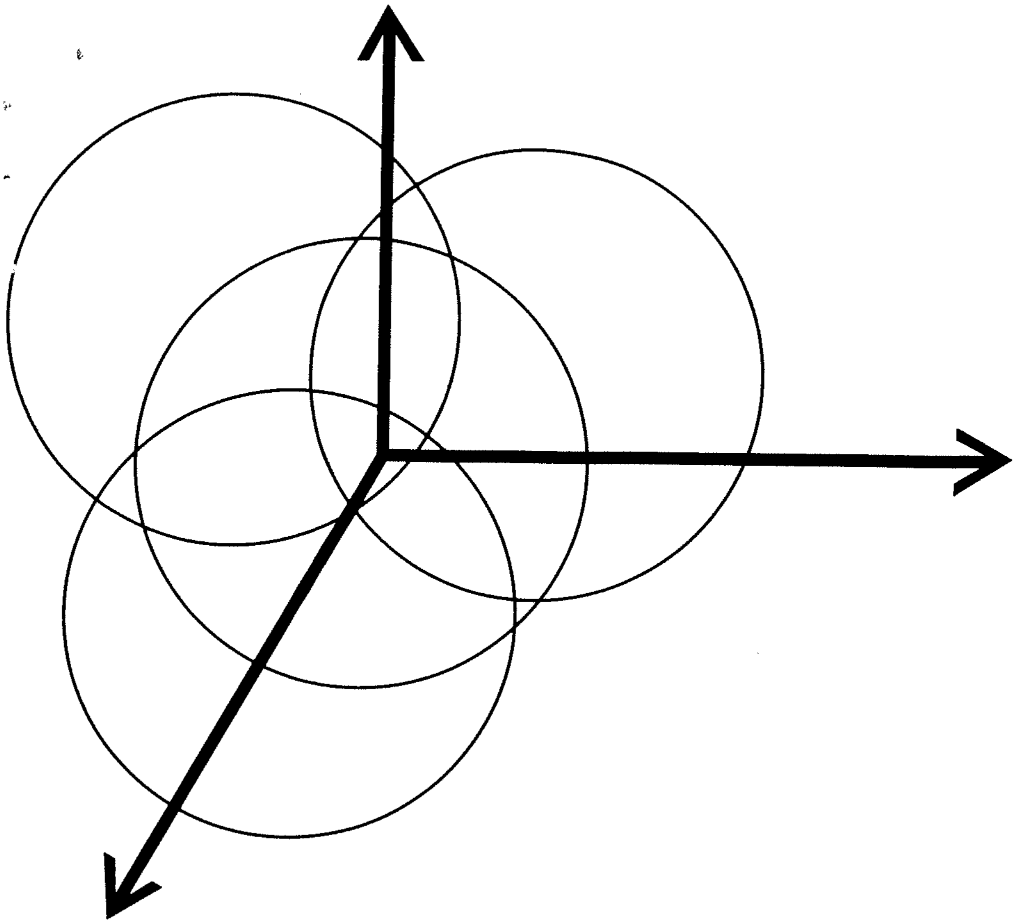

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SIXTEEN RUN DESIGNS OF HIGH PROJECTIVITY FOR FACTOR SCREENING

George E. P. Box[1] and John Tyssedal[2]

[1]Center for Quality and Productivity Improvement, University of Wisconsin-Madison, Madison, Wisconsin 53705 USA

[2]Department of Mathematical Sciences, The Norwegian University of Science and Technology, N-7034 Trondheim, Norway

ABSTRACT

A two level orthogonal array design for n observations with k factors and of projectivity P provides an (n, k, P) factor screen for which every projection into P space produces a complete 2^P factorial, possibly with certain points replicated. Box and Tyssedal (1) rigorously investigated the screening properties of such designs derived from fractional factorials and Plackett Burman orthogonal arrays (OA's). For example, they showed that these always provided (12, 11, 3) and (20, 19, 3) screens, but for 16 runs only a (16, 8, 3) screen could be generated. In this paper it is shown that designs derived from a different class of OA's due to Hall (2) can produce sixteen run designs that can screen a larger number of factors and that in particular (16, 12, 3) screens and also a (16, 14, 3) screen can be obtained.

