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One-factor-at-a-time designs of resolution V

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Abstract

Two classes of designs of resolution V are constructed using one-factor-at-a-time techniques. They facilitate sequential learning and are more economical in run size than regular 2_V^{k-p} designs. Comparisons of D efficiency with other designs are given to assess the suitability of the proposed designs. Their D_s efficiencies can be dramatically improved with the addition of a few runs.

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1. Introduction

At the beginning of an investigation there may be many potentially important factors. It is reasonable to assume that only a few of them will turn out to be important, but their identities are not known. Thus factor screening is needed. Many screening designs are available for this purpose, including the one-factor-at-a-time (OFAT) designs. Even though fractional factorial designs have well-known advantages over OFAT designs (e.g., Wu and Hamada, 2000, Section 3.7), the latter have several attractive features such as run size economy, fewer level changes and providing protection against the risk of premature termination of experiments. Running OFAT experiments is a sequential learning process. Use of OFAT designs allows investigators to find out more rapidly whether a factor has any effect. They continually receive information from each run rather than having to wait until the entire experiment is completed. They can monitor and react to data more rapidly than using orthogonal fractional factorial designs

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(OFFDs). If the magnitudes of the effects of interest are several times as large as the experimental error, there is no particular disadvantage with experimenting one factor at a time, especially when these effects do not need to be estimated precisely. Therefore, OFAT designs are still popular in physical experiments.

Before discussing different types of OFAT designs, we need a general definition of resolution (Webb, 1968). If all effects involving r or fewer factors are estimable, ignoring interactions of $r+1$ or more factors, the design is said to have resolution $2r+1$; if all effects involving $r-1$ or fewer factors are estimable, ignoring interactions of $r+1$ or more factors, the design is said to have resolution $2r$. In a resolution V design all main effects and two-factor interactions (henceforth abbreviated as 2fi's) are estimable, if all three-factor and higher-order interactions are ignored. Obviously, a resolution V design can also be considered as having resolution IV. We follow the convention that the maximum resolution is reported.

In the following discussion only factors with two levels are considered. Let $x_i = (x_{i1}, x_{i2}, \ldots, x_{in})$ denote the ith treatment, where x_{ij} is the level of factor j and takes the value -1 or 1. We assume the model

$$E(y_i) = \alpha_0 + \sum_{s=1}^{n} x_{is}\alpha_s + \sum_{r=2}^{n}\sum_{s=1}^{r-1} x_{is}x_{ir}\alpha_{sr}, \tag{1}$$

where y_i is the observation for treatment i, α_0 is the grand mean, α_s is the main effect of factor s, α_{sr} is the interaction between factors r and s, and so on. In model (1) all the three-factor or higher-order interactions are omitted.

Daniel (1973) classified OFAT designs into five categories, each having a different informative pattern. Two types of OFAT designs of resolution V are considered in this paper. In Section 2, standard OFAT designs, which vary one factor or one pair of factors from standard conditions, are constructed. In Section 3, strict OFAT designs, which vary one factor from the preceding treatment, are constructed. Comparisons with other designs in terms of run size and D-efficiency are given in Section 4. The D_s efficiencies of individual effects can be dramatically improved by adding a few runs (see Section 5). Concluding remarks are given in Section 6.

2. Standard OFAT designs of resolution V

These designs are constructed as follows:

(i) one run, treatment 0, with all factors at the low level;
(ii) n runs, treatments $1, \ldots, n$ in which each factor is in turn at the high level while others at the low level;
(iii) n runs, treatments $n+1, \ldots, 2n$ in which each factor is in turn at the low level while others at the high level;
(iv) one run, treatment $2n+1$ in which all factors are at the high level;
(v) $(n-1)(n-2)/2$ runs, treatments ij for $1 \leqslant i < j \leqslant n-1$ in which the ith and jth factors are at the high level and others at the low level.

The $2n+2$ runs from (i) to (iv) form a fold-over design of resolution IV. It was given in Cotter (1979), who did not mention the fold-over property. It is the fold-over of a standard OFAT design from a standard condition, i.e., a treatment in which all factors are at the low level. Part (v) is obtained by changing factors one-pair-at-a-time from the standard condition. It will be shown that adding part (v) makes it a resolution V design.

