Combined Array Experiment Design

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Abstract: Experiment plans formed by combining two or more designs, such as orthogonal arrays, primarily with 2- and 3-level factors, creating multi-level arrays with subsets of different strength are proposed for computer experiments. The specific illustrations are designs for 5-level factors with fewer runs than generally required for 5-level orthogonal arrays of strength 2 or more. At least five levels for each input are desired to allow for runs at a nominal value, two values either side of nominal but within a normal, anticipated range, and two more extreme values either side of nominal. This number of levels allows for a broader range of input combinations to test the input combinations where a simulation code operates. Five-level factors also allow the possibility of up to 4th order polynomial models for fitting simulation results, at least in one dimension. By having subsets of runs with more than strength 2, interaction effects may also be considered. Also, the resulting designs have a "checker-board" pattern in lower-dimensional projections, in contrast to the grid projection that occurs with orthogonal arrays.

Keywords: Computer experiments, experiment design, fractional factorial design, orthogonal arrays, correlation coefficient

1. INTRODUCTION

The context for this paper is planning runs of a non-stochastic computer code for the purpose of assessing important inputs from among p inputs. As in McKay (1995), "important" input(s) are identified based on comparison of R^2, an estimate of the correlation coefficient associated with the goodness of fit to the simulated output Y of an analysis of variance model based on a subset of inputs X_s. The following is a formula for R^2 based on a subset of inputs X_s:

$$R^2(X_s) = \frac{\sum_{i \in X_s} \sum_j (y_{i\cdot} - y_{\cdot\cdot})^2}{\sum_{i \in X_s} \sum_j (y_{ij} - y_{\cdot\cdot})^2}$$

where the subscript i varies over distinct values of the s inputs identified in X_s, the subscript j varies over "replicate" experiments corresponding to a fixed value of the inputs X_s, and the "dot" subscript indicates the standard average. "Replicate" is in quotes since no true replicates are done. The computer simulation output is non-stochastic in that the output is fully determined by specification of the input with no variation in output for repeated runs of the code for identical input. Variation in the output is induced solely by variation in the inputs. The (p-s) inputs identified by $X-X_s$ may differ while X_s is fixed and this is the basis of pseudo-replicate, or "replicate" runs for fixed values of X_s. The value $y_{i\cdot}$ will be identically y_{ij} if there are no pseudo-replicate runs. If this is the case for every value of the inputs identified by X_s, then R^2 will have a value identically 1. Otherwise, R^2 is between 0 and 1. This reasoning leads to considering experiment designs such that, for subsets of inputs of a specified size $s<p$, a sampling of values for that subset of inputs is required such that "replicates" determined by a sample of values for the remaining inputs occur, for at least one of the values of the subset of inputs. This is a property of factorial experiment designs, or orthogonal arrays, which naturally suit this analysis approach, per Moore and McKay (2002). However, in order to obtain non-degenerate values of R^2 for subsets of 2 or more inputs, orthogonal arrays of strength 2 or more are dictated.

The specific illustrations of experiment designs are for 5-level factors with fewer runs than generally required for 5-level orthogonal arrays of strength 2 or more. In statistical experiment design, particularly as used in industrial physical experiments, factorial experiments with 2 or 3 level factors are common. Here, at least five levels for each input are desired to allow for runs at a nominal value, two values either side of nominal but within a normal, anticipated range, and two more extreme values either side of nominal. This number of levels allows for a broader range of input combinations to test the input combinations where a simulation code operates. Five-level factors also allow the possibility of up to 4^{th} order polynomial models for fitting the simulation results, at least in one dimension.

