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Identifying Minimum *G* Aberration Designs from Hadamard Matrices of Order 28

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Two-level fractional factorial designs are among the most widely used statistical experimental strategies for the simultaneous study of the effects of several variables. In general, factorial designs consist of a fixed number of levels for each of the variables (factors) under investigation and all combinations of these factor levels. The combinations of factor levels represent the conditions at which the response will be measured, and a combination of factor levels at which an experiment is to be carried out is called a *run*. Since identifying active factors is often an early phase in a sequential experimental strategy, we would like to run the fewest number of levels of the factors while still learning about their impacts. Consequently, two-level factorial designs are popular choices for "screening" – that is, identifying which of the many factors under investigation really affects the response. To study the effects of k factors each at two levels, + and −, a two-level *full* factorial design consists of all 2^k combinations of factor levels. The two-level *fractional* factorial designs specify a carefully selected subset, or fraction, of the 2^k combinations of factor levels and are therefore extremely useful when a large number of factors is being investigated and/or the experimental runs are expensive or time consuming to conduct. That is, two-level fractional factorials are favored because of their *run size economy*. We consider the broad class of orthogonal two-level factorial designs that can be constructed from the columns of Hadamard matrices. A Hadamard matrix of order n, say $\boldsymbol{M}$, is an orthogonal $n \times n$ matrix with entries 1 or −1, so that $\boldsymbol{M}^T \boldsymbol{M} = n\boldsymbol{I}$ where $\boldsymbol{I}$ is the $n \times n$ identity matrix. For such a matrix to exist, n must be a multiple of four (except for the trivial cases $n = 1$ and $n = 2$), and a library of Hadamard matrices of every order up to $n = 256$ is available at N.J.A. Sloane's web site, *www.research.att.com/~njas*. For notational ease, we often use + and − to represent 1 and −1, respectively. Hadamard matrices may be normalized so the first column is all +'s. Removing this first column gives a Hadamard design, $\boldsymbol{H}$, with n runs and $n-1$ columns. The orthogonal property of Hadamard matrices means that designs constructed from the columns of Hadamard matrices have the same number of +'s and −'s in each design column and the four combinations (+, +), (+, −), (−, +), and (−, −) occur with the same frequency in every two design columns. From each Hadamard matrix of order n, there are ${}_{n-1}C_m$ possible designs of n runs and m factors. A survey on applications of Hadamard matrices in design theory can be found in Hedayat and Wallis (1978).

Aliasing of effects is the price paid for run size economy in fractional factorial designs. Two effects are aliased when it is not possible to distinguish the estimate of one effect from the estimate of the other. The *regular* fractional factorials exhibit a simple aliasing structure in that any two effects can be estimated independently or are fully aliased. For example, take a design that exhibits full aliasing between the main effect of factor A and the effect of the three-factor interaction between factors B, C, and D. The data from such a design will yield an estimate of the sum of these effects, $A + BCD$, but is not capable of distinguishing the estimate of A from the estimate of BCD. Fortunately, the effects of three-factor interactions tend to be negligible.

The regular fractional factorial designs are most commonly used and are readily available in the literature. See, for example, Wu and Hamada (2000) and Box et al. (1978). However, the number of runs in a regular design must be a power of two, leaving large gaps in the available choices of run size. In contrast, *nonregular* fractional factorial designs can be constructed for run sizes that are multiples of four, filling in the gaps in available run sizes left by the regular designs. The nonregular designs exhibit partial aliasing of effects. Using an example similar to the one above, the data from a nonregular design in which A and BCD are partially aliased with an aliasing coefficient of 1/3 will yield an estimate of the main effect of factor A plus one third the effect of the three-factor interaction BCD, denoted by $A + 1/3\ BCD$. By comparison, the aliasing coefficients in a regular design are either ±1 or 0, corresponding to effects that are fully aliased or are orthogonal (i.e., uncorrelated), respectively. The aliasing structures of nonregular designs are more complex than those of regular designs in that the number of partial aliases is much larger than the number of full aliases in a regular design, making the aliasing structure difficult to disentangle. However, partially aliased effects may be jointly estimable, as shown in Hamada and Wu (1992). Moreover, since nonregular designs can be constructed for run sizes that are multiples of four, they provide a distinct advantage over regular designs in *run size economy* and *run size flexibility*. For example, nonregular designs of 20, 24, and 28 runs fill in the gap left by the 16-run and 32-run regular fractional factorials.