Key Words: Orthogonal array; Factorial design; Projectivity; Screening design.

Consider an $n \times n$ orthogonal matrix **H** which has a first column of 1's and in which the sum of squares of the elements of each row and column is n. Then **H** may be written as $[1 \mid \mathbf{G}]$ and the $n - 1$ elements of each row of **G** define a point in a $n - 1$ dimensional space at a distance $\sqrt{n-1}$ from the origin. Also, since the sums of products of the elements in any two rows of **G** are identical, the n points so defined are the vertices of the regular n–dimensional simplex in some orientation or other. For example, in two dimensions, they are the three vertices of the equilateral triangle, in three dimensions the four vertices of the regular tetrahedron and so on.

In general, they can define the n design points of an orthogonal experimental arrangement for $n - 1$ factors that can take continuous values (see e.g. (3)); however particular interest attaches to those orientations of the simplex for which the elements of **G** are $-1's$ and $+1's$ so that **H** is an orthogonal array. Later these elements are denoted by minus and plus signs and each column of **G** will be referred to as a contrast column since it must contain equal numbers of these signs. Examples are the designs provided by Plackett-Burman (PB) (4) available when $n = 4\,m$, m a positive integer, for $n \leq 100$, except for $n = 92$, and also, when n is a power of two, the saturated fractional factorial designs (5) with which the corresponding PB designs are then identical. (In what follows designs obtained by renumbering rows, renumbering contrast columns, or switching all the signs in a contrast column are regarded as equivalent.) When $n = 4$, for example, the design points are the vertices of a regular tetrahedron, at a distance from the origin and oriented so that their coordinates are $(-1, -1, 1)$; $(1, -1, -1)$; $(-1, 1, -1)$; $(1, 1, 1)$, or the equivalent points obtained by switching all signs. Such orthogonal arrangements can be used as "main effect plans" (6), but the present paper is concerned with their projective properties which allow them to be used as "factor screens" (see e.g. (7)).

At the preliminary stage of an experimental investigation we may, in Juran's words, be attempting to "distinguish the vital few (factors) from the trivial many". In these circumstances a model that may sufficiently approximate reality is that, out of a larger number k of the tested factors, only a small subset, typically 2 or 3, are expected to be active. This principle of parsimony thus postulates that out of the whole k dimensional factor space, there is an active subspace of lower dimension within which all real changes in the measured response occur. The purpose of a screening design is to find this active subspace.

We believe that the first objective should be the identification of this active subspace followed by an examination of the nature of such activity, (see e.g. (8) and (9)). This view is supported by the following considerations.

a) while it is frequently true that factor activity can be usefully described in terms of a low order Taylor expansion, (see e.g. (10), it does not follow that the order of such effects form a hierarchy validating so-called heredity principles; for example, in regions of the factor space close to "optimal" conditions (and hence of particular interest) it is likely that the main effects of quantitative factors estimating first order derivatives will be small, but that two factor interactions estimating mixed second order derivatives may be large (see e.g. (11)).

b) many natural phenomena, see (12), are not best represented in terms of main effects and interactions at all. A response may occur, for example, only when there is a "critical mix" of a number of experimental factors, qualitative or quantitative. For example, a binary critical mix is required for sexual reproduction. In three dimensions a tertiary critical mix is required to make gun powder. Such a tertiary mix provides a possible explanation when one experimental point of the factorial cube, often at the extreme conditions, gives a response widely different from all the others; a binary active mix is suggested when two points on one edge of the cube give extreme results different from the rest, see e.g. (13) and (14). While such factor spaces are certainly active, this activity is not economically described in terms of polynomials or of main effects and interactions.

