SOME REMARKS ON CHEMICAL BALANCE WEIGHING DESIGNS

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Introduction.

When it is required to find out the weights of several light objects on a chemical balance, it is possible to increase the precision of estimation by weighing the objects in suitable combinations. Let there be p objects to be weighed and assume that N weighings are made on a chemical balance. Let

$x_{\alpha i}=-1$, if the i-th object is placed on the right pan in the α-th weighing,

$=1$, if the i-th object is placed on the left pan in the α-th weighing,

$=0$, otherwise; $\alpha=1,\ldots\ldots,N,\ i=1,\ldots\ldots\ldots,p$.

The observational equations from the N weighings may be written as

$$Y=Xw+e,$$

where $Y=(y_1, y_2, \ldots\ldots, y_N)'$ is the vector of observed weights, $X=(x_{\alpha i})$ is the design matrix, $w=(w_1, \ldots\ldots, w_p)'$ is the vector of true weights and $e=(e_1, \ldots\ldots, e_N)'$ is an $N\times 1$ vector of random errors with $E(e)=0$, $E(ee')=\sigma^2 I$, where 0 is an $N\times 1$ null vector and I is the N-th order unit matrix. Assuming that there is no bias in the balance, for the estimation of p weights from N equations, we must have $N \geqslant p$. If $X'X$ is non-singular, the least-squares estimates are given by

$$\hat{w}=(X'X)^{-1} X'Y, \text{ with covariance matrix as } (X'X)^{-1}\sigma^2,$$

The problem is to choose the design matrix X in such a manner that the variance factors are minimised.

Various methods of construction of X are available in literature. One such method is to employ the incidence matrix of a balanced incomplete block (BIB) design. Consider a BIB design with parameters v, b, r, k, λ. The incidence matrix $N^*=(n_{ij})$ for this design is defined as

$$n_{ij}=1, \text{ if the } j\text{-th treatment occurs in } i\text{-th block,}$$
$$=0, \text{ otherwise.}$$

The design matrix X for the chemical balance design is then obtained by replacing in N^*, 0 by -1. If the chosen BIB design is symmetrical, and the design is used for weighing $p(=v)$ objects, no degrees of freedom are left for the estimation of error variance. In such a situation, the whole design may be repeated once (or more) to get sufficient d.f. for the estimation of error variance.

The present paper aims at suggesting certain alternatives to the "repeated" design.

2. Some Known Results in Matrix Algebra

In this section we state some results in matrix algebra, which will be used later.

Let A be a matrix defined as

$$A=(a-b)\, I_n+bJ_{nn}, \tag{2.1}$$

where a and b are scalars, I_n is the n-th order unit matrix and J_{nn} is an $n\times n$ matrix with unit elements everywhere. Then, the two distinct latent roots of A are $\theta_1=a-b$ and $\theta_2=a+(n-1)\, b$ with respective multiplicities $\alpha_1=n-1$ and $\alpha_2=1$. Consequently,

$$\text{Det. }(A)=(a-b)^{n-1}\, [a+(n-1)\, b] \tag{2.2}$$

The inverse of A is given by

$$A^{-1}=(c-d)\, I_n+dJ_{nn}, \tag{2.3}$$

where

$$c=[a+(n-2)\, b]\, /\, [(a-b)\, \{a+(n-1)\, b\}] \tag{2.4}$$
$$d=-b/[(a-b)\{a+(n-1)\, b\}]. \tag{2.5}$$

3. Designs and Relative Efficeinces:

3.1. Let N^* be the incidence matrix of a symmetrical *BIB* design with parameters $v=b$, $r=k$, λ. Replace the zero in N^* by -1 and call the derived matrix as N_1. Then, the "repeated" design matrix for a chemical balance design is given by

$$D_1 : \qquad X=\begin{bmatrix} N_1 \\ N_1 \end{bmatrix}. \tag{3.1}$$

For this design, we have,

$$(X'X)_{D_1} =)2v-\alpha)\, I_v+\alpha J_{vv}, \tag{3.2}$$

where $\quad \alpha=2\,[v-4\,(r-\lambda)]$.

