RANDOMIZED FRACTIONAL WEIGHING DESIGNS

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0. Introduction and summary. Consider the problem of estimating unbiasedly a linear function, $\lambda'\omega$, $\omega' = (\omega_1, \cdots, \omega_p)$, of p weights $\omega_1, \cdots, \omega_p$ $(0 < \omega_i < \infty$ for all $i = 1, \cdots, p)$ when the number of possible weighing operations, n, is smaller than p. Assume further that the weighing design is of the chemical type (each entry of the design matrix can assume one of the values -1, 0, $+1$). A weighing design in which the number of weighing operations is smaller than the number of objects, $n < p$, will be called a *fractional weighing design*. A fractional weighing design is singular. As is well known, if a non-randomized weighing design is singular, one cannot estimate unbiasedly each of the p weights. Some linear functions $\lambda'\omega$ can be estimated, however, unbiasedly. For example, the sum of all p weights can be estimated unbiasedly by a singular weighing design in which, at each weighing operation, all the objects are placed on one pan. Such a singular weighing design is in fact optimal. One can not attain the same precision in estimating the sum of all the p weights by any non-singular design (see K. S. Banerjee [1]). Some linear functions of the weights can thus be estimated, with a sufficient degree of precision, on the basis of a number of weighing operations, n, smaller than the number of weights, p.

A. M. Mood [4] has shown that if the design matrix of a non-singular weighing design is a Hadamard matrix (if it exists) then the design is optimal. We shall therefore study fractional weighing designs based on Hadamard matrices. If p is such that no Hadamard matrix of order p exists, we shall consider the smallest integer p' larger than p, for which a Hadamard matrix exists and add $(p' - p)$ dummy weights. The linear functions $\lambda'\omega$ can be extended in a way that assigns the dummy weights the coefficient zero. We shall then consider randomized fractional weighing designs which are constructed by choosing at random n rows, independently and with replacement, from the given Hadamard matrix according to a probability vector ξ of order p. Every such row specifies a weighing operation to be performed. Non-randomized fractional designs are special cases of the randomized designs under consideration. It is well known that if the weighing design is fractional $(n < p)$ then not all the linear functions $\lambda'\omega$ are estimable under non-randomized designs.

It is shown in the present paper that any linear function $\lambda'\omega$ can be estimated unbiasedly under a proper randomization scheme. Optimal randomization procedures depend on the functional λ. Complete class of unbiased estimation procedures is given for any linear function $\lambda'\omega$. It is shown that every functional λ specifies a subset of, say r $(1 \leqq r \leqq p)$, admissible weighing operations (rows of the Hadamard matrix); in the sense that if other weighing operations are chosen then, either the estimation procedure is biased, or has a variance larger

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than the one that can be attained under the admissible weighing operations. It is also proven that if each of the r admissible weighing operations ($1 \leqq r \leqq p$) is chosen with probability equal to $1/r$, then the corresponding unbiased estimator has a uniformly (in ω and σ^2) minimum variance, relative to all the above specified randomization procedures. The formulae of the unbiased estimator of $\lambda'\omega$ and its variance are extended in Section 4 to the case of random choice without replacement, of n rows out of the r admissible ones. This randomization procedure improves the results that can be obtained under the best randomization procedure with replacement.

Finally, the relationship of the present study to the studies of S. Ehrenfeld and S. Zacks [2], [3] is discussed in Section 5.

1. Randomized fractional weighing designs and unbiased estimators. Let (X) be a square Hadamard matrix, corresponding to a non-singular weighing design of order p. If p weighing operations are performed, and if Y_i ($i = 1, \cdots, p$) represents the reading of the ith weighing operation then it is assumed that:

$$\mathbf{Y} = (X)\omega + \boldsymbol{\varepsilon} \tag{1.1}$$

where $Y' = (Y_1, \cdots, Y_p)$, and where $\boldsymbol{\varepsilon}$ is a random (error) vector satisfying $E\{\boldsymbol{\varepsilon}\} = 0$ and $E\{\boldsymbol{\varepsilon}\boldsymbol{\varepsilon}'\} = \sigma^2 I$. For the actual derivations in the present paper it is not necessary to assume any further properties of the distribution of $\boldsymbol{\varepsilon}$. However, in order to justify the restriction to linear estimators we assume the common assumption that $\boldsymbol{\varepsilon} \sim N(\mathbf{0}, \sigma^2 I)$.

The matrix (X) has the properties: All the entries of (X) are ± 1.

(i) $(X)1 = (p, \mathbf{0}'_{p-1})'$, where $\mathbf{1}' = (1, 1, \cdots, 1)$ of order p and $\mathbf{0}'_{p-1} = (0, \cdots, 0)$ of order $p - 1$;

(ii) $\mathbf{1}'(X) = (p, \mathbf{0}'_{p-1})$;

(iii) $(X)'(X) = (X)(X)' = pI$.

Let ξ be a probability vector of order p and let (Ξ) be a diagonal matrix of order p, whose diagonal elements are the components of ξ. (Ξ) will be called a randomization procedure matrix. A random choice of one row of (X) is performed according to the probability vector ξ. Let (J) be a diagonal matrix, representing a choice of one row of (X), whose diagonal elements are

$$\begin{aligned} J_i &= 1, \quad \text{if the } i\text{th row of } (X) \text{ is chosen} \\ &= 0, \quad \text{otherwise.} \end{aligned} \tag{1.2}$$

(J) will be called an allocation matrix. Obviously, $E\{(J)\} = (\Xi)$. Suppose n rows of (X) are chosen independently and according to the same probability vector ξ. Let $(J^{(j)})$ ($j = 1, \cdots, n$) denote the allocation matrix of the jth weighing operation. Let $\mathbf{Y}^{(j)}$ ($j = 1, \cdots, n$) be identically distributed random vectors, satisfying model (1.1). We restrict the discussion to fractional designs ($1 \leqq n \leqq p$). The n randomly allocated weighing operations yield the random vectors $(J^{(1)})\mathbf{Y}^{(1)}, \cdots, (J^{(n)})\mathbf{Y}^{(n)}$. Let $\mathbf{Z}^{(n)} = \sum_{j=1}^{n} (J^{(j)})\mathbf{Y}^{(j)}$. The vector $\mathbf{Z}^{(n)}$ is of order p. The components of $\mathbf{Z}^{(n)}$ correspond to the randomly chosen components of $\mathbf{Y}^{(1)}, \cdots, \mathbf{Y}^{(n)}$; all the other $(n - p)$ components of $\mathbf{Z}^{(n)}$ are zero.