Active subspaces may be identified using the projective properties of statistical designs. A $n \times k$ design **D** with n observations and k factors each at 2 levels will be said to be of projectivity P if it is such that a complete 2^P factorial design (possibly with some points replicated) is generated by every subset of P of the factors. The resulting design will then be called a (n, k, P) screen. In particular, designs obtained from orthogonal arrays provide (n, n − 1, 2) screens with n/4 replicated points at each of the 4 vertices of a projected square. In what follows we use the customary notation 2_R^{k-m} to denote a $1/2^m$ fraction of a 2^k factorial design of resolution R; where the resolution of a fractional design is the length of the shortest word in its defining contrasts. It is easy to show that the projectivity of a design of resolution R is $P = R - 1$ (7). All fractional factorial designs having $k < n - 1$ can be obtained by dropping columns from the corresponding saturated design, and when these columns are suitably chosen arrangements of greater projectivity can be obtained. Thus, a design of projectivity $P = 3$ for $k = n/2$ factors can always be obtained by dropping a particular set of $\frac{n}{2} - 1$ columns from the saturated factorial arrangement. For example, Figure 1 shows a 16×16 factorial orthogonal array (FOA) here referred to as $\mathbf{H}_1$ that is obtained by associating the factors A, B, C, ..., R with the orthogonal columns of all main effects and interactions of a 2^4 factorial design in the pseudo factors a, b, c, d. The ordering of the columns is chosen so that a 2_{IV}^{8-4} fractional factorial design is produced by dropping all but the first eight contrast columns; this design thus provides a (16, 8, 3) screen with duplicated 2^3 factorials in every one of the 56 choices of $P = 3$ factors from the $k = 8$ factors tested. Similarly a (16, 5, 4) screen is provided, for example, by using only columns A, B, C, D and R from this FOA.

		a	*b*	*c*	*d*	*abc*	*abd*	*acd*	*bcd*	*ab*	*ac*	*ad*	*bc*	*bd*	*cd*	*abcd*
	I	A	B	C	D	E	F	G	H	J	K	L	M	P	Q	R
1	+	-	-	-	-	-	-	-	-	+	+	+	+	+	+	+
2	+	+	-	-	-	+	+	+	-	-	-	-	+	+	+	-
3	+	-	+	-	-	+	+	-	+	-	+	+	-	-	+	-
4	+	+	+	-	-	-	-	+	+	+	-	-	-	-	+	+
5	+	-	-	+	-	+	-	+	+	+	-	+	-	+	-	-
6	+	+	-	+	-	-	+	-	+	-	+	-	-	+	-	+
7	+	-	+	+	-	-	+	+	-	-	-	+	+	-	-	+
H_1 8	+	+	+	+	-	+	-	-	-	+	+	-	+	-	-	-
9	+	-	-	-	+	-	+	+	+	+	+	-	+	-	-	-
10	+	+	-	-	+	+	-	-	+	-	-	+	+	-	-	+
11	+	-	+	-	+	+	-	+	-	-	+	-	-	+	-	+
12	+	+	+	-	+	-	+	-	-	+	-	+	-	+	-	-
13	+	-	-	+	+	+	+	-	-	+	-	-	-	-	+	+
14	+	+	-	+	+	-	-	+	-	-	+	+	-	-	+	-
15	+	-	+	+	+	-	-	-	+	-	-	-	+	+	+	-
16	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+

Figure 1. $\mathbf{H_1}$ is rearranged as a factorial orthogonal array (FOA) with the first eight contrast columns forming a 2_{IV}^{8-4} design.

By analogy with the saturated fractional factorials it had been conjectured that PB designs would provide (n, n − 1, P) screens with projectivity only 2. However a computer search by Bisgaard in 1987 (15), showed that such designs could be of projectivity higher than 2 and in particular, that every one of the 165 three-dimensional projections of the PB designs with n = 12 (m = 3 was a full 2^3 factorial design with four replicated runs which themselves formed a half-replicate main-effect plan. It was therefore a (12, 11, 3) screen. Thus compared with a 2_{IV}^{8-4} design this 12 run design could screen three additional factors with four fewer runs. Further computer evaluation by Lin and Draper (16) showed that similar results were possible for some, but not all, of the remaining (PB) designs. They referred to a projection in which half the vertices of the projected factorial cube were replicated t times and the remainder of the vertices s = m − t times as a (t, s) projection. Thus, for example, each of the 165 three-dimensional projections of the 12-run orthogonal array design was a (1, 2) projection. Computer studies of the aspects of the projective rationale for orthogonal arrays have been made by Wang and Wu (17) and by Lin (18).