"Optimal" fractions are those for which potentially important effects are not aliased with each other. When no *a priori* knowledge exists about which effects are potentially active, the hierarchical ordering principle (Wu and Hamada, 2000) suggests that lower order effects (e.g., main effects) are more likely to be important than higher order effects (e.g., three-factor interactions). For regular designs, optimal fractions are chosen according to the well-known resolution (Box and Hunter, 1961) and minimum aberration (Fries and Hunter, 1980) criteria. These criteria cannot be applied to nonregular designs, and there were no systematic criteria for comparing different nonregular designs until recently. Deng and Tang (1999) proposed minimum *G* aberration (short for "generalized minimum aberration") for this purpose. For a subset of k columns from a Hadamard design, $s = \{c_1, c_2, \ldots, c_k\}$, define

$$J_k(s) = \left| \sum_{i=1}^{n} c_{i1} c_{i2} \cdots c_{ik} \right| \qquad (1)$$

where c_{ij} is the ith component of column c_j. $J_1(s) = J_2(s) = 0$ because the designs taken from Hadamard matrices are orthogonal. For a regular design, the only possible values of $J_k(s)$ are 0 and n, corresponding to orthogonality and full aliasing, respectively. $J_k(s)$ values between 0 and n correspond to partial aliasing, as found in nonregular designs. Values of $J_k(s)$ closer to n indicate more serious aliasing among the columns of s, and values closer to 0 indicate less serious aliasing among the columns of s. For the set $s = \{c_1, c_2, c_3\}$ of three columns, $J_3(s)/n$ is the absolute value of the aliasing coefficient of main effect c_1 and the two-factor interaction c_2c_3. Therefore, large $J_3(s)$ values provide the worst scenario – a potentially large amount of contamination of two-factor interactions on the estimation of main effects. When $n = 28$ runs, the possible values of $J_3(s)$ are 28, 20, 12, and 4. Then, for example, when $J_3(s) = 20$, the data will yield an estimate of the main effect c_1 plus (or minus) 20/28 of the effect of the two-factor interaction c_2c_3, denoted by $c_1 + 20/28\ c_2c_3$. On the other hand, when $J_3(s) = 4$, the data will yield an estimate of $c_1 + 4/28\ c_2c_3$. The potential amount of contamination of the c_2c_3 two-factor interaction on the estimation of main effect c_1 is less for lower values of $J_3(s)$.

The *confounding frequency vector* of a design is built up from its $J_k(s)$ values, and two designs of the same size are compared by their confounding frequency vectors. Let $F_k(D)$ be the vector which contains the frequencies of the different $J_k(s)$ values for design D. Define the confounding frequency vector of D as $F(D) = [F_3(D), F_4(D), \ldots, F_m(D)]$. Deng and Tang (2002) showed that only two or three leading terms in $F(D)$ are needed to classify and rank designs. Consequently, we use the abbreviated confounding frequency vector $F(D) = [F_3(D), F_4(D), F_5(D)]$ as the classification and ranking criterion. As an example, the top and second-ranked designs of $n = 24$ runs and $m = 8$ columns found by a complete search of Hadamard matrices of order 24 in Deng and Tang (2002) have (abbreviated) confounding frequency vectors $F(D_1) = [(0, 0, 0, 56)_3, (0, 0, 70, 0)_4, (0, 0, 0, 56)_5]$ and $F(D_2) = [(0, 0, 6, 50)_3, (0, 0, 52, 18)_4, (0, 0, 18, 38)_5]$. For 24 runs, the possible values of $J_k(s)$ are 24, 16, 8, and 0 and the four components of $F_k(D)$ are the number of subsets of k columns with $J_k(s) = 24, 16, 8$, and 0, in that order from left to right. The confounding frequency vectors indicate that in the second-ranked design D_2, there are six subsets of three columns for which the aliasing coefficient between the main effects and two-factor interactions is $\pm 8/24 = \pm 1/3$ whereas in the top-ranked design D_1, all the main effects can be estimated independently of two-factor interactions since each of the ${}_8C_3 = 56$ subsets of three columns yields $J_3(s) = 0$. (In practice, the last components in $F_3(D)$, $F_4(D)$, and $F_5(D)$ can be omitted since these values can be determined by the previous entries.) To compare two designs according to the minimum *G* aberration criterion, compare the entries of their confounding frequency vectors from left to right. Let r be the smallest number for which $F_r(D_1)$ not equal to $F_r(D_2)$. Use the $[i]$ nomenclature for a particular element of a vector. If $F_r(D_1)[i] < F_r(D_2)[i]$ are the leftmost entries of $F_r(D_1)$ and $F_r(D_2)$ that are not equal, then D_1 is said to have less *G* aberration than D_2, and D_1 is preferred. If no design has less *G* aberration than D_1, then D_1 is said to have minimum *G* aberration.