These designs allow the estimation of all the main effects and 2fi's. First, all the main effects and the sum of 2fi's involving the ith factor, $i = 1, \ldots, n$ are estimable if three-factor or higher-order interactions are negligible (Cotter, 1979). As a matter of fact, Cotter proved that $[(y_{2n+1} - y_{n+j}) + (y_j - y_0)]/4$ is a linear unbiased estimator of α_j, where $y_0, y_1, \ldots, y_{2n+1}$ are the observations in (i)–(iv). Second, it can be shown that $[(y_{ij} - y_j) - (y_i - y_0)]/4$ is an unbiased estimator of α_{ij}, where y_{ij} are the observations in (v). Thus α_{ij} is estimable. Note that these estimators are not the best linear unbiased estimators. The latter can be obtained numerically via the least squares but no closed form is available.

The standard OFAT designs can be effectively used in the following situations. Suppose an experimenter is interested in estimating the main effects but is unwilling to assume that 2fi's are negligible. Therefore, a resolution IV design (e.g., the $2n+2$ runs given in (i)–(iv)) should be used in the initial experiment. If it turns out that factor 1 is significant, one would like to investigate all the 2fi's involving factor 1. Because $[(y_{1j} - y_j) - (y_1 - y_0)]/4$ is a linear unbiased estimator of α_{1j}, only treatments $(1, j)$ for $1 < j \leqslant n-1$ in (v) need to be added to the initial experiment. If two or more factor are significant, say, factors 2 and 3, then a similar argument shows that only treatments 12, 13, 23, $2j$, $3j$ for $4 \leqslant j \leqslant n-1$ in (v) need to be added in order to estimate all the 2fi's involving 2 and 3. In such situations only a portion of the runs in (v) is needed for estimating a specific set of 2fi's. Therefore, we can view this adaptation as a *sequential* and *abridged* version of the "full" standard OFAT design. It is especially economical when there are many factors but few are significant.

3. Strict OFAT designs of resolution V

The design given in Table 1 consists of several parts divided by lines. It is *saturated* because its run size $(n^2+n+2)/2$ is minimally required for estimating the main effects and 2fi's with n factors. The treatments are expressed by symbols so that the high (and resp. low) level of each factor is indicated by the presence (and resp. absence) of the corresponding number. For example, 123 denotes a treatment in which factors 1, 2, 3 are at the high level and others at the low level. Symbol (1) denotes a treatment with all factors at the low level. Daniel (1973) gave a strict OFAT design with five factors but did not extend it to more factors.

The first $2n$ runs in Table 1 form a fold-over design of resolution IV. All the main effects are estimable regardless of the 2fi's. It can be shown that

$$[(y_{1,\ldots,j} - y_{1,\ldots,j-1}) - (y_{j+1,\ldots,n} - y_{j,\ldots,n})]/4 \tag{2}$$

Table 1
A strict OFAT design of resolution V with n factors ($n^* = n-1$ for even n and $=n$ for odd n)

Run	Observation	Treatment	Estimable effect
1	y_0	(1)	
2	y_1	1	
3	$y_{1,2}$	12	
4	$y_{1,2,3}$	123	
$\vdots$	$\vdots$	$\vdots$	
n	$y_{1,2,\ldots,n-1}$	$12\cdots(n-1)$	
$n+1$	$y_{1,2,\ldots,n}$	$12\cdots n$	
$n+2$	$y_{2,\ldots,n}$	$2\cdots n$	
$n+3$	$y_{3,\ldots,n}$	$3\cdots n$	
$\vdots$	$\vdots$	$\vdots$	
$2n-1$	$y_{n-1,n}$	$(n-1)n$	
$2n$	y_n	n	
$2n+1$	$y_{1,n}$	$1n$	α_{1n}
$2n+2$	$y_{1,n-1,n}$	$1(n-1)n$	$\alpha_{1(n-1)}$
$\vdots$	$\vdots$	$\vdots$	$\vdots$
$2n+(n-2)$	$y_{1,3,\ldots,n}$	$13\cdots n$	α_{13}
$2n+(n-2)+1$	$y_{1,3,\ldots,n-1}$	$13\cdots(n-1)$	α_{2n}
$2n+(n-2)+2$	$y_{1,3,\ldots,n-2}$	$13\cdots(n-2)$	$\alpha_{2(n-1)}$
$\vdots$	$\vdots$	$\vdots$	$\vdots$
$2n+(n-2)+(n-3)$	$y_{1,3}$	13	α_{24}
$\vdots$	$\vdots$	$\vdots$	$\vdots$
$\frac{n^2+n+2}{2}$	$y_{1,3,5,7,\ldots,n^*}$	$1357\cdots n^*$	$\alpha_{(n-2)(n-1)}$