Under the assumption that the distribution function of $\mathbf{Y}$ is normal, $\mathbf{Z}^{(n)}$ is a complete sufficient statistic. Denote by (Ξ^*) a non-singular random procedure matrix, corresponding to a probability vector, ξ^*, having positive components. Notice that the non-randomized designs cannot be represented by ξ^*. The unbiased estimator (1.3) has, therefore, no non-randomized particular form. The non-randomized analogue $p^{-1}(X)'\mathbf{Z}^{(n)}$ is not unbiased if $n < p$.

LEMMA 1. *If (Ξ^*) is any non-singular randomization procedure matrix then the estimator*

$$\hat{\boldsymbol{\omega}}^{(n)}(\xi^*) = (np)^{-1}(X)'(\Xi^*)^{-1}\mathbf{Z}^{(n)} \tag{1.3}$$

is the unique unbiased linear estimator of $\boldsymbol{\omega}$, for every $n \geqq 1$.

PROOF. To prove that (1.3) is an unbiased estimator one has only to substitute $E\{\mathbf{Z}^{(n)}\} = n(\Xi^*)(X)\boldsymbol{\omega}$. We show now that (1.3) is unique. Suppose $(A)\mathbf{Z}^{(n)}$ is any unbiased estimator of $\boldsymbol{\omega}$, where (A) is a $p \times p$ matrix. Then $E\{[(np)^{-1}(X)'(\Xi^*)^{-1} - A]\mathbf{Z}^{(n)}\} = 0$. From this we obtain the equality, $n(A)(\Xi^*)(X) = I$. But since $(X^{-1}) = p^{-1}(X)'$, one obtains $(A)(\Xi^*) = (np)^{-1}(X)'$. Hence $(A) = (np)^{-1}(X)'(\Xi^*)^{-1}$. This establishes the uniqueness of (1.3). The one-to-one correspondence is between randomization procedures, represented by ξ^*, and unbiased estimations (1.3). A decision problem, to be studied in the sequel, is which procedure yields the optimal estimator. According to Lemma 1, any randomization procedure ξ^* combined with the estimator $\boldsymbol{\lambda}'\hat{\boldsymbol{\omega}}^{(n)}(\xi^*)$, yields the unique unbiased estimator of a given linear function $\boldsymbol{\lambda}'\boldsymbol{\omega}$. However, this class of randomized procedures, associated with probability vectors ξ^*, is not always complete. It depends on the functional $\boldsymbol{\lambda}$. For example, the best unbiased procedure for estimating $\mathbf{1}'\boldsymbol{\omega}$ is to choose the first row of (X) with probability one, and estimate $\mathbf{1}'\boldsymbol{\omega}$ by the arithmetic mean of the observed values. This procedure is not included in the above class since only the first row of (X) is chosen. We extend therefore the class of unbiased estimators to obtain complete classes of unbiased estimation procedures of any function $\boldsymbol{\lambda}'\boldsymbol{\omega}$.

Let $\boldsymbol{\lambda}$ be any linear functional, and consider the transformation:

$$\boldsymbol{\alpha} = p^{-1}(X)\boldsymbol{\lambda}. \tag{1.4}$$

Since the row vectors of (X) form an orthogonal basis of the Euclidean space $E^{(p)}$, the components of $\boldsymbol{\alpha}$ are the coordinates of $\boldsymbol{\lambda}$ in terms of this basis. Indeed, $\boldsymbol{\lambda}' = \sum_{i=1}^{p} \alpha_i \mathbf{X}_i'$, where $\mathbf{X}_i'$ $(i = 1, \cdots, p)$ is the ith row vector of (X). Suppose that r components of $\boldsymbol{\alpha}$ are different from zero, say $\alpha_{i_1} \neq 0, \cdots, \alpha_{i_r} \neq 0$. Let $\xi(i_1, \cdots, i_r)$ be any probability vector whose i_1th, i_2th, $\cdots$, i_rth components are positive, and all the other components are zero. Let $(\Xi(i_1, \cdots, i_r))$ be the corresponding randomization procedure matrix. For every randomization procedure matrix (Ξ) define

$$(\Xi^-) = \begin{bmatrix} \xi_1^- & & 0 \\ & \ddots & \\ 0 & & \xi_p^- \end{bmatrix} \tag{1.5}$$

where, for $i = 1, \cdots, p$,

$$\begin{aligned} \xi_i^- &= \xi_i^{-1}, \quad \text{if} \quad \xi_i > 0 \\ &= 0, \quad \text{if} \quad \xi_i = 0. \end{aligned}$$

(Ξ^-) is a generalized or pseudo-inverse of (Ξ) (see Price [5]).

LEMMA 2. *If the only components of* α *which are different from zero are* $\alpha_{i_1}, \cdots, \alpha_{i_r}$ $(1 \leqq r \leqq p)$ *then, under randomization procedure* $\xi(i_1, \cdots, i_r)$, *the estimator*

$$(1.6) \quad \lambda'\hat{\omega}^{(n)}(\xi(i_1, \cdots, i_r)) = \cdot(np)^{-1}\lambda'(X)'(\Xi^-(i_1, \cdots, i_r))\mathbf{Z}^{(n)}$$

is unbiased.

