A TOPOLOGICAL FORMULATION OF AN UNSOLVED PROBLEM IN FRACTIONAL FACTORIAL DESIGNS

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ABSTRACT

This paper presents a rigorous contribution towards the mathematical understanding of some of the problems which arise in fractional factorial designs. Specifically, it shows how choosing a saturated main effect fractional replicate of the 2^n factorial is equivalent to choosing a simplex in the n-dimensional Euclidean space E^n. The formulation of this equivalence is achieved by employing certain important concepts in topology. A complete illustration is given using the 2^3 factorial as an example. Statistical terminology has been limited to as to make the paper accessible to any mathematician with a slight understanding of statistics.

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1. Introduction and Background. In the ensuing developments we will be working in the Euclidean space E^n whose vectors will be written as column vectors x or as row vectors by writing the transpose $x' = (\xi_1\xi_2\cdots\xi_n)$, where $\xi_i \in R$ is the i^{th} coordinate with respect to the standard orthonormal basis vectors $e_1' = (100\cdots0)$, $e_2' = (010\cdots0),\cdots,e_n' = (00\cdots01)$. The inner product of two vectors x and y is defined as $\langle x,y\rangle = \sum_{i=1}^{n}\xi_i\eta_i$ and the distance between these points is $\langle x-y, x-y\rangle^{\frac{1}{2}}$.

Let $T = \{x' = (\xi_1\xi_2\cdots\xi_n),\ \xi_i \in \{0,1\}\}$. The set T has cardinality 2^n and it is known as the complete set of treat combinations of the 2^n factorial. We introduce an ordering on T by defining $x < y$ if and only if the decimal representation of $x' = (\xi_1\xi_2\cdots\xi_n)$ is less than the decimal representation of $y' = (\eta_1\eta_2\cdots\eta_n)$, where x' and y' are in T. In statistical theory we typically enrich the set T with a $2^n \times 1$ observation vector $Y^*(T)$, an element of which is of the form $y_{(\xi_1\xi_2\cdots\xi_n)}$, where $(\xi_1\xi_2\cdots\xi_n) \in T$. The assumed model for the observation vector $Y^*(T)$ is given

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by: (i) $E[Y^*(t)] = \mu(T)$ and $Var\ [Y^*(T)] = \sigma^2 I$, where E is the expectation operator, $\mu(T)$ is a $2^n \times 1$ column vector of unknown means with a typical element written as $\mu_{(\xi_1\xi_2\cdots\xi_n)}$, where $(\xi_1\xi_2\cdots\xi_n) \in T$; $Var\ [Y^*(T)]$ is the variance-covariance matrix of $Y^*(T)$ and I is a square identity matrix of order 2^n. (ii) The $2^n \times 1$ parametric vector $\beta^*(T) = 2^{-n}X^{*\prime}(T)\mu(T)$, where an element of $\beta^*(T)$ is written as $A_1^{\xi_1}A_2^{\xi_2}\cdots A_n^{\xi_n}$, $(\xi_1\xi_2\cdots\xi_n) \in T$, and $X^*(T)$ is a square (-1,1)-matrix such that $X^{*\prime}(T)X^*(T) = X^*(T)X^{*\prime}(T) = 2^n I$, represents the well-known vector of factorial effects. Note that $X^*(T)$ is simply a Hadamard matrix of order 2^n and we know that this always exists. Explicitly we may order the rows and columns of $X^*(T)$ using the ordered elements of T. Doing this we have that an element in the $(\gamma_1\gamma_2\cdots\gamma_n)^{th}$ row and $(\alpha_1\alpha_2\cdots\alpha_n)^{th}$ column $a_{(\gamma_1\gamma_2\cdots\gamma_n)}^{(\alpha_1\alpha_2\cdots\alpha_n)}$ of $X^*(T)$ is equal to $(2\gamma_1-1)^{\alpha_1}(2\gamma_2-1)^{\alpha_2}\cdots(2\gamma_n-1)^{\alpha_n}$, where $(\alpha_1\alpha_2\cdots\alpha_n)$ and $(\gamma_1\gamma_2\cdots\gamma_n)$ are in T. Note further that the decimal ordering imposed on T guarantees that $A_1^0A_2^0\cdots A_n^0$ will be the first component of $\beta^*(T)$.

Clearly, the above reparametrization leads us to $E[Y^*(T)] = X^*(T)\beta^*(T)$, and, it is actually this equation which one writes in practice. The pair $\{T, \beta^*(T)\}$ is usually called the full replicate of the 2^n factorial, because the basic intention is to estimate the vector of effects $\beta^*(T)$ using the observation vector $Y^*(T)$, which arises from the consideration of all elements of T. The matrix $X^*(T)$ is called the design matrix and the matrix $X^{*\prime}(T)X^*(T)$ is called the information matrix for the full replicate $\{T, \beta^*(T)\}$.

