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SOME COMBINATORIAL PROBLEMS AND RESULTS IN FRACTIONAL REPLICATION

by

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1. INTRODUCTION

In a mimeographed paper (distributed at the Spring Statistical Meetings at Tallahassee in 1965, Raktøe (see Federer and Raktøe (1965)) and, in his Ph.D. dissertation, Paik (1968) threw new light on the combinatorial structure of saturated main effect plans from an s^m factorial experiment. As a consequence, many combinatorial problems became evident. In a series of papers by Paik and Federer (1966, 1970a, 1970b, 1970c), Raktøe and Federer (1969a, 1969b, 1970a, 1970b, 1970c), and Werner (1970), several combinatorial structures and problems were investigated and formulated. Some of these are discussed below.

If we designate the s^m factorial single-degree-of-freedom effects by an $s^m \times 1$ column vector $\underline{\beta}$, the $s^m \times s^m$ columnwise-orthogonal design matrix of coefficients by X , and the $s^m \times 1$ vector of $N = s^m$ observations by \underline{Y} , then the expected value of the observation vector is $E(\underline{Y}) = X\underline{\beta}$. If $p < N$ observations from the complete set of N observations are selected and if p of the N parameters are to be estimated, a saturated fractional replicate of the s^m factorial results. If we let \underline{Y}_p be the $p \times 1$ column vector of observations, $\underline{\beta}_p$ be the

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$p \times 1$ column vector of parameters to be estimated, and β_{N-p} be the $(N-p) \times 1$ column vector of parameters aliased with those in β_p , then we may write the p observational equations for the fractional replicate, omitting the error vector, in the form: $X_{11}\beta_p + X_{12}\beta_{N-p} = \underline{Y}_p$, where

$$X = (X_1 : X_2) = \begin{pmatrix} X_{11} & \vdots & X_{12} \\ & \vdots & \\ X_{21} & \vdots & X_{22} \end{pmatrix}, X_1 \text{ is an } N \times p \text{ matrix}$$

of coefficients corresponding to the parameters in β_p , X_2 is an $N \times (N-p)$ matrix of coefficients corresponding to the parameters in β_{N-p} , X_{11} is a $p \times p$ matrix constructed by taking any p rows of X_1 and the corresponding observations from \underline{Y} to form \underline{Y}_p , X_{12} is a $p \times (N-p)$ matrix determined by the selection of the rows in X_{11} , X_{21} is an $(N-p) \times p$ matrix of the remaining rows in X_1 after X_{11} has been formed, and X_{22} is an $(N-p) \times (N-p)$ matrix resulting from X_2 after the p rows in X_{12} have been removed.

The combinatorial problems considered are concerned with the characterization of the matrix X_{11} . In particular, some of the following questions arise about the nature of X_{11} :

- (i) How many possible plans of X_{11} exist?
- (ii) Can any of these plans be generated from a given plan, i.e., is there a set of generators which can be used to generate all possible plans?
- (iii) For any given s^m factorial, how many generators and how many plans per generator are there?
- (iv) What values are possible for the determinant of X_{11} ?
- (v) Are there only n values of $||X_{11}||$, the absolute value of the determinant, for the 2^n factorial for $n > 2$?

- (vi) How many plans are associated with each value of $\|X_{11}\|$?
- (vii) What is the nature of the aliasing structure of $X_{11}^{-1}X_{12}$, given that X_{11}^{-1} is either an inverse or a generalized inverse of X_{11} , for each generator? for each value of $\|X_{11}\|$?
- (viii) What are the variances for the estimates of the parameters in β_p , given that X_{11}^{-1} exists, for all the plans derivable from a given generator or from a given value of $\|X_{11}\|$?
- (ix) How many plans are associated with singular X_{11} ?
- (x) How many plans are associated with the maximum value of $\|X_{11}\|$?
- (xi) Is there an algorithm for deriving all generators from any given generator for a specified value of $\|X_{11}\|$?
- (xii) Is there an algorithm for obtaining all generators from any specified generator?
- (xiii) Given that results are available for the 2^n factorial, how do they extend to the s^m and the $(q \times r \times t \dots)$ factorials?
- (xiv) Is there a transformation of X which will aid in characterizing X_{11} ?
- (xv) What is the frequency distribution of plus ones in X_{11} for fractional replicates from the 2^n factorial?
- (xvi) What is the frequency distribution of plus ones in X_{11} for the generators of fractional replicates in the 2^n factorial?
- (xvii) How does the frequency of plus ones in X_{11} for fractional replicates of the 2^n factorial relate to values of $\|X_{11}\|$?
- (xviii) Since the columnwise-orthogonal matrix X has rank N , what are the possible ranks for the matrix X_{11} and its corresponding matrix X_{22} ?