With a criterion now available for assessing the goodness of nonregular fractional factorial designs, methods for the construction of good designs were needed. By complete search of all possible designs from Hadamard matrices, Deng, Li, and Tang (2000) and Deng and Tang (2002) produced a comprehensive catalog of minimum *G* aberration designs of 12, 16, and 20 runs and a partial catalog of designs of 24 runs (accommodating up to eight factors). However, the number of comparisons required in a complete search for larger designs is enormous (e.g., for 28 runs and 10 factors, there are 4×10^9 designs to compare), rendering a complete search impractical. To solve this problem, efficient computational algorithms based on forward selection and backward elimination of columns of Hadamard matrices were studied in Ingram and Tang (2001). Improvements to these algorithms led to an excursion-at-target algorithm that allows the efficient exchange of columns after reaching the target design and thereby bypasses local minimum *G* aberration designs. The excursion-at-target algorithm was implemented in the construction of minimum *G* aberration designs of 24 runs for nine or more factors, and these designs are presented in Ingram (2000).

Designs of 28 runs are needed to further fill the gap in available run sizes left by the regular designs (no regular designs exist for run sizes between $n = 16$ and $n = 32$) and to offer more run size flexibility to experimenters. However, the excursion-at-target algorithm needed some major improvements to handle the complicated 28-run case. While it performed adequately in searching the 60 nonequivalent Hadamard matrices of order 24, it lacked the efficiency and stability to effectively search the 487 nonequivalent Hadamard matrices of order 28. To increase the stability of the program, memory usage was made more efficient. More sophisticated data structures were introduced to reduce the amount of memory used in each iteration. After the searches are performed, all necessary output is written to an output file to free up the memory for the next round of searches. In addition to these changes, the algorithm is now more generalized, allowing the construction of designs for any run size. Details on the original excursion at target algorithm appear in Ingram (2000). A complete discussion of the improvements made to the original algorithm along with the S-PLUS code appear in Belcher-Novosad (2002).

The upgraded excursion-at-target algorithm has now been implemented in the construction of designs of 28 runs. Competing designs include the regular designs of 32 runs, and therefore comparisons between the best 32-run designs and the best 28-run designs are of interest. Let m denote the number of factors accommodated by a design. For $m = 6$-16, the regular 32-run designs are such that all main effects can be estimated independently of two-factor interactions. The 28-run designs for $m = 6$-16 exhibit the weakest level of partial aliasing between main effects and two-factor interactions but may compete with the 32-run designs in terms of number of clear effects (Wu and Hamada, 2000).

For $m = 17$-27, the best regular designs of 32 runs all contain full aliasing between main effects and two-factor interactions, whereas the best 28-run designs exhibit only partial aliasing between main effects and two-factor interactions. For example, the minimum or near-minimum G aberration design of 28 runs and 17 factors found by the excursion-at-target algorithm has confounding frequency vector $F(D_{28\times 17}) = [(0, 0, 59, 621)_3, (0, 28, 262, 2090)_4, (0, 72, 2361, 3755)]$. The possible $J_k(s)$ values for $n = 28$ are (28, 20, 12, 4) for $k = 3$, 4 and (24, 16, 8, 0) for $k = 5$. A $J_3(s)$ value of 28 indicates full aliasing between main effects and two-factor interactions, whereas $J_3(s)$ values of 20, 12, and 4 indicate partial aliasing that decreases in severity with decreasing values of $J_3(s)$. The confounding frequency vector for design $D_{28\times 17}$ shows that the most serious level of aliasing is that exhibited by the columns contained in the 59 subsets of three columns with $J_3(s)$=12. The two-factor interactions contained in these 59 subsets are partial aliases of main effects with aliasing coefficient $\pm 12/28 = \pm 0.43$. At the same time, the best regular design of 32 runs and 17