PROOF. Without loss of generality, assume that the components of α which are different from zero are the first r ones $(1 \leqq r \leqq p)$, i.e., $i_1 = 1, \cdots i_r = r$. Let $(\alpha_r^*)' = (\alpha_1, \cdots, \alpha_r)$. Similarly, let

$$(\Xi_r^*) = \begin{bmatrix} \xi_1 & & 0 \\ & \ddots & \\ 0 & & \xi_r \end{bmatrix}.$$

(Ξ_r^*) is non-singular of rank r. According to (1.5),

$$(\Xi^-) = \left[\begin{array}{c:c} (\Xi_r^*)^{-1} & 0 \\ \hdashline 0 & 0 \end{array}\right]. \qquad \text{Hence,}$$

$$(1.7) \qquad (\Xi^-)E\{\mathbf{Z}^{(n)}\} = n(\Xi^-)(\Xi)(X)\omega = n\left[\begin{array}{c:c} I_r & 0 \\ \hdashline 0 & 0 \end{array}\right](X)\omega.$$

According to (1.4)

$$\begin{aligned} \lambda'E\{\hat{\omega}^{(n)}(\xi(1, \cdots, r))\} &= (\lambda'/np)(X)'(\Xi^-)E\{\mathbf{Z}^{(n)}\} \\ (1.8) \qquad &= ((\alpha_r^*)', \mathbf{0}'_{p-r})\left[\begin{array}{c:c} I_r & 0 \\ \hdashline 0 & 0 \end{array}\right](X)\omega \\ &= ((\alpha_r^*)', \mathbf{0}'_{p-r})(X)\omega = p^{-1}\lambda'(X)'(X)\omega \\ &= \lambda'\omega. \end{aligned}$$

For example, the case of $\lambda = \mathbf{1}$ yields $\alpha' = (1, \mathbf{0}'_{p-1})$. The randomization procedure to use is therefore $\xi'(1) = (1, 0, \cdots, 0)$, which is actually a non-randomized design. In other words, the weighing operation corresponding to the first row of (X) is performed with probability one, n times independently. In this case

$$r = 1, \qquad (\Xi(1)) = \begin{bmatrix} 1 & & & \\ & 0 & & \\ & & \ddots & 0 \\ 0 & & & 0 \end{bmatrix}$$

and

$$(1.9)\qquad \hat{\boldsymbol{\omega}}^{(n)}(\xi(1)) = (np)^{-1}(\mathbf{1} \vdots 0_{p\times(p-1)}) \sum_{j=1}^{n} \begin{pmatrix} Y_1^{(j)} \\ \mathbf{0}_{p-1} \end{pmatrix} = (np)^{-1} \sum_{j=1}^{n} Y_i^{(j)} \mathbf{1}.$$

Hence,

$$(1.10)\qquad 1'\hat{\boldsymbol{\omega}}^{(n)}(\xi(1)) = n^{-1} \textstyle\sum_{j=1}^{n} Y_1^{(j)} = \sum_{j=1}^{p} \omega_i + n^{-1} \sum_{j=1}^{n} \epsilon_1^{(j)}$$

which is the best unbiased estimator of the sum of weights. Moreover, Var $\{1'\hat{\boldsymbol{\omega}}^{(n)}(\xi(1))\} = \sigma^2/n$. We shall prove now that if all the components of $\boldsymbol{\alpha} = p^{-1}(X)\boldsymbol{\lambda}$ are different from zero, one cannot estimate unbiasedly $\boldsymbol{\lambda}'\boldsymbol{\omega}$ by a randomization procedure having a singular matrix (Ξ).

LEMMA 3. *Let $\boldsymbol{\alpha}$ be the transform* (1.4) *of $\boldsymbol{\lambda}$. If all the components of $\boldsymbol{\alpha}$ are different from zero then there is no randomization procedure $\xi(i_1, \cdots, i_r)$, with $1 \leqq r < p$, which yields unbiased estimators of $\boldsymbol{\lambda}'\boldsymbol{\omega}$.*

PROOF. Without loss of generality, assume that $(i_1, \cdots, i_r) = (1, \cdots, r)$ accordingly,

$$(1.11)\qquad \boldsymbol{\lambda}'\hat{\boldsymbol{\omega}}^{(n)}(\xi(1, \cdots, r) = \boldsymbol{\lambda}'(np)^{-1}(X)' \begin{bmatrix} \xi_1^{-1} & & & \vdots & \\ & \ddots & 0 & \vdots & 0 \\ 0 & & \xi_r^{-1} & \vdots & \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ & 0 & & \vdots & 0 \end{bmatrix} \mathbf{Z}^{(n)}$$

$$= n^{-1}\boldsymbol{\alpha}' \begin{bmatrix} \xi_1^{-1} & & & \vdots & \\ & \ddots & 0 & \vdots & 0 \\ 0 & & \xi_r^{-1} & \vdots & \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ & 0 & & \vdots & 0 \end{bmatrix} \mathbf{Z}^{(n)}.$$

Since,

$$(1.12)\qquad E\{\mathbf{Z}^{(n)}\} = n \begin{bmatrix} \xi_1 & & & \vdots & \\ & \ddots & 0 & \vdots & 0 \\ 0 & & \xi_r & \vdots & \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ & 0 & & \vdots & 0 \end{bmatrix} (X)\boldsymbol{\omega}$$

one obtains,

$$(1.13)\qquad E\{\boldsymbol{\lambda}'\hat{\boldsymbol{\omega}}^{(n)}(\xi(1, \cdots, r))\} = \boldsymbol{\alpha}' \begin{bmatrix} I_r & \vdots & 0 \\ \cdots & \cdots & \cdots \\ 0 & \vdots & 0 \end{bmatrix} (X)\boldsymbol{\omega}.$$

But if

$$\alpha' \begin{bmatrix} I_r & \vdots & 0 \\ \cdots & \vdots & \cdots \\ 0 & \vdots & 0 \end{bmatrix} (X) = \lambda', \tag{1.14}$$

then

$$\alpha' \begin{bmatrix} I_r & \vdots & 0 \\ \cdots & \vdots & \cdots \\ 0 & \vdots & 0 \end{bmatrix} = p^{-1}\lambda'(X)' = \alpha'. \tag{1.15}$$

This contradicts the assumption that the last $(p - r)$ components of α_p are different from zero. Hence, $E\{\lambda'\hat{\omega}^{(n)}(\xi(1, \cdots, r))\} \neq \lambda' w$ whenever $1 \leqq r < p$.