The requirement for strength 2 or more arrays, in addition to requiring factors to have 5 levels, leads to orthogonal arrays with unacceptably large numbers of runs in some situations. Moore and McKay (2002) present a 625 run orthogonal array for up to 26 5-level factors that is strength 3. In fact, for 625 runs the maximum number of 5-level factors for which a strength 2 orthogonal array exists is 156. The maximum number for which a strength 3 array exists in 625 runs is 26 5-level factors, and the maximum number for a strength 4 array is 6 5-level factors. For 125 runs, the maximum strength for a 5-level orthogonal array is 3 and inequalities in Hedayat, et al (1999) show that the maximum number of 5-level factors that could be accommodated by a strength 3 orthogonal array in 125 runs is 5. Although it is conceivable that in computer experiments hundreds of runs might be achievable, for the problem at hand less than, or on the order of 100 runs of the computer code are acceptable. Additionally, often computer codes have at least tens of inputs and for the illustrations here no fewer than 7 inputs are considered.

As a result of these requirements, experiment plans formed by combining two or more designs, such as orthogonal arrays primarily with 2- and 3-level factors, creating multi-level arrays with subsets of different strength are proposed for computer experiments. Experiments constructed in this way will be referred to as combined array experiments, or combined arrays. Construction of combined arrays is illustrated in Section 2, specifically including investigation of 2-level and 3-level orthogonal arrays used to construct 5-level combined arrays. Additional analysis considerations, optimal experiment design properties and space-filling properties are discussed in Section 3 for combined arrays. Conclusions are in Section 4.

2. COMBINED ARRAYS

In the following, combined array experiments are constructed by combining 2- and 3-level fractional factorial experiments, or orthogonal arrays, creating 5-level arrays with subsets of different strength. The resulting combined array is not orthogonal although, obviously, subsets of runs are orthogonal arrays. While 5-levels are formed and the underlying arrays are orthogonal, clearly the concepts can be extended to form any number of levels for the factors and to combine arrays that are not orthogonal although the arrays should have some specified, desirable properties.

Factorial experiments are experiments for inputs, called factors, with a finite number of discrete values, referred to as levels, so if each input has K levels and there are p inputs then there are K^P possible distinct runs referred to as the K^P factorial design space. The K levels could be associated with K equal probability content intervals for a continuous input. If the experiment plan consisted of the entire K^P factorial design space, then for each pair of inputs (subsets of size 2) there are K^2 values (levels) with K^{P-2} "replicates" for each value. Obviously this extends to subsets of inputs of size s in the obvious way. For relatively moderate K and even small sizes for p the full product space of possible experiment runs quickly becomes unmanageably large, even given the ability to run the simulation code thousands of times. As stated previously, inputs with at least 5 levels are desired and only 5-level factors are considered in the following.

Orthogonal array experiment designs are subsets of full factorial designs, also referred to as fractional factorial designs, with reduced runs obtained by relaxing the property that for any subset of inputs there are "replicate" inputs for each value of the subset. Wu and Hamada (2000) and Hedayat, et al (1999) are good references on orthogonal arrays, in addition to several older texts on statistical experiment design and fractional factorial experiments by John (1971) and Raktoe, et al (1981). For K levels identified by elements in the set L={0,1,2,…,k-1}, an $N\times p$ array X with entries from L is an orthogonal array with K levels, strength t ($0\leq t\leq p$) and index λ if every $N\times t$ sub-array of X contains each t-tuple based on L exactly λ times as a row. An array with parameters N (number of runs), p (number of factors), k (number of levels for each factor), and t (strength) is denoted OA(N,p,k,t). From this definition, a strength t orthogonal array with index λ is a set of p-dimensional factorial design points such that if one considers any t-dimensional projection then every point in the K^t factorial design space is replicated λ times. Likewise, any projection of dimension smaller than t, say s<t, consist of $\lambda * K^{(t-s)}$ replicates of the K^S factorial design space. A full K^P factorial design space is itself an OA(K^P,p,K,p) with index unity, that is $\lambda=1$. To reduce the number of runs from the full factorial design, a compromise is made on strength in orthogonal arrays. In a strict sense, fractional factorial designs may be any subset of the full factorial design space but often this terminology, or the term regular fractional factorial, is reserved for subsets that form an orthogonal array. For K prime, fractions of resolution III, IV and V defined in John (1971) or Raktoe, et al (1981) correspond to orthogonal arrays of strength 2, 3, and 4 respectively for which "replicate" runs occur for X_s including all values in the K^S grid, where $s\leq t$ and, respectively, t=2, 3, and 4 is the strength of the array.