is an unbiased estimator of α_j for $j = 1,2,\ldots,n$. Furthermore,

$$[(y_{1,\ldots,j} - y_{1,\ldots,j-1}) + (y_{j+1,\ldots,n} - y_{j,\ldots,n})]/4 \tag{3}$$

is an unbiased estimator of the linear combination of 2fi's involving factor j, i.e., $\alpha_{1j} + \cdots + \alpha_{(j-1)j} - \alpha_{j(j+1)} - \cdots - \alpha_{jn}$, for $j = 1,2,\ldots,n$. In (2) and (3), $y_{1,\ldots,j} = y_0$ for $j = 0$ and $y_{j,\ldots,n} = y_0$ for $j = n+1$.

In order to de-alias 2fi's, more runs need to be added in Table 1. It can proceed as follows. Since the interaction between any factors a and b can be estimated by $(y_{ab} + y_0 - y_a - y_b)/4$ in model (1), $(y_{1,n} + y_0 - y_1 - y_n)/4$ is a linear unbiased estimator of α_{1n}. Noting that y_0, y_1, y_n are in the first $2n$ runs, if the $(2n+1)$th run is treatment $1n$, then α_{1n} is estimable and the strict OFAT property is kept. Continuing with treatment $1n$, since $(y_{1,n-1,n} + y_n - y_{n-1,n} - y_{1,n})/4$ is a linear unbiased estimator of $\alpha_{1(n-1)}$ and y_n, $y_{n-1,n}$, $y_{1,n}$ have been taken, treatment $1(n-1)n$ is needed in order to estimate

$\alpha_{1(n-1)}$ and keep the strict OFAT property. Repeating this procedure for part 2 of Table 1, by adding the $(2n+n-2)$th run (i.e., treatment $134\ldots n$), α_{13} is estimable. Recall that $\alpha_{12}+\alpha_{13}+\cdots+\alpha_{1n}$ is estimable from (3) and $\alpha_{13}, \alpha_{14}, \ldots, \alpha_{1n}$ are estimable, thus α_{12} is estimable by subtraction. The added runs and the corresponding estimable 2fi's are given in rows $2n+1$ to $2n+n-2$ of Table 1. Therefore, all the 2fi's involving factor 1 are estimable if the first $2n+n-2$ runs in Table 1 are performed. Next we de-alias 2fi's involving factor 2. Note that $(y_{1,2,3,\ldots,n}+y_{1,3,4,\ldots,n-1}-y_{1,3,4,\ldots,n}-y_{1,2,3,\ldots,n-1})/4$ is a linear unbiased estimator of α_{2n} and all the terms except $y_{1,3,4,\ldots,(n-1)}$ are among the first $2n+n-2$ runs. Adding treatment $134\ldots(n-1)$ as the $(2n+(n-2)+1)$th run will keep the strict OFAT property and allow α_{2n} to be estimated. Repeating this procedure for part 3 of Table 1, by adding treatment 13 as the $(2n+(n-2)+(n-3))$th run, α_{24} is estimable. As $\alpha_{12}-\alpha_{23}-\cdots-\alpha_{2n}$ is estimable from (3), α_{23} is estimable as the other terms in the sum are estimable. Generally, for $k, j=0,1,\ldots,n$,