Since the PB designs for n = 2^k were identical with saturated fractional factorials, they had projectivity of only 2 and Plackett and Burman employed various other modes of generating for the remaining designs. Mathematical analysis (1) showed that these modes of generation decided projectivity, see also (19). In particular that: designs with m > 1 odd, *P* must equal to 3; 2n × 2n designs obtained by "doubling" an n × n orthogonal array were always of projectivity P = 2; cyclic designs had P = 3 except when they formed a factorial array, and hence had P = 2.

In particular for $n \leq 84$ the six designs having $n = 8, 16, 32, 40, 56$ and 64 were only of projectivity $P = 2$, but the remaining 14 designs all had $P = 3$.

Box and Tyssedal (1) also mentioned that further analysis showed that an additional class of orthogonal arrays due to Hall (2) could produce designs of greater projectivity. In particular, for $n = 16$, in addition to the FOA $\mathbf{H_1}$ there were four additional orthogonal arrays which we have here labeled $\mathbf{H_2}$, $\mathbf{H_3}$, $\mathbf{H_4}$ and $\mathbf{H_5}$. (For convenience, our mode of labeling the arrays differs from that used by Hall.) The first three of these could generate (16, 12, 3) screens and $\mathbf{H_5}$ could generate a (16, 14, 3) screen. Now designs of small or moderate size are usually of most interest for factor screening; in particular the sixteen run fractional factorial array referred to above has been widely use as a (16, 8, 3) screen. The main purpose of this paper is to derive and categorize 16 run designs obtained from Hall's arrays with even better projectivity properties.

As explained, Figure 1 shows the standard FOA 16×16 array $\mathbf{H_1}$ generated by a 2^4 factorial in factors a, b, c and d with columns renumbered A, B, ..., R arranged so that the first eight contrast columns terminated by the double line produce the familiar 2_{IV}^{8-4} design yielding a (16, 8, 3) screen. Figures 2, 3 and 4 show Hall's $\mathbf{H_2}$, $\mathbf{H_3}$ and $\mathbf{H_4}$ arrays rearranged so that their first eight contrast columns are again those of the 2_{IV}^{8-4} design. In (20) it is shown that in each case addition of four appropriate columns produces a (16, 12, 3) screen. Double lines are again used to show the termination of the columns that generate the screen. In Figure 5 Hall's $\mathbf{H_5}$ array is rearranged so that its first six contrast columns are

$\mathbf{H_2}$

	a	b	c	d	abc	abd	acd	bcd					ab	ac	bc
	A	B	C	D	E	F	G	H	J_2	K_2	L_2	M_2	P_2	Q_2	R_2
1	-	-	-	-	-	-	-	-	+	-	-	-	+	+	+
2	+	-	-	-	+	+	+	-	-	+	-	-	-	-	+
3	-	+	-	-	+	+	-	+	-	-	+	-	-	+	-
4	+	+	-	-	-	-	+	+	-	-	-	+	+	-	-
5	-	-	+	-	+	-	+	+	+	+	+	-	+	-	-
6	+	-	+	-	-	+	-	-	+	+	-	+	-	+	-
7	-	+	+	-	-	+	+	-	+	-	+	+	-	-	+
8	+	+	+	-	+	-	-	-	-	+	+	+	+	+	+
9	-	-	-	+	-	+	-	+	-	+	+	+	+	+	+
10	+	-	-	+	+	-	-	+	+	-	+	+	-	-	+
11	-	+	-	+	+	-	+	-	+	+	-	+	-	+	-
12	+	+	-	+	-	+		-	+	+	+	-	+	-	-
13	-	-	+	+	+	+	-	-	-	-	-	+	+	-	-
14	+	-	+	+	-	-	+	-	-	-	+	-	-	+	-
15	-	+	+	+	-	-	-	+	-	+	-	-	-	-	+
16	+	+	+	+	+	+	+	+	+	-	-	-	+	+	+

$$\begin{matrix} J_2: \\ K_2: \\ L_2: \\ M_2: \end{matrix} \quad \overset{\begin{matrix} ad & bd & cd & abcd \end{matrix}}{\begin{bmatrix} + & + & - & + \\ - & + & - & - \\ + & - & - & - \\ - & - & - & + \end{bmatrix}} \times \frac{1}{2}$$