Then, it is known from Dey (1971) that Det. $(X'X)_{D_1}>0$, for $v\neq 2r$. Using the results of section 2, the variance of any estimated weight is given by

$$\text{Var. } (\hat{w}_i)_{D_1} =\sigma^2[(v-2r)^2-v+4\,(r-\lambda)]\;/\;\{8\,(r-\lambda)\,(v-2r)^2\} \tag{3.3}$$

and the covariance between any two estimated weights is

$$\text{Cov. } (\hat{w}_i, \hat{w}_j)_{D_1} =\sigma^2[4(r-\lambda)-v]\;/\;\{\,8\,(r-\lambda)\,(v-2r)^2\}. \tag{3.4}$$

As alternatives to the "repeated" design, we suggest the following designs, namely D_2, D_3, D_4, D_5.

$$D_2 : \qquad X=\begin{bmatrix} N_1 \\ N_2 \end{bmatrix}, \tag{3.5}$$

where N_1 is as in (3.1) and N_2 is the incidence matrix of the complementary *BIB* design of N^*. Clearly, N_2 is the incidence matrix of the design with parameters

$$v'=v,\ b',=v,\ r'=v-r=k',\ \lambda'=v-2r+\lambda.$$

We have,

$$(X'X)_{D_2} =\{5\,(r-\lambda)\}\, I_v+(2v-6r+5\lambda)\, J_{vv}. \tag{3.6}$$

Using the results of section 2, one can easily prove that Det. $(X'X)_{D_2} > 0$. The variance-covariance of the estimated weights are given by:

$$\text{Var. } (\hat{w}_i)_{D_2} = \frac{\sigma^2\{(2v-r)+(v-2)(2v-6r+5\lambda)\}}{5(r-\lambda)\{(v-2r)^2+(v-r)^2\}} \quad \ldots(3.7)$$

$$\text{Cov. } (\hat{w}_i, \hat{w}_j)_{D_2} = \frac{-(2v-6r+5\lambda)\sigma^2}{5(r-\lambda)\{(v-2r)^2+(v-r)^2\}} \quad \ldots(3.8)$$

$$D_3: \qquad X = \begin{bmatrix} N_1 \\ J_{vv} \end{bmatrix} \text{ or } X = \begin{bmatrix} N_1 \\ -J_{vv} \end{bmatrix}. \quad \ldots(3.9)$$

Here, instead of repeating N_1, we take v additional weighings with all the v objects in the left or right pan. In fact, the two designs in (3.9) are equally efficient. We have,

$$(X'X)_{D_3} = \{4(r-\lambda)\}I_v + \{2v-4(r-\lambda)\}J_{vv}. \quad \ldots(3.10)$$

It is easy to see that Det. $(X'X)_{D_3} > 0$. Also,

$$\text{Var. } (\hat{w}_i)_{D_3} = \frac{\sigma^2\{2v+(v-2)(2v-4r+4\lambda)\}}{4(r-\lambda)\{v^2+(v-2r)^2\}}, \quad \ldots(3.11)$$

$$\text{Cov. } (\hat{w}_i, \hat{w}_j)_{D_3} = \frac{-(2v-4r+4\lambda)\sigma^2}{4(r-\lambda)\{v^2+(v-2r)^2\}}. \quad \ldots(3.12)$$

$$D_4: \qquad X = \begin{bmatrix} N_1 \\ N_3 \end{bmatrix} \quad \text{or} \quad X = \begin{bmatrix} N_1 \\ N_4 \end{bmatrix}, \quad \ldots(3.13)$$

where N_3 is a square matrix of order v, derived from I_v by replacing the zero by -1. N_4 is derived from N_3 by replacing in N_3, 1 by -1 and -1 by 1. The two designs in (3.13) are equally efficient. The designs in (3.13) amount to saying that with N_1 we take v additional weighings in each of which only one object is placed on one pan and the $(v-1)$ objects are placed on the other pan.