A direct conclusion from Lemma 3 is that the unbiased estimators of a single component of ω, ω_1 say, based on fractional designs $(1 \leqq n < p)$, can be attained only under randomization procedures which assign positive probabilities $\xi_i > 0$ $(i = 1, \cdots, 1)$ to all the p rows of (X). Indeed, the transform of $\lambda = (1, 0, \cdots 0)'$ is $\alpha = p^{-1}1$.

In a similar manner one can show that if the number of components of α which are different from zero is r $(1 \leqq r < p)$ then $\lambda'\omega$ is not estimable unbiasedly by using either a probability vector, ξ, whose number of positive components is less than r, or a probability vector whose positive components do not correspond to the non-zero components of α. This is formulated in the following lemma.

LEMMA 4. *If the non-zero components of α have indices $i_1, \cdots, i_r$ $(1 \leqq r < p)$, and if $\xi(i_1^*, \cdots, i_{r'}^*)$ represents a randomization procedure then $\lambda'\omega$ is estimable unbiasedly by* (1.6) *if, and only if, $r' \geqq r$ and $i_1^* = i_1, \cdots, i_r^* = i_r$.*

Every randomization procedure which yields an unbiased estimator in (1.6) will be called *an unbiased randomization procedure.*

2. The variance of an unbiased estimator of $\lambda'\omega$. We start the derivation of the variance function with the assumption that the randomization procedure matrix (Ξ) is non-singular. We shall modify the results then to the general case.

LEMMA 5. *If (Ξ) is non-singular, then the covariance matrix of* (1.3) *is,*

$$\mathfrak{V}(\hat{\omega}^{(n)}(\xi^*)) = (\sigma^2/np^2)\sum_{i=1}^{p} \xi_i^{-1}\mathbf{X}_i\mathbf{X}_i' + (np^2)^{-1}\sum_{i=1}^{p} \xi_i^{-1}(\mathbf{X}_i'\omega)^2\mathbf{X}_i\mathbf{X}_i' - n^{-1}\omega\omega' \tag{2.1}$$

where $\mathbf{X}_i'$ is the ith row of (X) $(i = 1, \cdots, p)$.

PROOF. From the definition (1.3) it follows that

$$\mathfrak{V}(\hat{\omega}^{(n)}(\xi^*)) = (n^2p^2)^{-1}(X')(\Xi)^{-1}\mathfrak{V}(\mathbf{Z}^{(n)})(\Xi)^{-1}(X). \tag{2.2}$$

Since $(J^{(1)})\mathbf{Y}^{(1)}, \cdots, (J^{(n)})\mathbf{Y}^{(n)}$ are independent and are identically distributed,

$$\mathfrak{V}(\mathbf{Z}^{(n)}) = \sum_{j=1}^{n} \mathfrak{V}((J^{(j)})\mathbf{Y}^{(j)}) = n\mathfrak{V}((J)\mathbf{Y}). \tag{2.3}$$

The covariance matrix of $(J)\mathbf{Y}$ can be determined according to the formula

$$\mathfrak{V}((J)\mathbf{Y}) = E\{\mathfrak{V}((J)\mathbf{Y} \mid (J))\} + \mathfrak{V}(E\{(J)\mathbf{Y} \mid (J)\}). \tag{2.4}$$

However, $\mathfrak{V}((J)\mathbf{Y} \mid (J)) = \sigma^2(J)$, and $E\{(J)\mathbf{Y} \mid (J)\} = (J)(X)\omega$. Hence,

$$(2.5)\quad n\mathfrak{V}((J)\mathbf{Y}) = n\sigma^2(\Xi) + nE\{(J)(X)\omega\omega'(X)(J)\} - n(\Xi)(X)\omega\omega'(X)'(\Xi).$$

Substitution of (2.5) in (2.2) yields,

$$(2.6)\quad \mathfrak{V}(\hat{\omega}^{(n)}(\xi^*)) = (\sigma^2/np^2)(X)'(\Xi)^{-1}(X) + (np^2)^{-1}(X)'(\Xi)^{-1} \cdot E\{(J)(X)\omega\omega'(X)'(J)\}(\Xi)^{-1}(X) - n^{-1}\omega\omega'.$$

Since (Ξ) is diagonal, we have

$$(2.7)\quad (X)'(\Xi)^{-1}(X) = \sum_{j=1}^{p} \xi_j^{-1}\mathbf{X}_j\mathbf{X}_j'.$$

Furthermore,

$$(2.8)\quad (J)(X)\omega\omega'(X)'(J) = \|J_iJ_j(\mathbf{X}_i'\omega)(\mathbf{X}_j'\omega)\|.$$

But since,

$$(2.9)\quad \begin{aligned} J_iJ_j &= J_i, \quad \text{if} \quad i = j, \\ &= 0, \quad \text{if} \quad i \neq j. \end{aligned}$$

We obtain,

$$(2.10)\quad E\{(J)(X)\omega\omega'(X)'(J)\} = (\Xi)\begin{bmatrix} (\mathbf{X}_1'\omega)^2 & & & 0 \\ & \ddots & & \\ & & \ddots & \\ 0 & & & (\mathbf{X}_p'\omega)^2 \end{bmatrix}.$$

Finally, by substituting (2.7) and (2.10) in (2.6) we obtain the expression (2.1).