$$\frac{1}{4}\,[y_{1,3,5,\ldots,2k+1,j,j+1,\ldots,n}+y_{1,3,5,\ldots,2k-1,j+1,j+2,\ldots,n}$$
$$-y_{1,3,5,\ldots,2k+1,j+1,j+2,\ldots,n}-y_{1,3,5,\ldots,2k-1,j,j+1,j+2,\ldots,n}], \tag{4}$$

is a linear unbiased estimator of $\alpha_{2k+1,j}$, where $1 \leqslant 2k+1 < j \leqslant n$; $y_{1,3,5,\ldots,2k-1,j+1,\ldots,n}=y_0$ for $k=0$ and $j=n$; $y_{1,3,5,\ldots,2k+1,j+1,j+2,\ldots,n}=y_{1,3,\ldots,2k+1}$ for $j=n$; $y_{1,3,5,\ldots,2k-1,j,j+1,\ldots,n}=y_{j,j+1,\ldots,n}$ for $k=0$, and

$$\frac{1}{4}\,[y_{1,3,5,\ldots,2k-1,2k+1,2k+3,2k+4,\ldots,j-1}+y_{1,3,5,\ldots,2k-1,2k+1,2k+2,2k+3,2k+4,\ldots,j}$$
$$-y_{1,3,5,\ldots,2k-1,2k+1,2k+2,2k+3,\ldots,j-1}-y_{1,3,5,\ldots,2k-1,2k+1,2k+3,2k+4,\ldots,j}], \tag{5}$$

is a linear unbiased estimator of $\alpha_{2k+2,j}$, where $2 \leqslant 2k+2 < j \leqslant n$, $y_{1,3,5,\ldots,2k+1,2k+3,2k+4,\ldots,j-1}=y_{1,3,\ldots,2k+1}$ for $j=2k+3$. Continuing the de-aliasing process as above, all the 2fi's can be estimated. Since only $(n-1)(n-2)/2$ 2fi's need to be estimated through adding runs to the first $2n$ treatments in Table 1, the strict OFAT design of resolution V has $2n+(n-1)(n-2)/2=(n^2+n+2)/2$ runs. Because the design is saturated (i.e., it has a square model matrix), the linear unbiased estimators given in (2), (4) and (5) for strict OFAT designs are unique and thus are the best linear unbiased estimators if the errors are independent with mean 0 and constant variance.

The main difference from standard OFAT designs is the strict OFAT property. Because of this property, all the treatments in Table 1 must be performed in the given order and the effects are de-aliased in the same order. If there is prior knowledge of factor importance in the experiment, the most important factor should be taken as the first in strict OFAT designs so that the interactions involving this factor can be estimated earlier than others. Moreover, strict OFAT designs have the minimum sequential level changes. They are desirable if it is difficult or time-consuming to change factor levels or to reset the apparatus.

As an illustration, a six-factor strict OFAT design of resolution V is given in Table 2, where lower case and capital letters stand for factors and effects respectively. From Table 2, it takes 16 runs to estimate AB, AC, and AE and 22 runs to estimate AB, CD, and DE. On the other hand, the standard OFAT design would require 17 runs to estimate either set of effects. Since AF is the first 2fi that is de-aliased in Table 2, we

Table 2
A six-factor strict OFAT design of resolution V

Run	Treatment	Estimable effects
1	(1)	
2	a	$A-(AB+AC+AD+AE+AF)$
3	ab	$B+(AB-BC-BD-BE-BF)$
4	abc	$C+(AC+BC-CD-CE-CF)$
5	$abcd$	$D+(AD+BD+CD-DE-DF)$
6	$abcde$	$E+(AE+BE+CE+DE-EF)$
7	$abcdef$	$F+(AF+BF+CF+DF+EF)$
8	$bcdef$	$A,\ AB+AC+AD+AE+AF$
9	$cdef$	$B,\ AB-BC-BD-BE$
10	def	$C,\ AC+BC-CD-CE-CF$
11	ef	$D,\ AD+BD+CD-DE-DF$
12	f	$E,\ AE+BE+CE+DE-EF$
		$F,\ AF+BF+CF+DF+EF$
13	af	AF
14	aef	AE
15	$adef$	AD
16	$acdef$	$AC,\ AB$
17	$acde$	BF
18	acd	BE
19	ac	$BD,\ BC$
20	acf	CF
21	$acef$	$CE,\ CD$
22	ace	$DF,\ DE$

can assign factors to letters a to f so that the 2fi that is most likely to be significant is represented by AF. This would only require 13 runs with the strict OFAT design.