For D_4, we have

$$(X'X)_{D_4} = (4r-4\lambda+4)\, I_v + [2v-4(r-\lambda+1)]J_{vv}. \quad (3.14)$$

Further,

$$\text{Det. } (X'X)_{D_4} = [4(r-\lambda+1)]^{v-1}[(v-2r)^2+(v-2)^2]. \quad \ldots(3.15)$$

Thus, Det. $(X'X)_{D_4}>0$, if $v>2$ or $v\neq 2r$. If $v=2$, v should be different from $2r$, whereas if $v=2r$, v is always greater than 2. The variance-covariance expressions are as follows :—

$$\text{Var. } (\hat{w}_i)_{D_4}=\frac{\sigma^2\{2v+(v-2)(2v-4r+4\lambda-4)\}}{4(r-\lambda+1)[(v-2)^2+(v-2r)^2]}, \quad \text{...(3.16)}$$

$$\text{Cov. } (\hat{w}_i, \hat{w}_j)_{D_4}=\frac{-(2v-4r+4\lambda-4)\sigma^2}{4(r-\lambda+1)[(v-2)^2+(v-2r)^2]} \quad \text{...(3.17)}$$

$$D_5 : \quad X=\begin{bmatrix} N_1 \\ I_v \end{bmatrix} \text{ or } X=\begin{bmatrix} N_1 \\ -I_v \end{bmatrix}. \quad \text{...(3.18)}$$

In the above design, we take with N_1, v additional weighings in each of which only one object is placed on one pan, the others being not included in that weighing. For the designs in (3.18),

$$(X'X)_{D_5}=[4(r-\lambda)+1]I_v+[v-4r+4\lambda]J_{vv}. \quad \text{...(3.19)}$$

$$\text{Det. } (X'X)_{D_5}>0.$$

$$\text{Var. } (\hat{w}_i)_{D_5}=\frac{\sigma^2[(v+1)+(v-2)(v-4r+4\lambda)]}{[4(r-\lambda)+1][1+(v-2r)^2]} \quad \text{...(3.20)}$$

$$\text{Cov. } (\hat{w}_i, \hat{w}_j)_{D_5}=\frac{-(v-4r+4\lambda)\sigma^2}{[4(r-\lambda)+1][1+(v-2r)^2]}\cdot \quad \text{...(3.21)}$$

3·2. We have noted above that the design D_1 exist, whenever $v\neq 2r$. As such, for the purpose of comparison, we restrict our study to the following two series of symmetrical BIB designs for constructing N_1 :

S_1 : $v=b=4t-1$, $r=k=2t-1$, $\lambda=t-1$, $t\geqslant 1$.*

S_2 : $v=b=s^2+s+1$, $r=k=s+1$, $\lambda=1$, s is a prime-power.

The series S_1 is known for many values of t and it is surmised that it exists for all values of t. The solutions for this series of designs is available in Takeuchi (1962) for all t satisfying $1<t\leqslant 15$.

Substituting the parameters of S_1 in the expressions (3.3), (3.7), (3.11), (3.16) and (3.20) we get,

*For $t=1$, the design of the series S_1 is not a BIB design ; however, this does not affect our subsequent results.

$$\text{Var. } (\hat{w}_i)_{D_{11}} = \sigma^2/4t. \quad \ldots(3.22)$$

$$\text{Var. } (\hat{w}_i)_{D_{21}} = \frac{(4t^2-t+2)\sigma^2}{5t(1+4t^2)}. \quad \ldots(3.23)$$

$$\text{Var. } (\hat{w}_i)_{D_{31}} = \frac{(16t^2-12t+4)\sigma^2}{4t(16t^2-8t+2)}. \quad \ldots(3.24)$$

$$\text{Var. } (\hat{w}_i)_{D_{41}} = \frac{(16t^2-28t+16)\sigma^2}{(4t+4)(16t^2-24t+10)}. \quad \ldots(3.25)$$

$$\text{Var. } (\hat{w}_i)_{D_{51}} = \frac{3\sigma^2}{2(4t+1)}. \quad \ldots(3.26)$$

In the above expressions, D_{i1} $(i=1, 2,\ldots, 5)$ denotes the design D_i when S_1 is used.