Some of the above questions have been answered or partially answered but some appear to be exceedingly difficult. In order to complete the theory for saturated fractional replicates from an s^m factorial, it is necessary to have answers to all of the above questions. Since the $(1, -1)$ coefficient matrix can

be transformed to a (0,1) matrix (see e.g., Raktoe and Federer (1970a)), answers to the above questions also extend the theory of (0,1) and (1,-1) matrices. Since the rows of X, and consequently of X_{11} , are all distinct, there are $\binom{N}{p}$ ways of forming saturated fractional replicate plans. Paik (1968) and Paik and Federer (1970a) have shown that generators can be produced, each of which will generate s^m plans, s a power of a prime, provided that the generator does not form a group. Only for the case that $p = s^k$, $k < m$, is it possible for a generator to form a group. Raktoe and Federer (1970c) have determined the number of generators for $p = m(s-1) + 1$, s a power of a prime number, and for saturated main effect plans from an s^m factorial.

Paik and Federer (1966, 1970a) and Paik (1968) have found that $||X_{11}||$, the absolute value of $|X_{11}|$, can take on the following values for specified factorials:

	Possible values of $ X_{11} $
2^3	$2^2, 0^*$
2^3	$2(2^3), 2^3, 0$
2^4	$3(2^4), 2(2^4), 2^4, 0$
3^2	$2(2^2)(3^2), 2^2(3^2), 0$
3^3	$4(2^3)(3^3), 3(2^3)(3^3), 2(2^3)(3^3), 2^3(3^3), 0$

* occurs with zero frequency.

From the above Paik and Federer (1970a) were lead to the conjecture that $||X_{11}||$ can take the values $[s(s-1)(s-2)...1]^2 [m(s-1)-i]$ for $i = s-1, s, s+1, \dots, m(s-1)$. Since Paik has produced a counter example to the above conjecture for $s = 5$, it may hold only for $s = 2$ and/or 3. The fact that $||X_{11}||$ takes only a relatively small number of values appears to be unknown to most writers of statistical literature.

Only Webb (1965) appears to have been aware of this fact. Writers of mathematical literature also appear to be unaware of this. A proof of the number of values and the values that $||X_{11}||$ can take would be an important development in mathematics and in the theory of fractional replication.

Metropolis and Stein (1967) obtained a lower bound on the number of singular $(0,1)$ matrices in the class having distinct rows (i.e., those from the 2^n factorial). Raktoe and Federer (1970b) obtained a lower bound on the number of singular saturated main effect plans from an s^m factorial. The general problem is formulated precisely in a mathematical form, and these two bounds are discussed and compared in the second section of this paper. Thus, some characterizations of X_{11} have been made when X_{11} is singular. In addition, Raktoe and Federer (1970a) have given some characterizations of X_{11} when $||X_{11}||$ achieves its maximal value. It appears that mathematicians having been mostly concerned with studying X_{11} when $||X_{11}||$ achieves its maximum value. The study of $||X_{11}|| \neq 0$ or a maximum has been neglected; knowledge of other values of $||X_{11}||$ is important in selecting fractional replicates with desirable aliasing properties (see Paik and Federer (1970a)). Some information on the aliasing structure of $X_{11}^{-1}X_{12}$ and on the variances of the estimated parameters in $\underline{\beta}_p$ has been obtained by Paik and Federer (1970c).

Werner (1970) has obtained the frequency distribution of ones in $(0,1)$ matrices with distinct rows and of ones in the generators for saturated main effect plans from the 2^n factorial. Some of her results are presented in the third section of this paper.