$P_2 = ab$

$Q_2 = ac$

$R_2 = bc$

Figure 2. $\mathbf{H_2}$ is rearranged so that a (16, 12, 3) screen is obtained from the first 12 contrast columns by adding the four columns J_2, K_2, L_2 and M_2.

		a	b	c	d	abc	abd	acd	bcd							ab
		A	B	C	D	E	F	G	H	J_3	K_3	L_3	M_3	P_3	Q_3	R
	1	-	-	-	-	-	-	-	-	+	-	-	-	+	+	+
	2	+	-	-	-	+	+	+	-	-	+	-	-	-	+	-
	3	-	+	-	-	+	+	-	+	-	-	+	-	-	-	-
	4	+	+	-	-	-	-	+	+	-	-	-	+	-	-	+
	5	-	-	+	-	+	-	+	+	+	+	+	-	-	-	+
	6	+	-	+	-	-	+	-	+	+	-	+	+	-	+	-
	7	-	+	+	-	-	+	+	-	+	+	-	+	+	-	-
H_3	8	+	+	+	-	+	-	-	-	-	-	+	+	+	+	+
	9	-	-	-	+	-	+	+	+	-	+	+	+	+	+	+
	10	+	-	-	+	+	-	-	+	+	+	-	+	+	-	-
	11	-	+	-	+	+	-	+	-	+	-	+	+	-	+	-
	12	+	+	-	+	-	+	-	-	+	+	+	-	-	-	+
	13	-	-	+	+	+	+	-	-	-	-	-	+	-	-	+
	14	+	-	+	+	-	-	+	-	-	-	+	-	+	-	-
	15	-	+	+	+	-	-	-	+	-	+	-	-	-	+	-
	16	+	+	+	+	+	+	+	+	+	-	-	-	+	+	+

	ad	bd	cd	abcd	ac	bc
J_3	+	+	-	+		
K_3			-	-	-	+
L_3			-	-	+	-
M_3	-	-	-	+		
P_3	+	-			+	+
Q_3	-	+			+	+

$\times \frac{1}{2}$

$R_3 = ab$

Figure 3. $\mathbf{H_3}$ is rearranged so that a (16, 12, 3 screen is obtained from the first 12 contrast columns by adding the four columns J_3, K_3, L_3 and M_3.

		a	b	c	d	abc	abd	acd	bcd							
		A	B	C	D	E	F	G	H	J_4	K_4	L_4	M_4	P_4	Q_4	R_4
	1	-	-	-	-	-	-	-	-	+	+	+	+	+	+	+
	2	+	-	-	-	+	+	+	-	+	-	-	+	-	-	+
	3	-	+	-	-	+	+	-	+	-	-	+	+	+	-	-
	4	+	+	-	-	-	-	+	+	+	-	+	-	-	+	-
	5	-	-	+	-	+	-	+	+	-	-	-	-	+	+	+
	6	+	-	+	-	-	+	-	+	-	+	-	+	-	+	-
	7	-	+	+	-	-	+	+	-	-	+	+	-	-	-	+
H_4	8	+	+	+	-	+	-	-	-	+	+	-	-	+	-	-
	9	-	-	-	+	-	+	+	+	+	+	-	-	+	-	-
	10	+	-	-	+	+	-	-	+	-	+	+	-	-	-	+
	11	-	+	-	+	+	-	+	-	-	+	-	+	-	+	-
	12	+	+	-	+	-	+	-	-	-	-	-	-	+	+	+
	13	-	-	+	+	+	+	-	-	+	-	+	-	-	+	-
	14	+	-	+	+	-	-	+	-	-	-	+	+	+	-	-
	15	-	+	+	+	-	-	-	+	+	-	-	+	-	-	+
	16	+	+	+	+	+	+	+	+	+	+	+	+	+	+	+

	ab	ac	ad	bc	bd	cd	abcd
J_4	+		-	+		+	
K_4		+		+		-	+
L_4			+			+	+
M_4	-	+			+	+	
P_4	+	+	+				
Q_4	+				+		+
R_4		-	+	+	+		

$\times \frac{1}{2}$

Figure 4. $\mathbf{H_4}$ is rearranged so that the first 12 contrast columns gives a (16, 12, 3) screen.