According to Lemma 5, if ω is estimated by (1.3) then the variance of the unbiased estimator of $\lambda'\omega$ is:

$$(2.11)\quad \mathrm{Var}\{\lambda'\hat{\omega}^{(n)}(\xi^*)\} = (np^2)^{-1}\sum_{i=1}^{p}\xi_i^{-1}(\sigma^2 + (\mathbf{X}_i'\omega)^2)(\lambda'\mathbf{X}_i)^2 - n^{-1}(\lambda'\omega)^2.$$

In particular, for $\lambda = 1$ we obtain,

$$(2.12)\quad \mathrm{Var}\{1'\hat{\omega}^{(n)}(\xi^*)\} = (n\xi_1)^{-1}(\sigma^2 + (1'\omega)^2) - n^{-1}(1'\omega)^2.$$

Letting ξ_1 approach 1 we get,

$$(2.13)\quad \lim_{\xi_1 \to 1} \mathrm{Var}\{1'\hat{\omega}(\xi^*)\} = \sigma^2/n$$

which is the variance of the best unbiased estimator of $1'\omega$. The best unbiased estimator of $1'\omega$ can be approached by a sequence of estimators of the type $\hat{\omega}^{(n)}(\xi^*)$, whose variances approach (from above) σ^2/n. We shall see later that this result can be extended to the case of any linear function $\lambda'\omega$.

In case the vector α has some zero components we apply the unbiased estimator (1.6). The general formula of the covariance matrix of an unbiased es-

timator $\hat{\omega}^{(n)}(\xi)$ of the type defined by (1.6) is, in analogy to (2.1),

$$(2.14)\quad \mathfrak{V}(\hat{\omega}^{(n)}(\xi)) = (\sigma^2/np^2)\sum_{i=1}^{p}\xi_i^{-}\mathbf{X}_i\mathbf{X}_i' + (np^2)^{-1}\sum_{i=1}^{p}\xi_i^{-}(\mathbf{X}_i'\omega)^2\mathbf{X}_i\mathbf{X}_i' - n^{-1}\omega^*(\omega^*)'$$

where ξ_i^{-} are defined as in (1.5); and ω^* is:

$$(2.15)\quad \omega^* = p^{-1}(X)'I(i_1, \cdots, i_r)(X)\omega$$

and where $I(i_1, \cdots, i_r)$ is a diagonal matrix of order p, whose i_1th, $\cdots$, i_rth diagonal elements are equal to unity and all the other elements are zero. The proof of (2.14) is carried out step by step like the proof of Lemma 5, replacing the inverse of (Ξ^*) by the generalized inverse of $(\Xi(i_1, \cdots, i_r))$. According to (2.14) the variance of an unbiased estimator of $\lambda'\omega$ is given by,

$$(2.16)\quad \mathrm{Var}\{\lambda'\omega^{(n)}(\xi)\} = (np^2)^{-1}\sum_{i=1}^{p}\xi_i^{-}[\sigma^2 + (X_i'\omega)^2](\lambda'X_i)^2 - n^{-1}(\lambda'\omega)^2.$$

Indeed,

$$\begin{aligned} n^{-1}\lambda'\omega^*(\omega^*)'\lambda &= (np^2)^{-1}\lambda'(X)'I(i_1, \cdots, i_r)(X)\omega\omega'(X)' \\ &\quad \cdot I(i_1, \cdots, i_r)(X)\lambda \\ &= n^{-1}\alpha'I(i_1, \cdots, i_r)(X)\omega\omega'(X)'I(i_1, \cdots, i_r)\alpha \\ &= n^{-1}\alpha'(X)\omega\omega'(X)'\alpha = n^{-1}\lambda'\omega\omega'\lambda. \end{aligned} \tag{2.17}$$

The comparison of (2.11) and (2.17) leads to the following theorem:

THEOREM 1. *If λ is a linear functional whose transformed functional α (1.4) has r $(1 \leqq r \leqq p)$ non-zero components then, for any unbiased randomization procedure with ξ, there exists an unbiased randomization with a probability vector ξ^+, having r positive components, which is at least as good as ξ:* and if the number *of positive components in ξ is $r' > r$, then ξ^+ is strictly better than ξ.*

PROOF. Suppose that the non-zero components of α are $\alpha_{i_1}, \cdots, \alpha_{i_r}$ $(1 \leqq i, < \cdots < i_r \leqq p)$. $\lambda'\hat{\omega}^{(n)}(\xi^*)$ is an unbiased estimator of $\lambda'\omega$. Compare its variance (2.11) to that of $\lambda'\hat{\omega}^{(n)}(\xi(i_1, \cdots, i_r))$, (2.16). Since $\lambda'\mathbf{X}_i \neq 0$ only if $i = i_1, \cdots, i_r$ we obtain,

$$(2.18)\quad \mathrm{Var}\{\lambda'\hat{\omega}^{(n)}(\xi^*)\} = (np^2)^{-1}\sum_{j=1}^{r}\xi_{ij}^{-1}[\sigma^2 + (\mathbf{X}_{ij}'\omega)^2](\lambda'\mathbf{X}_{ij})^2 - n^{-1}(\lambda'\omega)^2.$$

But since all the components of ξ^* are positive then, if $r < p, 0 < \sum_{j=1}^{r}\xi_{ij} < 1$. Consider the randomization procedure given by the probability vector $\xi^*(i_1, \cdots, i_r)$, whose components are,

$$\begin{aligned} \xi_i^* &= \xi_{ij}/(\textstyle\sum_{j=1}^{r}\xi_{ij}), \qquad \text{if} \quad i = i_j \quad (j = 1, \cdots, r), \\ &= 0, \qquad\qquad\qquad\quad \text{otherwise}, \end{aligned} \tag{2.19}$$

$\xi_{ij}^* > \xi_{ij}$ for all $j = 1, \cdots, r$. Hence

$$(2.20)\quad \mathrm{Var}\{\lambda'\hat{\omega}^{(n)}(\xi^*(i_1, \cdots, i_r))\} = (np^2)^{-1}\sum_{j=1}^{r}(\xi_{ij}^*)^{-1}\sigma^2 + (\mathbf{X}_{ij}'\omega)^2(\lambda'\mathbf{X}_{ij})^2 - n^{-1}(\lambda'\omega)^2 < \mathrm{Var}\{\lambda'\hat{\omega}^{(n)}(\xi^*)\}.$$

Hence, if $r < p$ the variance of the unbiased estimator under $\xi^*(i_1, \cdots, i_r)$ is strictly smaller than that of the unbiased estimator under ξ^*. Equality of variance holds only if $r = p$. If the given unbiased randomization procedure is represented by ξ which has r' positive components and $r' > r$ then $\sum_{j=1}^{r} \xi_{i_j} < 1$ and, according to (2.19) the variance attained by (1.6) under $\xi^*(i_1, \cdots, i_r)$ is smaller than that attained under ξ.