2. SOME COMBINATORIAL PROBLEMS OF SINGULAR SATURATED

MAIN EFFECT PLANS OF THE 2^n FACTORIAL

In this section some additional unsolved problems and first attempts at solving them are presented. The results are associated with the enumeration of saturated main effect plans of the 2^n factorial. Special attention is devoted to the class of singular saturated plans and two lower bounds to its cardinality are discussed.

First, let us consider the general combinatorial problem. Let G be the set of n -tuples of the form (x_1, x_2, \dots, x_n) , with $x_i \in \{0, 1\}$. Further let A_{n+1} be the set of $(n+1) \times (n+1)$ matrices of the form $[1:D]$, where 1 is a column of $+1$'s and the rows of D are $n+1$ distinct elements of G . Note that the cardinality of A_{n+1} is $\binom{2^n}{n+1}$. If $\det [1:D]$ denotes the determinant of $[1:D]$, then an unsolved problem of considerable complexity is the determination of the precise range of $\det [1:D]'[1:D]$ or of $|\det [1:D]|$ for arbitrary n . A second and related problem is then to determine how many matrices belong to each possible value of $|\det [1:D]|$. These two problems can be considered as the general combinatorial problem of saturated main effect plans of the 2^n factorial. (See also Paik and Federer (1970a) and Raktoe and Federer (1970b)).

The above general problem was first enumerated by Paik (1968) and Paik and Federer (1970a) for $n = 2, 3$, and 4 . In a mimeographed note distributed at the Joint Statistical Meetings of August 1969 in New York City, the general problem was pointed out to the audience by one of the authors and possible methods of attack were indicated. This could be done, because the problem can be treated in terms of $(-1, 1)$ -matrices, $(0, 1)$ -matrices, polytopes, etc.

Possibly, the simplest problem to be solved is to find the number of matrices in A_{n+1} having determinant equal to zero, i.e., the determination of the cardinality of the singular class in A_{n+1} . Let us denote this singular class by $A_{n+1,0}$ and let $\delta_{n+1,0}$ be its cardinality. In a recent attempt to determine $\delta_{n+1,0}$ for arbitrary n , Raktoc and Federer (1970b) considered a subclass of A_{n+1} , this subclass being of the form $[1:B]$, where the $n+1$ rows of B were considered to be $(n+1)$ -subsets of the points belonging to a $(n-k)$ -flat of $EG(n,2)$, k being the largest positive integer such that $n \leq (2^{n-k}-1)$ for given n . (For further details concerning the more general setting of this subset, the reader is directed to Raktoc and Federer (1970b).) Denoting this subset by E_{n+1} and its cardinality by ϵ_{n+1} , the authors showed that:

$$\epsilon_{n+1} = a(n,k) \cdot 2^k \cdot \binom{2^{n-k}}{n+1} \quad \dots(2.1)$$

where:

$$a(n,k) = \prod_{i=0}^{k-1} [(2^{n-i}-1)(2^{k-i}-1)^{-1}] \quad \dots(2.2)$$

Denoting by $E_{n+1,0}$ the singular subclass of E_{n+1} and letting $\epsilon_{n+1,0}$ be the cardinality of $E_{n+1,0}$, the authors further showed (via a theorem first proved by Dowling (1970) that:

$$\epsilon_{n+1,0} = [a(n,k) - b(n,k)] \cdot [c(n,k)]^{-1} \cdot 2^k \binom{2^{n-k}}{n+1} \quad \dots(2.3)$$

where:

$$b(n,k) = \prod_{i=0}^{n-1} [(2^{n-k}-1)^{-i}] \quad \dots(2.4)$$

$$c(n,k) = 2^{(n-k)(n-k-1)} 2^{-1} \prod_{i=0}^{n-k-1} (2^{n-k-i}-1) \quad \dots(2.5)$$

This number now can be used as a lower bound to $\delta_{n+1,0}$.