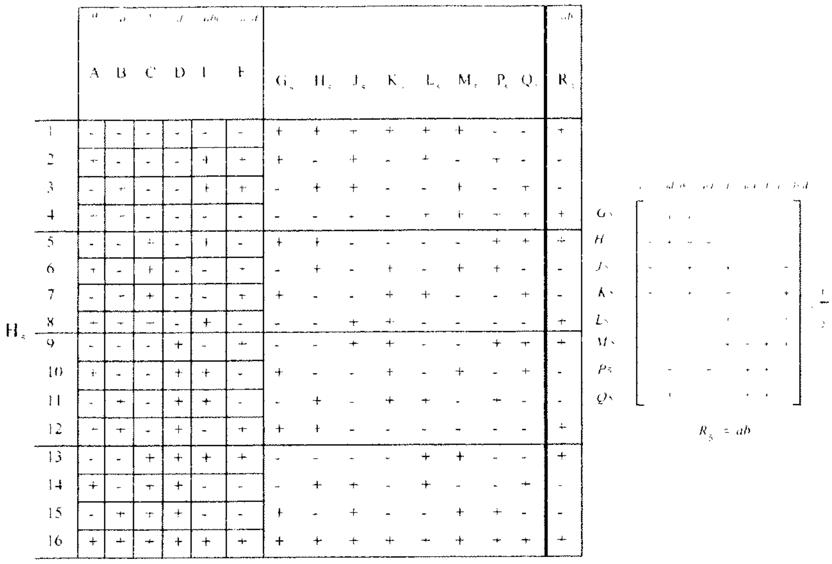


Figure 5. $\mathbf{H}_5$ is rearranged so that a (16, 14, 3) screen is obtained from the first 14 contrast columns.

those of a 2_{IV}^{8-4} design. The addition of the eight columns indicated then produces a (16, 14, 3) screen. Modified columns are denoted by subscripts, thus J_2 refers to the Jth column in $\mathbf{H}_2$, and so on.

Now since *all* orthogonal matrices of the form of **H** produce the basic simplex in some rotation or other, it must be possible to derive $\mathbf{H}_2$, $\mathbf{H}_3$, $\mathbf{H}_4$ and $\mathbf{H}_5$ by orthogonal transformation from $\mathbf{H}_1$. The appropriate transformations are easily obtained algebraically and are shown in Figures 2, 3, 4 and 5 accompanying each array with double lines delineating the transformation for each screen.

For example the design $\mathbf{H}_2$ is obtained by an orthogonal transformation of $\mathbf{H}_1$ with the first eight contrast columns the same as those for $\mathbf{H}_1$ and the remainder obtained by transformation of the last seven columns of $\mathbf{H}_1$ as indicated in Figure 2.

Thus for example

$$J_2 = \frac{1}{2}(ad + bd - cd + abcd)$$

The additional generators of $\mathbf{H}_2$ can then be obtained directly from the transformation matrix. For example, the above relation implies that

$$I = \frac{1}{2}(ADJ_2 + BDJ_2 - CDJ_2 + ABCDJ_2).$$

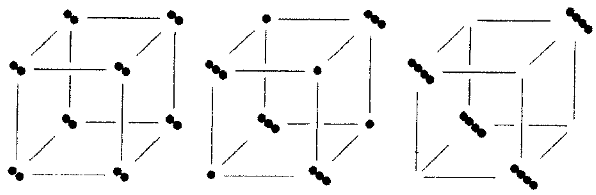
The generators for the $\mathbf{H_2}$ design are thus the four generators of the 2^{8-4}_{IV} design plus an additional seven supplied by the transformation matrix. A complete set of generators is thus

$$
\begin{aligned}
I &= ABCE = ABDF = ACDG = BCDH \\
&= \frac{1}{2}(ADJ_2 + BDJ_2 - CDJ_2 + ABCDJ_2) \\
&= \frac{1}{2}(-ADK_2 + BDK_2 - CDK_2 + ABCDK_2) \\
&= \frac{1}{2}(ADL_2 - BDL_2 - CDL_2 - ABCDL_2) \\
&= \frac{1}{2}(-ADM_2 - BDM_2 - CDM_2 + ABCDM_2) \\
\hline
&= ABP_2 = ACQ_2 = ABCR_2.
\end{aligned}
$$