Again, experiment design options for 5-level factors are desired. The number of levels is required to be 5: a nominal value (coded as 2), two values either side of nominal (referred to as inner limits, coded as 1 and 3) but with values that might be reasonably expected, and two values either side set a little further out (referred to as outer limits, coded as 0 and 4). The potential exists for failed runs at some of the extreme values. Less than 100 runs, or on the order of 100, could be done. Strength 3, at a minimum, is also desirable but that requires too many runs for a fully orthogonal array, on the order of 5^4=625 at a minimum, for 7 to 10 5-level factors. In reality, strength 3 is probably not absolutely required, that is the ability to assess a possibly unique effect for all 3 variable combinations of 5-level variables. Instead, this strength requirement reflects the experimenter's suspicion that there are potential interaction effects and the experimenter's desire to obtain some information about interactions from the experiment.

To obtain 5-level factors, 2-level and 3-level experiments designs are combined associating the levels of these two designs with 5-levels. The 2-levels are assigned the reasonable values either side of nominal (inner limits) and 3-levels assigned to nominal and the two extreme values (outer limits) either side of nominal. With this construct in mind, it is clear all that is required are desirable (high strength, allowing for run size limitations) 2-level and 3-level experiment designs. It is expected that a good (high strength) 2-level factorial design would yield main effects assessments independent of (at least pair-wise) cross factor interactions while a riskier (lower strength) 3-level factorial design would give somewhat more limited information on code functioning at nominal and extreme values of the factors. One would not run as much risk of losing information if code runs at extreme values fail since results on a good 2-level design would be obtained. However, there is potential for additional information over the limited 2-level factorial experiment, such as departure from linearity assessable with runs at the nominal values of factors as well as code performance at extremes. In the following, combined arrays are denoted CA(N,p,k,"i"t,"o"t) with parameters N (number of runs), p (number of factors), k (number of levels for each factor, here k=5), strength t labeled "i"t corresponding to the orthogonal array associated with the inner limits , and strength t labeled "o"t corresponding to the orthogonal array associated with the outer limits.

Substantial research and continuing development exists for constructing 2- and 3-level fractional factorial designs and the variety of methods and results in the literature are not surveyed here. Specific arrays are used to illustrate the construction of combined arrays. Hedayat, et al (1999) is a source of most constructions of these designs, and Tables 12.6 (c-e) on pages 326-327 of this text index constructed (fixed-level) orthogonal arrays for 2-level arrays with strength at least 3 and 3-level arrays with strength at least 2. Electronic data-bases containing these, and other, arrays can be found at the website:

www.research.att.com/~njas/oadir.

For seven factors, there is an OA(16,8,2,3), a 16-run orthogonal array for eight 2-level factors that is strength 3, and an OA(18,7,3,2), an 18 run orthogonal array for seven 3-level factors. Using only 7 of the 8 factors from an OA(16,8,2,3) combined with the OA(18,7,3,2), a CA(34,7,5,i3,o2) combined array is constructed. An OA(16,8,2,3), 2-level array is defined by columns x_1, …, x_8 such that the first four columns are the full 2^4 array and the remaining columns are defined by the following equations (with modulus 2 addition):

$x_5 = x_1 + x_2 + x_3$,

$x_6 = x_1 + x_2 + x_4$,

$x_7 = x_1 + x_3 + x_4$,

$x_8 = x_2 + x_3 + x_4$.