A different and interesting subset of A_{n+1} has also been investigated by Metropolis and Stein (1967). Putting their work in our context their subclass, call it A_n , consisted of matrices of the form $\begin{bmatrix} \cdot & 0' \\ 1 & \cdot \\ \cdot & \cdot \\ \cdot & D^* \\ \cdot & \cdot \end{bmatrix}$, where D^* is an $n \times n$ matrix with the rows being distinct non-zero elements of G and $0'$ is the zero element of G . Note that the cardinality δ_n of A_n is equal to $\binom{2^n - 1}{n}$. As pointed out by these two authors, the determination of the cardinality $\delta_{n,0}$ of the singular subclass $A_{n,0}$ of A_n is still unresolved. They obtained a lower bound to $\delta_{n,0}$ (their derivations are complex and would require at least a couple of pages, so that the reader is advised to read the paper) and they compared it with $\delta_{n,0}$ as enumerated by M. B. Wells (1967) for $n = 2, 3, 4, 5, 6$. Denoting the Metropolis-Stein lowerbound by $\epsilon_{n,0}$ we have the following illustrative table:

Table 2.1. Lower bounds to the number of singular plans for $n = 2, 3, 4, 5, 6$.

n	RAKTOE-FEDERER		METROPOLIS-STEIN	
	$\delta_{n+1,0}$	$\epsilon_{n+1,0}$	$\delta_{n,0}$	$\epsilon_{n,0}$
2	0	0	0	0
3	12	12	6	6
4	1360	1120	425	350
5	?	15680	65625	43260
6	?	86080	27894671	14591171

From table 2.1 it can be observed that the Raktœ-Federer bound becomes crude for $n > 4$ and noting the fact that A_n is contained in A_{n+1} we see that the Metropolis-Stein bound is much sharper for these values. There is hope that further work will improve the Raktœ-Federer bound.

3. FREQUENCY DISTRIBUTION OF ONES IN
(0,1)-MATRICES HAVING DISTINCT ROWS

Let D be an $(n+1) \times n$ matrix composed of zeros and ones such that the rows are all distinct. One problem related to characterizing D is to find the frequency distribution of ones in all possible fractional replicates with $n+1$ observations from the 2^n factorial. This problem is resolved here. Before presenting this result we state four lemmas without proof.

Lemma 3.1. Given a (0,1)-matrix D with T equal to the number of ones in the matrix, then the range of T is from n to n^2 for a total of n^2-n+1 values.

Lemma 3.2. Given the $\binom{2^n}{n+1}$ possible matrices D and letting the number of matrices having exactly T ones be denoted by $df(T)$, then the $df(n+k) = df(n^2-k)$ for $k = 0, 1, \dots, (n^2-n)/2$; that is, $df(T)$ is symmetric around the median value of T .

Let D^* be an $n \times n(0,1)$ -matrix having all rows distinct and no row containing all zeros.

Lemma 3.3: Given a (0,1)-matrix D^* with T^* equal to the number of ones in the matrix, the range of T^* is from n to n^2-n+1 for a total of n^2-2n+2 values.

Lemma 3.4: Given the $\binom{2^n-1}{n}$ possible matrices D^* and letting the number of matrices having exactly T^* ones be denoted by $d^*(T^*)$, then $d^*(n+k) = d^*(n^2-n-k)$ for $k = 0, 1, \dots, (n^2-2n-1)/2$ if n is odd and $k = 0, 1, 2, \dots, n(n-2)/2$ if n is even; that is with the exclusion of $T^* = n^2-n+1$, $d^*(T^*)$ is symmetric around the median value of T^* .

We are now ready to state the main result concerning the frequency distribution of ones in (0,1)-matrices having distinct rows:

Theorem 3.1: Given (0,1)-matrices D of size $(n+1) \times n$ with T ones and letting $df(T)$ equal the number of matrices D having exactly T ones, then

- (i) for $T = n$, $df(n) = 1$
- (ii) for $T = n+1$, $df(n+1) = \binom{c_0}{1} \binom{c_1}{n-1} \binom{c_2}{1}$, and
- (iii) for $T = n+k$, $k = 0, 1, \dots, (n^2-n)/2$,

$$df(T) = \sum_{\substack{\text{of all cases when} \\ \sum_{i=0}^n x_i = n+1 \\ \sum_{i=0}^n ix_i = n+k}} \prod_{j=0}^n \binom{c_j}{x_j},$$

where $c_j = \binom{n}{j} \equiv$ the number of unique $1 \times n$ row vectors with n ones and,
 $x_j = 0, 1, \dots, \binom{n}{j} \equiv$ the number of $1 \times n$ row vectors having j ones in the matrix
 D.