Alternatively the last seven generators may be written in the more compact form

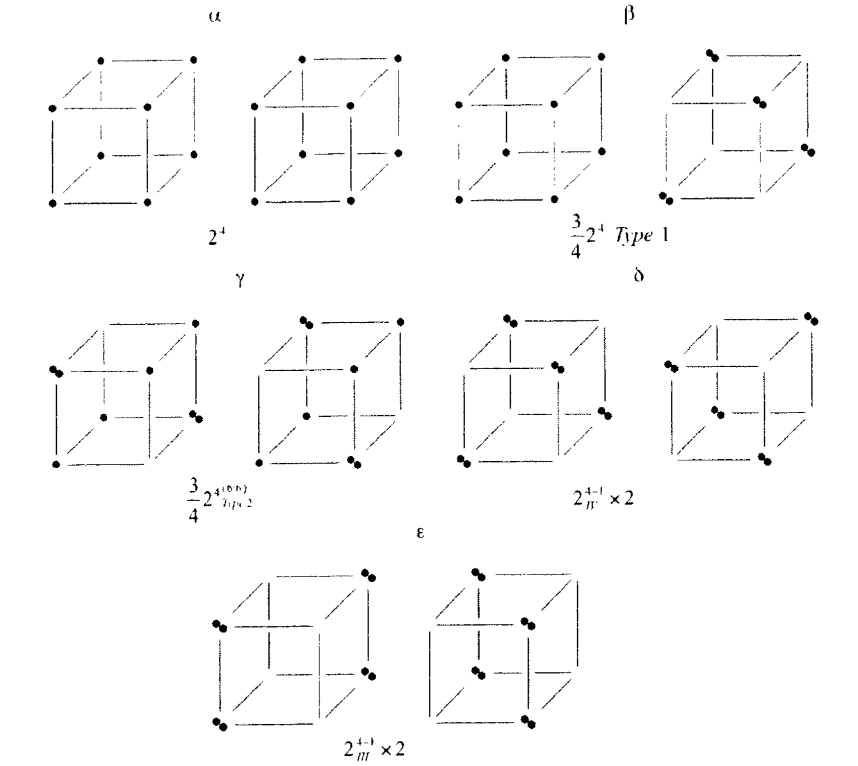
$$
\begin{aligned}
I &= \frac{1}{2}(ADJ_2 + BDJ_2 - CDJ_2 + ABCDJ_2) \\
&= -BCJ_2K_2 = -ACJ_2L_2 = -ABJ_2M_2 \\
\hline
&= ABP_2 = ACQ_2 = ABCR_2.
\end{aligned}
$$

Table 1. Number of 3-D Projections for the (16, k, 3) Designs



Generating Array	Screen	Number of Projections by Type (2, 2)	(3, 1)	(4, 0)	Total
$\mathbf{H_1}$	(16, 8, 3)	56 (100%)	0	0	56
$\mathbf{H_2}$	(16, 12, 3)	156 (71%)	64 (29%)	0	220
$\mathbf{H_3}$	(16, 12, 3)	156 (71%)	64 (29%)	0	220
$\mathbf{H_4}$	(16, 12, 3)	156 (71%)	64 (29%)	0	220
$\mathbf{H_5}$	(16, 14, 3)	252 (69%)	112 (31%)	0	364

Table 2. Number of 4-D Projections for the (16, k, 3) Designs



Generating Array	Screen	α	β	γ	δ	ε	Total
H_1	(16, 8, 3)	56 (80%)	0	0	14 (20%)	0	70
H_2	(16, 12, 3)	168 (34%)	0	288 (58%)	39 (8%)	0	495
H_3	(16, 12, 3)	152 (30%)	64 (13%)	256 (52%)	23 (5%)	0	495
H_4	(16, 12, 3)	144 (29%)	96 (19.5%)	240 (48.5%)	15 (3%)	0	495
H_5	(16, 14, 3)	252 (25%)	224 (22.5%)	504 (50.5%)	21 (2%)	0	1001

Where double lines are again used to delineate those identities that apply to the (16, 12, 3) screen. The following properties and results are all shown in (20).