Let D be an (n+1) $\times$ n matrix whose row vectors form a (n+1)-subset of T; D will be referred to as a fractional factorial design consisting of n+1 treatment combinations. Clearly, these rows are ordered because of the ordering on T. Further let $\beta' = (A_1^0A_2^0A_3^0\cdots A_n^0,\ A_1^1A_2^0A_3^0\cdots A_n^0,\ A_1^0A_2^1A_3^0\cdots A_n^0,\ \cdots,\ A_1^0A_2^0\cdots A_{n-1}^0A_n^1)$. This vector is called in statistics the column vector of main effects and the pair $\{D,\beta\}$ is called a saturated main effect replicate of the 2^n factorial. The idea is to estimate β using the (n+1) $\times$ 1 observation vector Y corresponding to D. The word saturated refers to the fact that the number of rows of D is equal to the number of components of β, which in this case is equal to n+1. It follows from the assumptions (i) and (ii) above that there is an induced model for Y, which we indicate by writing $E[Y] = X\beta + \bar{X}\bar{\beta}$, where X is a $(n\times 1) \times (n+1)$ submatrix of $X^*(T)$ determined by the elements in Y and the components of β and $\bar{X}$ is the $(n+1) \times (2^n-n-1)$ submatrix of $X^*(T)$ determined by the elements in Y and the components of the complementary $(2^n-n-1) \times 1$ column vector of effects $\bar{\beta}$, where $\beta^{*\prime} = (\beta' \,\vdots\, \bar{\beta}')$. The normal equations to obtain the least squares estimate $\hat{\beta}$ of β are given by the well-known system $X'X\hat{\beta} = X'Y$. The matrix $X'X$ is called the information matrix of the saturated main effect replicate $\{D,\beta\}$.

From the above considerations it is clear that there are $\binom{2^n}{n+1}$ possible fractional factorial designs. Consequently it is imperative to introduce certain criteria so that a choice can be made among the possible D's. In this paper we utilize the determinant of $X'X$ or since X is square the $|\det X|$, where the bars denote absolute value. This leads us to the following two fundamental questions, which are more general than the question of finding the D which results in maximum $|\det X|$: (a) What are the possible values of $|\det X|$? (b) What is the frequency of each possible value of $|\det X|$? These two questions have as of present not been resolved in all its generality. From earlier work it is well-known that $0 \leq |\det X| \leq (n+1)^{(n+1)/2}$. Clearly, the lower bound is achieved if X is singular and from Hadamard's theorem we know that the upper bound is achieved if and only if X is a Hadamard matrix. A necessary condition for the existence of such a matrix is that $n+1 \equiv 0 \pmod{4}$ or $n+1 = 2$. Whether this condition is sufficient has not been settled yet. For $n+1 \leq 200$ the smallest order which defies a construction as of today is the case $n+1 = 188$. The interested reader is referred to the numerous publications in this area, for example [4].

There are certain results in matrix algebra which supply us with relations among all the possible values of det X or of $(\det X)^2$. From a result in [7] and the structure of $X^*(T)$ it can be easily shown that the sum of squares of all the $\binom{2^n}{n+1}$ determinants is equal to $2^{n(n+1)}$. Also all the $\binom{2^n}{n+1}$ determinants are connected by $\binom{2^n}{n+1} - [2^n-n-1][n+1] - 1$ quadratic relations and these may be derived using the Bazin-Reiss-Picquet theorem mentioned in the same reference.