Proof:

Consider the matrix D as being composed of $n+1$ row vectors of size $1 \times n$ with each vector containing from zero to n ones with all elements not one being zero. Every row of D is unique (distinct) and the total number of ones, T , in D is equal to $n + k$, $k = 0, 1, \dots, n^2-n$ by lemma 3.1. Let t equal the smallest number of ones in any row vector of the matrix and let r equal the number of row vectors with t ones. When there are r row vectors with t ones, the remaining $n+1-r$ row vectors must contain $n+k-rt$ ones. If matrices are formed by starting with r row vectors with t ones in each and if

$$n+1-r > n+k-rt \quad \dots(3.1)$$

then no matrix exists because the number of row vectors left to choose is greater than the number of ones left to distribute. This results from the facts that

$$n+1-r = \sum_{i=t+1}^n x_i$$

and

$$n+k-rt = \sum_{i=t+1}^n ix_i ;$$

when $n+1-r > n+k-rt$, this means that

$$\sum_{i=t+1}^n x_i > \sum_{i=t+1}^n ix_i ,$$

i.e., that

$$0 > \sum_{i=t+1}^n (i-1)x_i .$$

But, by definition $0 \leq x_i \leq \binom{n}{i}$ and $t \geq 0$; therefore, the strict inequality can never hold.

If there are $n+k-rt$ ones left to distribute and if each remaining row vector that can be chosen has at least $t+1$ ones (by the definition of t), then the number of ones left must be equal to or greater than the number of ones required such that every remaining row vector has $t+1$ ones, i.e.,

$$n+k-rt \geq (t+1)(n+1-r) \quad \dots(3.2)$$

The inequality in (3.2) results from the fact that every row vector still to be selected has $t+1$ or more ones.

In proving the theorem we proceed part by part. First we shall prove part (i). Since there is only one, $\binom{n}{0} = 1$, possible unique zero row vector and since there are $\binom{n}{1} = n$ possible unique row vectors with one one each, then there is only one unique combination which will form an $(n+1) \times n$ matrix with

only n ones (There can be no negative ones in a $(0,1)$ matrix.). The formula is

$$\begin{pmatrix} c_0 \\ 1 \end{pmatrix} \begin{pmatrix} c_1 \\ n \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \begin{pmatrix} n \\ n \end{pmatrix} = 1, \text{ which proves part (i).}$$

To prove part (ii), note that if the zero row vector is selected, there are n row vectors left to choose and $n+1$ ones left to distribute. Therefore, if r row vectors with t ones each are selected from the remaining n row vectors, the following must hold (from 3.2)):

$$n+1-rt \geq (t+1)(n-r) ,$$

or

$$r \geq tn - 1 .$$

Since only n row vectors remain to be selected, $r \leq n$.

If $t > 1$, r becomes too large. When $t = 1$, r can either be n or $n-1$. For $r = n$,

$\sum_{i=1}^n ix_i = 0(1) + 1(n) \neq n+1$. If $r = n-1$, the following combinations are suitable:

$$\begin{pmatrix} c_0 \\ 1 \end{pmatrix} \begin{pmatrix} c_1 \\ n-1 \end{pmatrix} \begin{pmatrix} c_2 \\ 1 \end{pmatrix} \dots (3.3)$$

If the zero row vector is not selected as one of the rows of D , there are $n+1$ row vectors to be selected and $n+1$ ones to distribute. Therefore, from (3.2) the inequality,

$$r \geq t (n+1) ,$$

must hold in order for any possible matrices to exist. If $t = 1$, then $r = n+1$ but there are only n unique row vectors with one one. When $t > 1$, $r > n+1$ and therefore there are no possibilities except (3.3) which proves part (ii).