3. Optimal procedures. In the present section we study the problem of choosing an optimal randomization procedure, for estimating unbiasedly a given linear function $\lambda'\omega$.

According to Theorem 1, if α has r non-zero components ($1 \leqq r \leqq p$) then all unbiased procedures represented by probability vectors having exactly r corresponding positive components constitute a complete class. All other unbiased procedures are inadmissible. The problem is to choose an unbiased procedure from the complete class of all probability vectors, ξ, having r positive components. In the sequel we shall consider the following risk function:

$$(3.1) \qquad R(\omega, \xi; \lambda) = (np^2)^{-1} \sum_{i=1}^{p} \xi_i^{-1}[\sigma^2 + (\mathbf{X}_i'\omega)^2](\lambda'\mathbf{X}_i)^2.$$

Given σ^2, ω and λ, the probability vector ξ^0 which minimizes (3.1) has the components

$$(3.2) \quad \xi_i^0 = [\sigma^2 + (\mathbf{X}_i'\omega)^2](\lambda'\mathbf{X}_i)^2 / \sum_{j=1}^{p} [\sigma^2 + (\mathbf{X}_i'\omega)^2](\lambda'\mathbf{X}_i)^2, \quad i = 1, 2, \cdots, p.$$

Since $\lambda'\mathbf{X}_i = p\alpha_i$ for all $i = 1, \cdots, p$ we see $\xi_i^0 = 0$ whenever $\alpha_i = 0$. ξ^0 lies therefore in the interior of the open simplex of all probability vectors $\xi^*(i_1, \cdots, i_r)$, $1 \leqq r \leqq p$. Consider the probability vector $\xi_0^*(i_1, \cdots, i_r)$ which assigns equal probability to any of the r admissible rows of (X). According to (3.1),

$$(3.3) \quad R(\omega, \xi_0^*(i_1, \cdots, i_r); \lambda) = (r/np^2) \sum_{i=1}^{p} [\sigma^2 + (\mathbf{X}_i'\omega)^2](\lambda'\mathbf{X}_i)^2.$$

But this is equivalent to $R(\omega, \xi^0; \lambda)$ for all values of σ^2 and ω. Thus we have proven the following theorem.

THEOREM 2. *For any given linear function $\lambda'\omega$, if the transformed functional α has non-zero components at the i_1th, $\cdots$, i_rth places ($1 \leqq r \leqq p$), then the probability vector $\xi_0^*(i_1, \cdots, i_r)$ yields the best unbiased estimator of $\lambda'\omega$, uniformly in ω and σ^2.*

4. Extension to randomized procedures without replacement. Assume at the beginning that the functional λ is such that all the rows of (X) are admissible. We have proven in the previous section that if sampling of rows is with replacement then the best randomization procedure is to assign each row equal probability of choice. This randomization procedure can be improved by sampling of n rows out of p at random without replacement. That is, n rows are chosen in a way that assures every possible set of n rows the same probability $\binom{p}{n}^{-1}$ to be chosen. We give now the unbiased estimator of $\lambda'\omega$ and its variance. The statistical model under the present randomization procedure can be written as,

$$\mathbf{Z}^{(n)} = \begin{bmatrix} J_1 & & 0 \\ & \ddots & \\ 0 & & J_p \end{bmatrix} (X)\omega + \begin{bmatrix} J_1 & & 0 \\ & \ddots & \\ 0 & & J_p \end{bmatrix} \varepsilon, \tag{4.1}$$

where

$$\begin{aligned} J_i &= 1, \quad \text{if } i\text{th row is chosen} \quad (i = 1, \cdots, p) \\ &= 0, \quad \text{otherwise,} \end{aligned} \tag{4.2}$$

and where, $\epsilon_1, \cdots, \epsilon_p$ are identically distributed independent random variables, $E\{\varepsilon\} = \mathbf{0}$; $E\{\varepsilon\varepsilon'\} = \sigma^2 I$. Accordingly,

$$E\{Z^{(n)}\} = E \begin{bmatrix} J_1 & & 0 \\ & \ddots & \\ 0 & & J_p \end{bmatrix} (X)\omega = (n/p)(X)\omega. \tag{4.3}$$

Hence, the unbiased estimator (unique!) of ω, under this randomization procedure, is

$$\hat{\omega}^{(n)} = n^{-1}(X)'\mathbf{Z}^{(n)}. \tag{4.4}$$

A non-randomized fractional weighing design of size $1 \leqq n \leqq p$, is one in which n out of the p rows are chosen with probability 1. In case $n = p$, estimator (4.4) is the common least-squares estimator of ω.

It is easy to show that, under the present assumptions the covariance matrix of $\hat{\omega}^{(n)}$ is:

$$\begin{aligned} \mathfrak{V}(\hat{\omega}^{(n)}) = (\sigma^2/n)I + n^{-1}(1 - (n-1)/(p-1)) \\ \cdot [p^{-1} \textstyle\sum_{i=1}^{p} (\mathbf{X}_i'\omega)^2 \mathbf{X}_i\mathbf{X}_i' - \omega\omega']. \end{aligned} \tag{4.5}$$

Formula (4.5) differs from (2.1) only in the finite multiplier $(1 - (n-1)/(p-1))$ of the second term. Formula (4.5) yields the known result that when $n = p$, $\mathfrak{V}(\hat{\omega}^{(n)}) = (\sigma^2/p)I$. The variance of $\lambda'\hat{\omega}^{(n)}$ is $\lambda'\mathfrak{V}(\hat{\omega}^{(n)})\lambda$.