4. Comparisons with other designs

Because of orthogonality, OFFDs like 2_{V}^{k-p} require considerably more runs. This can be prohibitive if runs are expensive. Nonorthogonal resolution V designs with smaller run size have been proposed. Rechtschaffner (1967) (RECH) constructed saturated resolution V designs. Addelman (1969) and John (1962) constructed designs with fractions of full factorial designs. Diamond (1989) proposed some class A designs using regular or John's designs of resolution V with fewer factors plus regular or John's designs of resolution IV. Run size comparison of these designs with standard (STA) or strict (STR) OFAT designs is given in Table 3.

It is clear from Table 3 that strict OFAT and Rechtschaffner's designs are most economical. Both are saturated designs because their run size equals the number of parameters in model (1). Standard OFAT have two more runs than saturated designs. As the number of factors increases, standard OFAT designs are almost as economical as saturated designs. OFFDs are the worst because the degrees of freedom used to estimate high-order interactions get bigger as the number of factors grows. Other designs are

Table 3
Run size comparison of resolution V designs (NA indicates "not available")

No.of factors	RECH or STR-OFAT	STA-OFAT	Addelman	John	Diamond	OFFD
4	11	13	12	12	NA	16
5	16	18	16	24	NA	16
6	22	24	32	NA	28	32
7	29	31	40	48	36	64
8	37	39	48	48	44	64
9	46	48	64	96	69	128
10	56	58	64	96	81	128

Table 4
D efficiency comparison of resolution V designs (NA indicates "not available")

No. of factors	RECH	STR-OFAT	STA-OFAT	Addelman	John	Diamond
4	0.83	0.68	0.89	0.86	0.86	NA
5	1.00	0.54	0.73	0.77	0.93	NA
6	0.93	0.44	0.58	1.00	NA	0.84
7	0.79	0.36	0.46	0.89	0.93	0.71
8	0.66	0.30	0.37	0.88	0.89	0.61
9	0.55	0.32	0.30	0.83	0.95	0.73
10	0.46	0.26	0.25	0.76	0.94	0.61

between these two extremes. John's designs are larger than Addelman's and Diamond's. Addelman's and Diamond's designs are available up to 17 and 11 factors, respectively. By comparison, OFAT designs can be systematically constructed for any number of factors.

A commonly used criterion for design comparison is the D criterion, which measures the overall efficiency for effect estimation: $D=\det(X^tX)^{1/(k+1)}/N$, where $X=[\mathbf{1_N},x_1,\ldots,x_k]$, N is the run size, k is the number of effects and x_i is the coefficient vector of the ith effect, $i=1,2,\ldots,k$. $D=1$ if $\mathbf{1_N}$ and all the $x_i's$ are orthogonal to each other, i.e., when the design is orthogonal. Therefore, the D efficiency of OFFDs is 1. Table 4 shows the D efficiencies of various designs.

OFFDs are obviously the best, Addelman's, John's, Diamond's and RECH designs are in the middle, OFAT designs are the worst. The decrease in D efficiency reflects the increasing degree of nonorthogonality. There is a trade-off between run size and D efficiency because run size can be reduced by allowing nonorthogonality. Also standard OFAT designs have higher (and resp. lower) efficiency than strict OFAT designs if the number of factors is 4–8 (and resp. 9–10). For 4 factors, the D efficiency of standard OFAT design is the highest. OFAT designs are less D-efficient than

Rechtschaffner's designs. If estimation efficiency is the only concern, D-optimal designs should be used.