Admissible matrices D occur when the number of row vectors selected equals $n+1$ and when the number of ones totals $n+k$. If a row vector with i ones is needed, there are $\binom{n}{i} = c_i$ combinations from which to choose. If x_i row vectors with i ones are needed, there are $\begin{pmatrix} c_i \\ x_i \end{pmatrix}$ possible unique combinations. In our

notation, this is simply:

$$df(T) = \sum_{\text{when}} \prod_{j=0}^n \binom{c_j}{x_j} \dots (3.4)$$

$$\sum_{i=0}^n x_i = n+1$$

$$\sum_{i=0}^n ix_i = n+k$$

In order to perform the actual computations and in order to find all possibilities (as was done for part (ii)), the following breakdown of (3.4) is used:

$$df(T) = \binom{c_0}{1} \sum_{\text{when}} \prod_{j=1}^n \binom{c_j}{x_j} + \sum_{\text{when}} \prod_{j=1}^n \binom{c_j}{x_j} \dots (3.5)$$

$$\sum_{i=1}^n x_i = n \qquad \sum_{i=1}^n x_i = n+1$$

$$\sum_{i=1}^n ix_i = n+k \qquad \sum_{i=1}^n ix_i = n+k$$

The above expression allows consideration of whether or not the zero row vector is selected.

Once r row vectors with t ones are selected, the first part of (3.5) may be rewritten as:

$$\sum_{t=1}^n \sum_{r=tn+k}^{c_t \text{ or } n+1} \binom{c_t}{r} \sum_{\text{when}} \prod_{j=t+1}^n \binom{c_j}{x_j} \dots (3.6)$$

$$\sum_{i=t+1}^n x_i = n-r$$

$$\sum_{i=t+1}^n ix_i = n+k-rt$$

If $n-r > n+k-rt$ (from (3.1)), there are no possibilities, and only if $n+k-rt \geq (t+1)(n-r)$, from (3.2), are there any possibilities. In the first case,

the summation is zero and the next value of r and t can be tried. For the second case, the expression.

$$\sum_{j=t+1}^n \prod_{j=t+1}^n \begin{pmatrix} c_j \\ x_j \end{pmatrix}$$

when

$$\sum_{i=t+1}^n x_i = n-r$$

$$\sum_{i=t+1}^n ix_i = n+k-rt$$

may be partitioned in the same manner as the first term of (3.5) was to obtain (3.6).

If r_1 row vectors with t_1 ones each are selected, where t_1 is the second smallest number of ones in any row vector, the number of ones left is $n+k-rt-r_1t_1$ and the number of row vectors left to be chosen is $n+1-r-r_1$. To continue with this procedure, the following must hold:

$$n+k-rt-r_1t_1 \geq (n+1-r-r_1)(t_1+1),$$

or

$$r_1 \geq t_1(n+1) + (1-k) + r(t-t_1);$$

if

$$n+1-r-r_1 > n+k-rt-r_1t_1,$$

then no possibilities exist and a new path with a larger value for t must be tried. Whenever (3.1) holds the entire path is wrong and the first choice of t must be increased if possible. When t can no longer be increased, there are no more possibilities for choosing the zero row vector. This same procedure can be used for the second part of (3.5) and hence to complete the proof of part (iii). This completes the proof of the theorem and illustrates the procedure for computing $df(T)$.

The generators developed by Paik (1968) have a zero row vector in the first row. The remaining part of the matrix D is then D^* . The frequency distribution of ones in the matrix D^* is given in the following corollary.

Corollary 3.1: Given (0,1)-matrices D^* composed of n unique (0,1) row vectors with none of them being the zero row vector and letting $df^*(T^*)$ be the number of matrices D^* having a total of T^* ones, then

- (i) for $T^* = n$, $df^*(n) = 1$,
- (ii) for $T^* = n+1$, $df^*(n+1) = \binom{c_1}{n-1} \binom{c_2}{1}$, and
- (iii) for $T^* = n+k$, $k = 0, 1, \dots, n^2 - 2n + 2$,

$$df^*(T^*) = \sum_{\text{when}} \prod_{j=1}^n \binom{c_j}{x_j} .$$

$$\sum_{i=1}^n x_i = n$$

$$\sum_{i=1}^n ix_i = n+k$$

The proof of the corollary follows that given for theorem 3.1.

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