Table 1 lists the 16 design points in this OA(16,8,2,3) with levels coded as 0 and 1 and then recoded to the values either side of nominal (inner limits) coded as 1 and 3 for the 5-level factors denoted f_1, …, f_8:

Table 1: OA(16,8,2,3) and associated points in CA(34,7,5,i3,o2)

OA(16,8,2,3) Run/Input Coded {0,1}	x_1	x_2	x_3	x_4	x_5	x_6	x_7	x_8	CA(34,7,5,i3,o2) Run/Input Coded {1,3}	f_1	f_2	f_3	f_4	f_5	f_6	f_7	f_8
1	0	0	0	0	0	0	0	0	1	1	1	1	1	1	1	1	1
2	1	0	0	0	1	1	1	0	2	3	1	1	1	3	3	3	1
3	0	1	0	0	1	1	0	1	3	1	3	1	1	3	3	1	3
4	1	1	0	0	0	0	1	1	4	3	3	1	1	1	1	3	3
5	0	0	1	0	1	0	1	1	5	1	1	3	1	3	1	3	3
6	1	0	1	0	0	1	0	1	6	3	1	3	1	1	3	1	3
7	0	1	1	0	0	1	1	0	7	1	3	3	1	1	3	3	1
8	1	1	1	0	1	0	0	0	8	3	3	3	1	3	1	1	1
9	0	0	0	1	0	1	1	1	9	1	1	1	3	1	3	3	3
10	1	0	0	1	1	0	0	1	10	3	1	1	3	3	1	1	3
11	0	1	0	1	1	0	1	0	11	1	3	1	3	3	1	3	1
12	1	1	0	1	0	1	0	0	12	3	3	1	3	1	3	1	1
13	0	0	1	1	1	1	0	0	13	1	1	3	3	3	3	1	1
14	1	0	1	1	0	0	1	0	14	3	1	3	3	1	1	3	1
15	0	1	1	1	0	0	0	1	15	1	3	3	3	1	1	1	3
16	1	1	1	1	1	1	1	1	16	3	3	3	3	3	3	3	3

Hedayat, et al (1999) lists an OA(18,7,3,2) on page 20 and discusses construction in Chapter 3. The reader is referred to the text for construction and the design is listed here in Table 2 with standard {0,1,2} coding followed by coding for the nominal and extreme values (outer limits) for f_1, …, f_7:

Table 2: OA(18,7,3,2)) and associated points in CA(34,7,5,i3,o2)

OA(18,7,3,2) Run/Input Coded{0,1,2}	x_1	x_2	x_3	x_4	x_5	x_6	x_7	CA(34,7,5,i3,o2) Run/Input Coded {0,2,4}	f_1	f_2	f_3	f_4	f_5	f_6	f_7
1	0	0	0	0	0	0	0	17	0	0	0	0	0	0	0
2	1	1	1	1	1	1	0	18	2	2	2	2	2	2	2
3	2	2	2	2	2	2	0	19	4	4	4	4	4	4	4
4	0	0	1	2	1	2	0	20	0	0	2	4	2	4	0
5	1	1	2	0	2	0	0	21	2	2	4	0	4	0	0
6	2	2	0	1	0	1	0	22	4	4	0	2	0	2	0
7	0	1	0	2	2	1	1	23	0	2	0	4	4	2	2
8	1	2	1	0	0	2	1	24	2	4	2	0	0	4	2
9	2	0	2	1	1	0	1	25	4	0	4	2	2	0	2
10	0	2	2	0	1	1	1	26	0	4	4	0	2	2	2
11	1	0	0	1	2	2	1	27	2	0	0	2	4	4	2
12	2	1	1	2	0	0	1	28	4	2	2	4	0	0	2
13	0	1	2	1	0	2	2	29	0	2	4	2	0	4	4
14	1	2	0	2	1	0	2	30	2	4	0	4	2	0	4
15	2	0	1	0	2	1	2	31	4	0	2	0	4	2	4
16	0	2	1	1	2	0	2	32	0	4	2	2	4	0	4
17	1	0	2	2	0	1	2	33	2	0	4	4	0	2	4
18	2	1	0	0	1	2	2	34	4	2	0	0	2	4	4

Table 3 lists additional examples of combined arrays that could be formed in a like fashion to CA(34,7,5,i3,o2) based on arrays that are indexed in Hedayat, et al (1999).