5. Adding runs to boost efficiency

If the individual effect is of interest, D_s-efficiency should be used. The D_s-efficiency of the ith effect is defined as

$$D_s(i) = \{x_i^t x_i - x_i^t X(i)(X(i)^t X(i))^{-1} X^t(i) x_i\}/x_i^t x_i,$$

where $X(i)$ is obtained from X by deleting x_i. A low $D_s(i)$ value would indicate that the ith effect is estimated with low precision. It was observed that the D_s efficiencies of some effects in OFAT designs are small. One way to increase their D_s efficiencies is to add a few runs. Consider the six-factor strict OFAT design given in Table 2. The D_s-efficiency for any effect is 0.18. The extra runs can be added in batches or sequentially. Adding runs in batches can explore all the possible batches and choose one with the largest D_s increment. Adding runs sequentially will choose one run at a time to maximize the increment in D_s value. Choice between batch of runs and sequential runs varies with the practical situations. Consider, for example, the main effect A. The optimal batch of 1–3 runs and the corresponding D_s efficiencies are given in Table 5. It is clear that the D_s efficiency of factor a is dramatically improved by adding 1–3 runs. Since the angle between the two columns representing effect A and the grand mean, 63°, is the smallest, the column vector for A in the model matrix is unbalanced (with 16 +'s and 6 −'s). To compensate for the imbalance, factor a in the added runs is set at the low level. After adding one more run, the angle is increased to 67°. The D_s efficiency of effect A in the augmented design is 0.35. Two more runs can be added if we need a higher D_s efficiency. The angle between the two columns representing effect A and the grand mean is further increased to 71°. The D_s efficiency of effect A in the augmented design is 0.55. This explains why factor a is always set at the low level in the three runs added. The sequentially added runs and the corresponding D_s efficiencies for A are given in Table 6. Since adding runs sequentially explores fewer possibilities than adding runs in batches, the D_s efficiencies for adding 2 and 3 runs in Table 6 are smaller than those in Table 5.

A similar procedure can be applied to boost the D_s efficiency of any other effect. For instance, results of boosting the D_s efficiency of AB are given in Table 7.

Table 5
Runs added in batches for main effect A

D_s	0.18	0.35	0.55	0.69
Factors		a b c d e f	a b c d e f	a b c d e f
Runs		0 1 1 1 1 0	0 1 0 1 0 0	0 1 0 1 1 0
			0 1 1 0 0 0	0 1 1 0 0 0
				0 1 1 1 0 0

Table 6
Runs added sequentially for main effect A

D_s	0.18	0.35	0.50	0.64
Factors		a b c d e f	a b c d e f	a b c d e f
Runs		0 1 1 1 1 0	0 1 1 1 1 0	0 1 1 1 1 0
			0 1 0 0 0 0	0 1 0 0 0 0
				0 1 1 0 0 0

Table 7
Runs added in batches for 2fi AB

D_s	0.18	0.35	0.44	0.53
Factors		a b c d e f	a b c d e f	a b c d e f
Runs		0 1 0 0 0 0	0 1 0 0 0 0	0 1 0 0 0 0
			0 0 1 0 0 0	0 0 1 1 0 0
				1 1 0 0 0 1

Runs added sequentially for 2fi AB

D_s	0.18	0.35	0.44	0.53
Factors		a b c d e f	a b c d e f	a b c d e f
Runs		0 1 0 0 0 0	0 1 0 0 0 0	0 1 0 0 0 0
			1 1 0 1 1 1	1 1 0 1 1 1
				0 0 1 1 0 0

Coincidentally, the D_s efficiencies of AB in adding two or three runs sequentially and in batches are identical.

6. Conclusions

In spite of the popularity of orthogonal designs, OFAT designs continue to be used in physical experiments. The sequential build-up of the designs involves much fewer changes of factor levels and is amenable to sequential learning. This is attractive if level changes are costly or time-consuming. Even if the experiment is prematurely terminated, some main effects (and 2fi's in the case of resolution V OFAT designs) can still be estimated. The proposed OFAT designs of resolution V are economical in run size. Because the designs are far from orthogonal, the estimation efficiency is quite low. This can be boosted by adding a few runs chosen by the D_s criterion. (As pointed out by a referee, other criteria can be employed in choosing additional runs to boost efficiency.) Other disadvantages include lack of randomization and possible presence of trends. OFAT designs should be considered when the advantages outweigh the disadvantages.

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