We generalize now the estimation procedure for an arbitrary function $\lambda'\omega$. Let λ be such that α (1.4) has r $(1 \leqq r \leqq p)$ non-zero components. We shall assume that the number of weighing operations, n, is either smaller or equal to r or $n = kr$, $k = 2, 3, \cdots$ (k is the number of replications). Consider the case of $1 \leqq n \leqq r$. n rows are chosen at random, without replacement, from the r admissible rows of (X) (those corresponding to the non-zero components of α). Without loss of generality, assume that the admissible rows of (X) are the first r ones. This assumption implies also that $\lambda'\mathbf{X}_i = 0$ for all $r < i \leqq p$. Let

$$(J_{(r)}) = \left[\begin{array}{ccc:c} J_1 & & & 0 \\ & \ddots & & \vdots \\ & & J_r & \vdots \\ \hdashline \multicolumn{3}{c:}{\cdots\cdots\cdots} & \cdots \\ \multicolumn{3}{c:}{0} & 0 \end{array}\right] \tag{4.6}$$

where $J_i = 1, 0$ $(i = 1, \cdots, r)$ if the ith row of X_p is chosen or not. The statistical model is now,

$$\mathbf{Z}^{(n)} = (J_{(r)})[(X)\boldsymbol{\omega} + \boldsymbol{\varepsilon}]. \tag{4.7}$$

Accordingly, the unbiased estimate of $\lambda'\boldsymbol{\omega}$ is:

$$\lambda'\hat{\boldsymbol{\omega}}^{(n)} = (r/np)\lambda'(X)'\mathbf{Z}^{(n)}. \tag{4.8}$$

Indeed,

$$E\{\mathbf{Z}^{(n)}\} = (n/r)\begin{bmatrix} I_r & \vdots & 0 \\ \cdots & \vdots & \cdots \\ 0 & \vdots & 0 \end{bmatrix}(X)\boldsymbol{\omega}. \tag{4.9}$$

But, since the last $(p - r)$ components of $\lambda'X'$ are zeros, we have,

$$\lambda'(X)'\begin{bmatrix} I_r & \vdots & 0 \\ \cdots & \vdots & \cdots \\ 0 & \vdots & 0 \end{bmatrix} = \lambda'(X)'. \tag{4.10}$$

Hence, according to (4.8), (4.9) and (4.10), $E\{\lambda'\hat{\boldsymbol{\omega}}^{(n)}\} = \lambda'\boldsymbol{\omega}$. One can also prove that, whenever $1 \leqq n \leqq r$,

$$\begin{aligned}\text{Var}\{\lambda'\hat{\boldsymbol{\omega}}^{(n)}\} = (r/np)\sigma^2\lambda'\lambda + n^{-1}(1 - (n-1)/(r-1)) \\ \cdot[(r/p^2)\textstyle\sum_{i=1}^{r}(\mathbf{X}_i'\boldsymbol{\omega})^2(\lambda'\mathbf{X}_i)^2 - (\lambda'\boldsymbol{\omega})^2].\end{aligned} \tag{4.11}$$

This formula shows that whenever $r < p$, the optimal weighing design is singular, and consists of the r weighing operations corresponding to the r admissible rows of (X). This result solves a problem raised by K. S. Banerjee in [1], concerning the characterization of singular designs which are optimal.

Finally, it should be remarked that when $n = rk$ $(k = 2, 3, \cdots)$, k independent replicates of the optimal design are performed, and the estimate used is the average of the k corresponding estimates. The variance of the estimator of $\lambda'\boldsymbol{\omega}$ is obtained then by dividing (4.11) by k.

5. Relationship of the present results to optimal randomization procedures in fractional factorial designs. Optimal randomization procedures in fractional factorial designs were studied previously by S. Ehrenfeld and S. Zacks [2], [3]. The objective in these studies was to design, in some optimal manner, a $n/2^{m-s}$ fractional replicate of a 2^m factorial experiment $(1 \leqq s < m)$, in order to estimate and test hypotheses concerning a preassigned subset of 2^s parameters. The 2^m factorial model is similar to the chemical type weighing model. In both designs we use Hadamard matrices as design matrices. The main difference is that in the factorial model the number of parameters is $p = 2^m$ $(m = 1, 2, \cdots)$ while in the weighing problem the number of parameters is (to some extent) arbitrary. The Hadamard matrices for 2^m factorial models always exist, and are given by:

$$(C^{(2^m)}) = \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \otimes (C^{(2^{m-1})}), \qquad m = 1, 2, \cdots, \tag{5.1}$$

where

$$(C^{(2)}) = \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix},$$

and $\otimes$ denotes the Kronecker's direct multiplication operator. The relationship between the matrix $(C^{(2^m)})$ determined by (5.1) and the matrix X of order $p = 2^m$ of the type considered previously is: $X = (C^{(2^m)})'$. Let $N = 2^m$ and $S = 2^s$ $(s < m)$. Suppose that a fractional replication of size S is designed for estimating a pre-assigned subset of S parameters. Without loss of generality, suppose we are interested in the parameters $\beta_1, \cdots, \beta_S$. Denote by $\underline{\beta}_N$ the vector of all parameters, and by $\underline{\beta}_S$ the subvector of pre-assigned parameters $\underline{\beta}_N' = (\underline{\beta}_S', (\underline{\beta}^*_{N-S})')$. The randomization procedures studied by Ehrenfeld and Zacks in [2] are of two types. The first type, designated by RP I, is to classify the rows of $(C^{(N)})$ into $M = N/S$ blocks of S rows, according to usual classification rules of fractional replications, and then to choose one block at random (with equal probability). For the sake of the present discussion we can assume that the M blocks are constructed simply by assigning the first S rows to the first block, the second S rows to the second block, etc. The second type of randomization procedures, designated by RP II is to construct S blocks, each one of M rows of $C^{(N)}$, and to choose at random a row from each of the S blocks. Under the present assumption, the S blocks for RP II are the following: Block 1 contains all the $(1 + US)$th rows of $C^{(N)}$, where $U = 0, \cdots, M - 1$; Block 2 contains all the $(2 + US)$th rows of $C^{(N)}$, $U = 0, \cdots, M - 1$; etc. As proven in [2] the variances of the unbiased estimators of the individual parameters in $\underline{\beta}_S$ are:

$$\begin{aligned} \text{Var}\{\hat{\beta}_i\} &= \sigma^2/S + S^{-1}(1 - (S-1)/(N-1)) \\ &\qquad \cdot \textstyle\sum_{U=1}^{N/S-1} \beta^*_{i+US}, \quad \text{under RP I,} \\ &= \sigma^2/S + S^{-1}(1 - (S-1)/(N-1))1/((N/S) - 1) \\ &\qquad \cdot \textstyle\sum_{i=0}^{S-1} \sum_{U=1}^{N/S-1} \beta^*_{i+US}, \quad \text{under RP II.} \end{aligned} \tag{5.2}$$

for $i = 1, 2, \cdots, S$.

It is simple to show that the best unbiased estimators of the first S individual parameters can be obtained, according to the randomization procedures studied in the present paper, only if we choose S rows at random (without replacement) from the N rows of $C^{(N)}$ which are the admissible rows (denote this procedure by SAR-sampling admissible rows). Writing $\lambda_{(i)} = (0, \cdots, 1, 0, \cdots, 0, \underline{0}'_{N-S})$ for $i = 0, \cdots, S - 1$, we obtain from (4.11) that the variance of $\hat{\beta}_i$, under the SAR is,

$$\begin{aligned} \text{Var}\{\hat{\beta}_i \mid \text{SAR}\} &= \sigma^2/S + S^{-1}(1 - (S-1)/(N-1)) \\ &\qquad \cdot (\textstyle\sum_{j=0}^{N-1} \beta_j^2 - \beta_i^2), \quad i = 0, \cdots, S-1. \end{aligned} \tag{5.3}$$

The comparison of (5.2) and (5.3) shows that individual estimates of the pre-assigned parameters are generally better (have smaller variances) under RP I or RP II than under SAR.

We show now that for estimating certain linear functions of the pre-assigned parameters, the randomization procedures, studied in the previous sections, might be better than either RP I or RP II. Consider the linear functional $\lambda_N' = (1_S', 0_{N-S}')$. $\lambda_N'\beta_N$ is the sum of the pre-assigned parameters. Since $\alpha_N' = N^{-1}\lambda_N'(C^{(N)}) = c_1^{(N/S)} \otimes ((S/N), 0_{S-1}')$, where $c_1^{(N/S)'}$ is the first row vector of $(C^{(N/S)})$. Accordingly, $M = N/S$ components of α_N are non-zero. These are the 1st, $(1 + S)$st, $\cdots$ $(1 + (M - 1)S)$st components. According to the estimation procedures SAR, the function $1_S'\beta_S$ is estimated unbiasedly by choosing at random (without replacement) S rows out of the M admissible rows of $(C^{(N)})$. The admissible rows for SAR are the $(1 + US)$st, $U = 0, \cdots, M - 1$. If $M \leqq S$ it is sufficient to perform only M experiments, and the variance of the unbiased estimator (the average yield) will be σ^2/M. Assume that $S < M$. According to (4.16), a simple random sample of S rows out of the M admissible rows of $(C^{(N)})$ yields an unbiased estimator having a variance,

$$(5.4)\quad \mathrm{Var}\{1_S'\hat{\beta}_S \mid \mathrm{SAR}\} = \sigma^2/S + S^{-1}(1 - (S-1)/(M-1)) \sum_{U=1}^{M-1} (1_S'\beta_{(u)}^*)^2$$

where $\beta_{(u)} = (\beta_{1+uS}, \cdots, \beta_{(u+1)S-1})'$ for all $u = 0, \cdots, M - 1$.

On the other hand, under RP I, the covariance matrix of the unbiased estimator (conditional least squares estimator, see S. Zacks [6]) of β_S is,

$$(5.5)\quad \mathcal{V}(\hat{\beta}_S \mid \mathrm{RP\ I}) = (\sigma^2/S)I_S + \sum_{u=1}^{M-1} \beta_{(u)}^*(\beta_{(u)}^*)'.$$

Hence,

$$(5.6)\quad \mathrm{Var}\{1_S'\hat{\beta}_S \mid \mathrm{RP\ I}\} = \sigma^2 + \sum_{u=1}^{M-1} (1_S'\beta_{(u)}^*)^2.$$

The comparison of (5.4) with (5.6) shows that the randomization procedures discussed in the present paper may reduce the variance of a given linear function of $\lambda_S'\hat{\beta}_S$ considerably, over that attained by RP I. In the above example it was shown that

$$\mathrm{Var}\{1_S'\hat{\beta}_S \mid \mathrm{SAR}\} < S^{-1}\,\mathrm{Var}\{1_S'\hat{\beta}_S \mid \mathrm{RP\ I}\}.$$

A similar result can be demonstrated in comparing SAR with RP II. The conclusion from this analysis is that whenever we are concerned with a subvector of $S = 2^s$ $(s < m)$ parameters of a 2^m factorial system, if a non-singular design is optimal for a problem concerning the parameters of the corresponding 2^s factorial model, regarded as a complete factorial model, then RP I or RP II is superior to SAR. If a singular design is optimal for the reduced 2^s factorial model, then SAR is superior to RP I or RP II, for the estimation of the appropriate linear function.

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