Table 3: CA formed from binary and ternary OA

Binary OA	Ternary OA	CA
OA(16,8,2,3)	OA(18,7,3,2)	CA(34,7,5,i3,o2)
OA(24,12,2,3)	OA(27,13,3,2)	CA(51,12,5,i3,o2)
OA(32,16,2,3)	OA(27,13,3,2)	CA(59,13,5,i3,o2)
OA(64,14,2,3)	OA(27,13,3,2)	CA(91,13,5,i3,o2)
OA(64,14,2,3)	OA(54,25,3,2)	CA(118,14,5,i3,i2)
OA(128,15,2,4)	OA(54,25,3,2)	CA(182,15,5,i4,i2)

3. STATISTICAL ANALYSIS AND SPACE-FILLING FEATURES FOR COMBINED ARRAYS

Examining CA(34,7,5,i3,o2) in a similar way as an orthogonal array is evaluated, lower dimensional projections may be considered or, equivalently, multi-way tables of the counts of values of the factors that occur in the experiment design. For any two columns of the CA(34,7,5,i3,o2) experiment, the two-way table (Table 4) of values that occur in the design is:

Table 4 : Incidence of values for any two columns in CA(34,7,5,i3,o2)

“replicates”	fj=	0	1	2	3	4	totals
fi=							
0		2	0	2	0	2	6
1		0	4	0	4	0	8
2		2	0	2	0	2	6
3		0	4	0	4	0	8
4		2	0	2	0	2	6
Totals		6	8	6	8	6	34 runs

For a strength 2 orthogonal array this table would have the same values in every cell. For combined orthogonal arrays such as CA(34,7,5,i3,o2), there is a “checkerboard” pattern for the cells with non-zero and zero counts and the cells with non-zero counts may not have the same counts.

Considering any three factors in CA(34,7,5,i3,o2), the tables of values that occur are variants of one of the three tables labeled below as Table 5 for f_1, f_2, and f_3, Table 6 for f_1, f_2, and f_7, or Table 7 for f_3, f_5, and f_7. The variations that occur are that the rows that correspond to the even values of a factor may be permuted, although the marginal count values stay the same. There are 28 triples of factors, which have a 3-way table like Table 5, 6 triples correspond to Table 6, and factors f_3, f_5, and f_6 are the only ones with the pattern in Table 7.

Table 5: Values of f_1, f_2, and f_3 in the design CA(34,7,5,i3,o2).

“reps”	f_3=	0					1					2					3					4					total
	f_2=	0	1	2	3	4	0	1	2	3	4	0	1	2	3	4	0	1	2	3	4	0	1	2	3	4	
f_1=	0	1	0	1	0	0	0	0	0	0	0	1	0	0	0	1	0	0	0	0	0	0	0	1	0	1	6
	1	0	0	0	0	0	0	2	0	2	0	0	0	0	0	0	0	2	0	2	0	0	0	0	0	0	8
	2	1	0	0	0	1	0	0	0	0	0	0	0	1	0	1	0	0	0	0	0	1	0	1	0	0	6
	3	0	0	0	0	0	0	2	0	2	0	0	0	0	0	0	0	2	0	2	0	0	0	0	0	0	8
	4	0	0	1	0	1	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0	1	0	0	0	1	6
Total		2	0	2	0	2	0	4	0	4	0	2	0	2	0	2	0	4	0	4	0	2	0	2	0	2	34

Table 6: Values of f_1, f_2, and f_7 in the design CA(34,7,5,i3,o2).