There is a simpler way of looking at the fundamental problem stated above, namely in terms of (0,1)-matrices. This is achieved by postmultiplying X by a $(n+1) \times (n+1)$ triangular matrix $G = \frac{1}{2}\begin{bmatrix} 2 & 1' \\ 0 & I \end{bmatrix}$, where $\mathbf{1}$ is a $n \times 1$ column vector of 1's, 0 is a $n \times 1$ column vector of 0's and I is a $n \times n$ identity matrix. The matrix G represents a series of column operations on X and it has been successfully used earlier in [9, 12]. From elementary matrix algebra it follows that $XG = [\mathbf{1} \vdots D]$, so that $|\det X| = 2^n |\det[\mathbf{1} \vdots D]|$, where $\mathbf{1}$ is $(n+1) \times 1$ column vector of 1's and D is the design already defined above. Note that $[\mathbf{1} \vdots D]$ is a (0,1)-matrix with the first column equal to 1's. Such a matrix is referred to as a seminormalized (0,1)-matrix. It is now obvious that the fundamental problem which was stated above in terms of (-1,1)-matrices can now be stated in terms of (0,1)-matrices as: (a^*) What are the possible values of $|\det[\mathbf{1} \vdots D]|$? ($b^*$) What is the frequency of each possible value of $|\det[\mathbf{1} \vdots D]|$? Again these two questions have not been answered fully as of yet. Using G and Hadmard's theorem we see that $0 \leq |\det[\mathbf{1} \vdots D]| \leq 2^{-n}(n+1)^{(n+1)/2}$. Clearly, the lower bound is achieved if $[\mathbf{1} \vdots D]$ is singular and the upper bound is achieved by transforming a seminormalized Hadamard matrix utilizing G, i.e. by leaving the 1's unaltered and by setting the -1's to 0's. Hence, for $n+1 = 4t \leq 200$ the smallest order for which a maximal seminormalized (0,1)-matrix $[\mathbf{1} \vdots D]$ has not been constructed is the case n+1 = 188. Of course, there are also intimate connections between maximal $[\mathbf{1} \vdots D]$'s and other structures such as v,k,λ configurations, e.g. see [12, 13]. Recently Wells [15] has presented a complete answer to the two questions (a^*) and (b^*) for the cases $n+1 \leq 7$. It is obvious that this was done utilizing computers. Other authors such as Yang [16] and Ehlich [1] are engaged with cases other than $n+1 \equiv 0 \pmod 4$. Metropolis and Stein [6] and Raktoe and Federer [10] have presented bounds on the number of singular $[\mathbf{1} \vdots D]$'s. The last two authors utilized an external natural structure with which the set T could be enriched. Some other results relating to either combinatorial or analytical aspects have recently been presented by Paik and Federer [8], Raktoe and Federer [11], and Srivastava, Raktoe, and Pesotàn [14]. Also the interested reader should read an asymptotic result by Komlos [5] on the number of singular (0,1)-matrices in the class of all $k \times k$, (0,1)-matrices, this class having cardinality 2^{k^2}. Specifically he shows that as $k \to \infty$ the relative frequency of singular (0,1)-matrices goes to zero. It is highly desirable to have a similar result for our class consisting of $\binom{2^n}{n+1}$ seminormalized (0,1)-matrices. Limited calculations seem to bear out such an asymptotic result. Note that this is a subclass of the class considered by Komlos. Also, some of these problems and results and also other aspects were summarized in the paper [2]. Finally, from above it follows that the sum of squares of the values of det $[1 \vdots D]$ is equal to $2^{n(n-1)}$, the values being connected through $\binom{2^n}{n+1} - [2^n-n-1][n+1] - 1$ quadratic relations.

2. The Topological Formulation. To make this paper self-contained and to achieve what the title claims, we introduce formally the following definitions and results which can be found in most standard texts (e.g. [3]) containing the theory of polytopes:

Definition 2.1. A subset $A \in E^n$ is said to be affinely dependent if for some $x_1', x_2', \cdots, x_r' \in A$ and $\lambda_1, \lambda_2, \cdots, \lambda_r \in R$ the equation $\sum_{i=1}^{r} \lambda_i x_i' = 0'$ is satisfied, where $\sum_{i=1}^{r} \lambda_i = 0$ and at least one λ_i is nonzero. If no such equation is satisfied then A is said to be affinely independent.

As an example consider the set A = {(000), (010), (001), (011)} in E^3. Clearly, A is an affinely dependent set since: 1(000) - 1(010) - 1(001) + 1(011) = (000).

THEOREM 2.1. The set $A=\{x_1',x_2',\cdots,x_r'\}$ of points in E^n is affinely independent if and only if the matrix $[1 \vdots \tilde{A}]$ has rank r, where the matrix $\tilde{A}$ has as rows $x_1',x_2',\cdots,x_r'$.

Example. $A = \{(000), (100), (010), (001)\}$ in E^3 is affinely independent since rank $[1 \vdots \tilde{A}] = 4$, where the four points in A are row vectors of $\tilde{A}$.

Definition 2.2. A nondegenerate n-simplex is the convex hull of a set of n+1 affinely independent points, i.e. if $A=\{x_1',x_2',\cdots,x_{n+1}'\}$ and the x_i''s are affinely independent then the nondegenerate n-simplex = conv A = $\{x' \in E^n,\ x' = \sum_{i=1}^{r} \lambda_i x_i',\ x_i' \in A,\ 1 \le r < \infty,\ \lambda_i \ge 0,\ \sum_{i=1}^{r} \lambda_i = 1\}$. Clearly, a nondegenerate simplex then is the set of all convex combinations of finite subsets of A, which consists of n+1 affinely independent points in E^n. A degenerate n-simplex will be defined to be the convex hull of a set of n+1 affinely dependent points in E^n.

Example. The set of points in E^3 given by $A = \{(000), (100), (010), (001)\}$ determines a nondegenerate n-simplex. On the other hand the set $B = \{(000), (010), (001), (011)\}$ in E^3 produces a degenerate n-simplex.