In what follows, we shall use the notation $D_i \succ D_j$ to denote that the design D_i is "superior" to D_j, *i.e.*, Var. $(\hat{w}_i)_{D_i} <$ Var. $(\hat{w}_i)_{D_j}$. If, however, Var. $(\hat{w}_i)_{D_i} \leqslant$ Var. $(\hat{w}_i)_{D_j}$, the equality holding for certain values of t, we shall write $D_i \succ_{/} D_j$ (D_i is "at least as good as" D_j).

A comparison of the expressions (3.22) to (3.26) yields the following results.

(*i*) $D_2 \succ D_1$, for all $t \geqslant 1$.

(*ii*) $D_3 \succ D_1$, for all $t \geqslant 1$.

(*iii*) $D_4 \succ D_1$, for all $t > 1$.

(*iv*) $D_1 \succ D_5$, for all $t \geqslant 1$.

(*v*) $D_2 \succ_{/} D_3$, for all $t \geqslant 1$, equality holding for $t=1$.

(*vi*) $D_4 \succ D_2$, for $1 \leqslant t \leqslant 4$; $D_2 \succ D_4$ for $t \geqslant 5$.

(*vii*) $D_2 \succ D_5$, for all $t \geqslant 1$.

(*viii*) $D_4 \succ D_3$, for all $t \geqslant 1$.

(*ix*) $D_3 \succ D_5$, for all $t > 1$.

(*x*) $D_4 \succ D_5$, for all $t \geqslant 1$.

Now, consider the second series S_2. The variance expressions are as follows :

$$\text{Var. } (\hat{w}_i)_{D_{12}} = \frac{(s^3-2s^2-2s+5)\sigma^2}{8(s^2-s-1)^2}. \qquad \ldots(3.27)$$

$$\text{Var. } (\hat{w}_i)_{D_{22}} = \frac{(2s^3-2s^2-3s+6)\sigma^2}{5(2s^4-2s^3-s^2+2s+1)}. \qquad \ldots(3.28)$$

$$\text{Var. } (\hat{w}_i)_{D_{32}} = \frac{(s^3+3)\sigma^2}{4(s^4+s^2+2s+1)}. \qquad \ldots(3.29)$$

$$\text{Var. } (\hat{w}_i)_{D_{42}} = \frac{(s^4-2s^2+s+2)\sigma^2}{4(s+1)(s^4-s^2+1)}. \qquad \ldots(3.30)$$

$$\text{Var. } (\hat{w}_i)_{D_{52}} = \frac{(s^4-2s^3-2s^2+5s+1)\sigma^2}{(4s+1)(s^4-2s^3-s^2+2s+2)}. \qquad \ldots(3.31)$$

A comparison of the expressions (3.27) to (3.31) yields the following results.

(*i*) $D_1 \succ D_2$, for all s except for $s=2$, when $D_2 \succ D_1$.

(*ii*) $D_1 \succ D_3$, for all s except for $s=1, 2$, when $D_3 \succ D_1$.

(*iii*) $D_1 \succ D_4$, for all $s>2$. At $s=1$, $D_1 \equiv D_4$ and at $s=2$, $D_4 \succ D_1$.

(*iv*) $D_1 \succ D_5$, for all s.

(*v*) $D_2 \succ D_3$, for all $s>1$. At $s=1$, $D_3 \succ D_2$.

(*vi*) $D_2 \succ D_4$, for all $s \geqslant 5$. For $1 \leqslant s \leqslant 4$, $D_4 \succ D_2$.

(*vii*) $D_2 \succ D_5$, for all $s>1$. At $s=1$, $D_2 \equiv D_5$.

(*viii*) $D_4 \succ D_3$, for all $s>1$. For $s=1$. $D_3 \succ D_4$.

(*ix*) $D_5 \succ D_3$, for all $s>2$. For $s=1, 2$, $D_3 \succ D_5$.

(*x*) $D_4 \succ D_5$, for all s.

(The above results are based on actual computations for all permissible values of s in the range $1 \leqslant s \leqslant 500$).

4. SUMMARY

The present paper discusses various weighing designs suitable for the chemical balance problem. Some of these have been shown to be superior to the "repeated" design.

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