"reps"	f_7=	0					1					2					3					4					total
	f_2=	0	1	2	3	4	0	1	2	3	4	0	1	2	3	4	0	1	2	3	4	0	1	2	3	4	
f_1=	0	2	0	0	0	0	0	0	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0	1	0	1	6
	1	0	0	0	0	0	0	2	0	2	0	0	0	0	0	0	0	2	0	2	0	0	0	0	0	0	8
	2	0	0	2	0	0	0	0	0	0	0	1	0	0	0	1	0	0	0	0	0	1	0	0	0	1	6
	3	0	0	0	0	0	0	2	0	2	0	0	0	0	0	0	0	2	0	2	0	0	0	0	0	0	8
	4	0	0	0	0	2	0	0	0	0	0	1	0	1	0	0	0	0	0	0	0	1	0	1	0	0	6
Total		2	0	2	0	2	0	4	0	4	0	2	0	2	0	2	0	4	0	4	0	2	0	2	0	2	34

Table 7: Values of f_3, f_5, and f_7 in the design CA(34,7,5,i3,o2).

"reps"	f_7=	0					1					2					3					4					total
	f_5=	0	1	2	3	4	0	1	2	3	4	0	1	2	3	4	0	1	2	3	4	0	1	2	3	4	
f_3=	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	2	0	0	6
	1	0	0	0	0	0	0	2	0	2	0	0	0	0	0	0	0	2	0	2	0	0	0	0	0	0	8
	2	0	0	2	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	0	0	0	0	0	0	2	6
	3	0	0	0	0	0	0	2	0	2	0	0	0	0	0	0	0	2	0	2	0	0	0	0	0	0	8
	4	0	0	0	0	2	0	0	0	0	0	0	0	2	0	0	0	0	0	0	0	2	0	0	0	0	6
Total		2	0	2	0	2	0	4	0	4	0	2	0	2	0	2	0	4	0	4	0	2	0	2	0	2	34

A strength 3 orthogonal array would dictate that every cell in the 3-way tables has the same non-zero count. There are 125 cells, so, obviously, with only 34 runs not every cell can have a non-zero count. The trade-off with fewer runs than cells is to have non-zero count in as many cells as possible and have these cells "spread" around as much as possible. Visually, this is best achieved in Table 5 which is the associated table for 28 of the 35 possible triples of factors. Based on this observation, combined array designs do a good job of space-filling in lower dimensional projections that correspond to the strengths of the combined arrays. Specifically, CA(34,7,5,i3,o2) is a good space-filling design in its 2- and 3-dimensional projections.

Since the combined arrays have underlying structure of orthogonal arrays on subsets of runs, analyses investigating main effects and interactions are possible and there are "replicates" required for the comparison of R^2 as in McKay (1995) for identifying "important" input(s). In statistical experiments, 2- and 3-level experiments are common and relate to the fitting of polynomial regression models with degree 1 or 2, respectively. For 2-level factors, at most a first order, or linear, polynomial in a single factor can be modeled. For 3-level factors, a second order polynomial model can be fit. In the analysis of variance paradigm, 2-level factors allow fitting of linear main effects only while 3-level factors coincide with fitting linear and quadratic main effects. The requirement of strength 2 or 3 orthogonal arrays is associated with fitting of polynomial regression models without or with cross factor terms, respectively. In an analysis of variance interpretation, strength 2 corresponds to the ability to fit main effects only where at least some main effects are biased by possibly significant two-factor interactions. In the experiment design literature this type of experiment is referred to as a resolution III design. Strength 3 corresponds to a resolution IV design where only a main effects model is estimable but the main effects estimates are not biased by any two-factor interactions, although bias due to any higher order interactions exists. Strength 4 corresponds to a resolution V design where main effects and two-factor interactions are estimable, although again biased by any potentially non-negligible higher order interactions. The capacity of an experiment to evaluate assorted polynomial trends does not necessarily indicate that the polynomial is in any sense the replacement model, but as for analysis based on comparison of R^2 for different sets of inputs, it provides a means for identifying inputs that are most influential subject to the limits of the experiment design.

4. CONCLUSIONS

Combining 2- and 3-level orthogonal arrays leads to designs with 5-level factors but with full orthogonality compromised. The resulting array is not orthogonal but high strength is achieved with respect to some level combinations or a subset of runs and as a result there is the capacity to make assessment of important effects based on comparison of R^2 for different input sets as in McKay (1995). These properties are achieved with fewer runs than would be required for an orthogonal design for 5-level factors.

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