An interesting property of the (16, 12, 3) screen from $\mathbf{H_2}$:

Consider 3 sets of four columns which we will call S_1, S_2 and S_3 chosen as follows

$$S_1 = (A, B, C, E); \quad S_2 = (D, F, G, H); \quad S_3 = (J_2, K_2, L_2, M_2)$$

Table 3. Number of 3-D Projections for Saturated Designs

Generating Array	Number of 3-D Projections by Type (2, 2)	(3, 1)	(4, 0)	Total
$\mathbf{H}_1$	420 (92%)	0	35 (8%)	455
$\mathbf{H}_2$	372 (82%)	64 (14%)	19 (4%)	455
$\mathbf{H}_3$	348 (77%)	96 (21%)	11 (2%)	455
$\mathbf{H}_4$	336 (74%)	112 (25%)	7 (1%)	455
$\mathbf{H}_5$	336 (74%)	112 (25%)	7 (1%)	455

We know that eight columns of S_1 and S_2 taken together form a 2_{IV}^{8-4} design, we show in (20) that this is also true for the eight columns obtained from S_1 and S_3 and for the eight columns obtained from S_2 and S_3. Thus the (16, 12, 3) screen has the property of producing a 2_{IV}^{8-4} design for any two of these three sets of columns.

3-D Projections:

Screening properties of the (16, 12, 3) designs: Table 1 shows the number of projections in three dimensions of types (2, 2), (3, 1) and (4, 0) for the projectivity $P = 3$ screens derived from the various orthogonal arrays.

4-D Projections:

It is of interest to know how well these designs behave if there are four active factors. The results are shown in Table 2 where we denote the various types of projections by α, β, γ, δ and ε.

Screening properties of the saturated designs obtained from Hall's orthogonal arrays:

It is also of interest to consider projections properties of the saturated designs obtained from using the 15 contrast columns of $\mathbf{H}_1$, $\mathbf{H}_2$, $\mathbf{H}_3$, $\mathbf{H}_4$ and $\mathbf{H}_5$. Table 3 shows the number of projections in dimensions of types (2, 2), (3, 1) and (4, 0) for the projectivity $P = 2$ screens. We see that particular for $\mathbf{H}_4$ and $\mathbf{H}_5$ a remarkably small portion of the projections are of the undesirable (4, 0) type.

4-D Projections:

Table 4 shows the number of projections in 4 dimensions of types α, β, γ, δ and ε. It will be seen that the particular undesirable projections of type ε which

Table 4. Number of 4-D Projections for Saturated Designs

Generating Array	α	β	γ	δ	ε	Total
$\mathbf{H}_1$	840	0	0	105	420	1365
$\mathbf{H}_2$	600	192	288	57	228	1365
$\mathbf{H}_3$	480	288	432	33	132	1365
$\mathbf{H}_4$	420	336	504	21	84	1365
$\mathbf{H}_5$	420	336	504	21	84	1365

are absent for the 4-D projections of the (16, k, 3) screens now occur for the (16, 15, 2) screens.

We believe that some of the corresponding evaluations by Lin and Draper (21) are erroneous. In particular the number of 4-D projections for the 15 contrast columns must be $C_4^{15} = 1365$.

Pratical Applications of the Designs:

The (16, 12, 3) screns derived from $\mathbf{H_2}$, $\mathbf{H_3}$ and $\mathbf{H_4}$ are obtained by adding four extra columns to the 2_{IV}^{8-4} design which is associated in each case with the letters A, B, C, D, E, F, G and H. Any combination of three of these particular factors, therefore produces (2, 2) projections only. These are usually most desirable. The factors thought most likely to be important should therefore be associated with the first eight columns of these designs.

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