Remark. It is a convention in many branches of mathematics to refer to the points $x_1,x_2,\cdots,x_{n+1}$ of A as the vertices of the simplex. Pairs of affinely independent points then determine the edges or 1-faces, etc. For example, the simplex determined by the points (00), (10) and (01) in E^2 is a triangle whose vertices are these three points and whose sides are the edges given by the three pairs of points.

Definition 2.3. The unit n-cube in E^n is the set $\{x' = (\xi_1 \cdots \xi_n) \in E^n, 0 \le \xi_i \le 1, i = 1,2,\cdots,n\}$. It is well-known that this convex set has $2^{n-k}\binom{n}{k}$, k-faces, where $0 \le k \le n$.

For example, the unit 3-cube in E^3 has $2^{3-0}\binom{3}{0} = 8$, 0-faces or vertices, namely $\{(000), (100), (010), (001), (110), (101), (011), (111)\}$ and $2^{3-1}\binom{3}{1} = 12$, 1-faces or edges and $2^{3-2}\binom{3}{2} = 6$, 2-faces.

Definition 2.4. The volume of a nondegenerate n-simplex determined by the affinely independent points $x_1', x_2', \cdots, x_{n+1}'$ is given by the equation $V = \frac{1}{n!} |\det [1 \vdots \tilde{A}]|$, where $\tilde{A}$ has $x_1', x_2', \cdots, x_{n+1}'$ as its rows and 1 is an $(n+1) \times 1$ column vector of 1's.

Note that the volume of a degenerate simplex is 0 since in this case the n+1 points are affinely dependent so that the resulting determinant is 0.

From the above definitions and results it is quite clear that the fundamental problem of saturated main effect replicates can be formulated in terms of simplices of the n-cube in the space E^n. Specifically, if we identify the points in T with the vertices of the unit n-cube in E^n then a saturated main effect design D obviously determines an n-simplex. The n+1 vertices of the simplex are the rows of D. Since we are taking (n+1)-subsets of vertices out of the 2^n possible vertices of unit n-cube, clearly we will have $\binom{2^n}{n+1}$ simplices. Hence, formally we have proved the following:

THEOREM 2.2. The fundamental problem of saturated main effect replicates, namely: "(a) What are the possible values of $|\det X|$? and (b) What is the frequency of each possible value of $|\det X|$?", is equivalent to the following fundamental problem in topology: (a^{**}) What are the possible values of the volume of an n-simplex obtained by selecting (n+1) vertices of the unit n-cube in E^n, and, (b^{**}) What is the frequency of each possible value of the volume of the n-simplex?

3. Discussion and Examples. This fundamental problem in theorem 2.2 has not been settled by topologists yet. What we should realize is that theorem 2.2 provides us with an important tool to at least attack the fundamental problem of saturated main effect replicates of the 2^n factorial. This is the first paper which shows that problems in fractional replication can be formulated topologically and clearly a window has been opened through which light can pass so we may look better at some of the objects.

For example, if a saturated main effect replicate is singular , i.e. its design matrix has determinant equal to zero, then this means that the rows of D lead to a degenerate simplex in E^n. Thus counting the number of singular saturated main effect replicates is equivalent to counting the number of degenerate simplices among the $\binom{2^n}{n+1}$ possible ones. To search for an optimal saturated main effect replicate, i.e. a pair $\{D,\beta\}$ such that $|\det X|$ is maximum or equivalently $|\det [1 \vdots D]|$ is maximum, is by theorem 2.2 equivalent to searching among the $\binom{2^n}{n+1}$ possible ones that simplex which has maximum volume. Of course, there are many other similar equivalent statements possible now. Finally, in the future we hope to report results based on using affine transformations, since from earlier mentioned results we know that the sum of squares of the volumes of all the simplices is equal to $2^{n(n-1)}(n!)^{-2}$ and that they are connected through $\binom{2^n}{n+1} - [2^n-n-1][n+1] - 1$ quadratic relations.

To present a complete "dissection" let us consider the 3-cube in E^3-space. By selecting 4 vertices among the 8 possible ones we obtain 70 possible simplices. Of these 70 there are by a quick count 12 degenerate ones of which 6 are regular (squares) and 6 are irregular (rectangles). Among the remaining 58 nondegenerate ones there are precisely 2 which have maximal volume equal to $\frac{2}{6}$. Both of these are regular tetrahedra. The rest of them, i.e. 56, have volume equal to $\frac{1}{6}$ and partition into groups of 8, 24 and 24 such that the simplices within a group are geometrically identical or reflections of each other. Finally, from what has been presented in the previous section, we see that $\left[2(0^2) + 56\left(\frac{1}{6}\right)^2 + 2\left(\frac{2}{6}\right)^2\right] = \frac{2^6}{36}$ $= 2^{n(n-1)}(n!)^{-2}$ and the 70 possible volumes are connected through 53 quadratic relations.

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