Table 1. $D_{28\times 17}$: minimum or near-minimum G aberration design of 28 runs and 17 factors with confounding frequency vector $[(0, 0, 59, 621)_3, (0, 28, 262, 2090)_4, (0, 72, 2361, 3755_5)]$.

Run	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
1	+	+	+	+	+	-	-	-	-	-	-	-	+	+	+	+	-
2	-	-	-	-	-	+	+	+	-	-	-	-	+	+	+	-	+
3	-	-	-	-	-	-	-	-	+	+	+	+	+	+	+	+	+
4	+	-	+	+	-	-	+	-	+	-	-	+	-	+	-	+	+
5	+	-	+	-	+	+	-	-	-	-	+	-	-	-	+	+	+
6	+	-	-	+	+	-	-	+	+	+	-	-	+	-	-	+	+
7	-	+	+	-	-	-	+	+	-	-	+	+	+	-	-	+	+
8	-	+	-	+	-	+	-	+	+	+	-	+	-	-	+	+	+
9	-	+	-	-	+	+	+	-	-	+	+	-	-	+	-	+	+
10	+	-	+	-	-	-	+	+	+	+	+	-	-	+	-	-	-
11	+	-	-	+	-	+	-	+	-	-	+	+	+	-	-	-	-
12	+	-	-	-	+	+	+	-	+	+	-	+	-	-	+	-	-
13	-	+	+	+	-	+	-	-	+	-	+	+	-	+	+	-	-
14	-	+	+	-	+	-	-	+	+	+	+	-	+	-	+	-	-
15	-	+	-	+	+	-	+	-	-	+	-	+	+	+	-	-	-
16	+	+	+	-	-	-	+	+	-	+	-	+	-	-	+	+	-
17	+	+	-	+	-	+	-	+	-	+	+	-	-	+	-	+	-
18	+	+	-	-	+	+	+	-	+	-	+	+	+	-	-	+	-
19	-	-	+	+	-	+	+	-	-	+	-	-	+	-	+	+	-
20	-	-	+	-	+	+	-	+	+	-	-	+	+	+	-	+	-
21	-	-	-	+	+	-	+	+	+	-	+	-	-	+	+	+	-
22	+	+	+	-	-	+	-	-	+	+	-	-	+	+	-	-	+
23	+	+	-	+	-	-	+	-	+	-	+	-	+	-	+	-	+
24	+	+	-	-	+	-	-	+	-	-	-	+	-	+	+	-	+
25	+	-	+	+	+	+	+	+	-	+	+	+	+	+	+	-	+
26	-	+	+	+	+	+	+	+	+	-	-	-	-	-	-	-	+
27	-	-	+	+	+	-	-	-	-	+	+	+	-	-	-	-	+

factors has confounding frequency vector $F(D_{32\times 17}) = [(23, 0, 0, 0, 657)_3, (80, 0, 0, 0, 2300)_4, (194, 0, 0, 0, 5994)_5]$. The possible $J_k(s)$ values for n = 32 are (32, 24, 16, 8, 0) for all k. Therefore, the best design of 32 runs contains 23 subsets of three columns in which the main effects and two-factor interactions are *fully* aliased.

Design $D_{28\times 17}$ is given in Table 1. It was constructed from column numbers {1, 2, 4, 5, 6, 7, 8, 9, 13, 16, 17, 18, 19, 20, 21, 26, 27} of the 28[th] Hadamard matrix of order 28 (denoted had.28.28 in Sloane's library of Hadamard matrices) after normalizing and removing the first column of +'s. Complete design tables containing the minimum or near-minimum G aberration designs of 28 runs constructed by the excursion-at-target algorithm are being generated.

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