2. *Given a singular weighing design of rank $p - 1$, the weights of* *the objects will be efficiently estimated, for Mood's efficiency definition, by taking an additional weighing corresponding to the row vector* $[A_1\ A_2]$ *determined as in Lemma* 4.3. *The estimates of the weights thus obtained are given by* (4.16) *with the dispersion matrix* (4.17).

ILLUSTRATION 4.2.1. Let us consider the singular weighing design

$$\begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & -1 & 0 \\ 1 & -1 & 0 \end{bmatrix} \tag{4.18}$$

of rank 2. Since the first two column vectors of (4.18) are independent, we can choose them for our X_1. Then $J' = (\frac{1}{2}, \frac{1}{2})$. Lemma 4.3 dictates us to take the additional weighing corresponding to the row vector

$$(1, \quad 1, \quad -1), \tag{4.19}$$

in order to get maximum efficiency for Mood's efficiency definition, for the estimated weights of the objects. The estimates are given by

$$\hat{w} = \frac{1}{8}\begin{bmatrix} 2z + y_1 + y_2 + 2y_3 + 2y_4 \\ 2z + y_1 + y_2 - 2y_3 - 2y_4 \\ 2y_1 + 2y_2 - 4z \end{bmatrix} \tag{4.20}$$

with the dispersion matrix

$$\sigma^2 \begin{bmatrix} \frac{7}{32} & -\frac{1}{32} & -\frac{1}{16} \\ -\frac{1}{32} & \frac{7}{32} & -\frac{1}{16} \\ -\frac{1}{16} & -\frac{1}{16} & \frac{3}{8} \end{bmatrix} \tag{4.21}$$

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