

USING REGULAR FRACTIONS OF TWO-LEVEL DESIGNS TO FIND BASELINE DESIGNS

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Abstract: Mukerjee and Tang (2012) established the K -aberration criterion for baseline two-level designs. This paper explores the use of the regular fractions of two-level designs (2^{m-p} designs) to create baseline designs. Results are presented that establish relationships between the sequence of K -values for a baseline design and the word length pattern of the corresponding 2^{m-p} design. Based on these results, methodology for creating baseline designs that have good K -aberration characteristics is developed and demonstrated.

Key words and phrases: Baseline parameterization, minimum aberration, orthogonal array, regular design, word length pattern.

1. Introduction

The analysis of data from two-level factorial and fractional factorial designs is usually based on the definitions of effects (main effects and interactions) given by Box and Hunter (1961), where an effect measures the impact on the response of changes to the levels of one or more factors averaged over all possible combinations of levels for the remaining factors. As these definitions of effects produce an orthogonal set of contrasts for a 2^m design, we refer to them as the *orthogonal parameterization* of the linear model.

A much less common (but in some cases more appropriate) alternative is ‘the *baseline parameterization* of the linear model. In this case, a baseline level (the default or preferred level) is designated for each factor. Consider an experiment that explores avenues for improving an established process. The practitioner does not want to make extensive changes to the process but rather wishes to identify one or two high-impact factors. It would be natural to designate the current level of each factor included in the experiment as its baseline level. Under the baseline parameterization, an effect measures the impact on the response of changes to the levels of one or more factors given that the remaining factors are set to their baseline levels. Given the practitioner’s desire to keep most of the factors at their current levels, these definitions are more appropriate than the orthogonal parameterization definitions.

Mukerjee and Tang (2012) developed theory related to the optimality of baseline designs. They focused on main effects designs and showed that orthogonal arrays of strength two are universally optimal for estimating main effects. They also developed the K -aberration criterion to quantify how well a design guards against bias in the estimation of main effects caused by active interactions. This entails finding the sequence K_2, K_3, \dots where K_j measures the total amount of aliasing between all j th order interactions and main effects. Details of the derivation of this sequence can be found in Mukerjee and Tang (2012) and also in Li, Miller, and Tang (2014). The objective is to identify a design that sequentially minimizes K_2, K_3, \dots . This approach is justified by the effect hierarchy principle which states that interactions of the same order are equally likely to be active and that lower order interactions are more likely to be active than higher order ones – see Wu and Hamada (2009).

Definition 1. Consider two baseline designs \mathcal{D}_1 and \mathcal{D}_2 that are of the same size, each corresponding to an orthogonal array of strength 2. Let \bar{j} be the smallest integer j for which the values of K_j differ for \mathcal{D}_1 and \mathcal{D}_2 . If the value of $K_{\bar{j}}$ for \mathcal{D}_1 is less than that for \mathcal{D}_2 , then \mathcal{D}_1 has less K -aberration than \mathcal{D}_2 . A minimum K -aberration design is one such that no other design with less K -aberration exists.

Mukerjee and Tang (2012) developed an efficient complete search algorithm which they used to identify all of the minimum K -aberration designs for $N = 8, 12, \text{ or } 16$ runs. Li, Miller, and Tang (2014) used the same algorithm to identify the minimum K -aberration designs for $N = 20$ runs and $m \leq 13$ factors. For $m > 13$ factors, they found that the complete search algorithm was not feasible and developed an efficient incomplete search algorithm to find nearly optimal designs.

In this paper, we develop a theory for creating baseline designs that have good K -aberration characteristics using the regular fractions of the 2^m factorial designs. This approach is very efficient in that it is possible to use the word length pattern of the 2^{m-p} designs to identify those which will generate the best baseline designs – often it is possible to identify a single regular fraction in this regard. Although we cannot guarantee that a design generated in this manner is a minimum K -aberration design, we present evidence that suggests that this is often the case. We also show that for $N \leq 64$, it can be guaranteed that these designs will have a K -sequence that matches at least the leading value of the minimum K -aberration designs. Section 2 introduces notation and background that are needed for the main results of this paper. The main results are presented in Section 3. Section 4 demonstrates how our results can be applied to produce

Table 1. The model matrix for a 2^3 design for the orthogonal parameterization and for the baseline parameterization.

Orthogonal Parameterization Model Matrix								Baseline Parameterization Model Matrix							
<i>I</i>	<i>A</i>	<i>B</i>	<i>C</i>	<i>AB</i>	<i>AC</i>	<i>BC</i>	<i>ABC</i>	<i>I</i>	<i>A</i>	<i>B</i>	<i>C</i>	<i>AB</i>	<i>AC</i>	<i>BC</i>	<i>ABC</i>
+1	-1	-1	-1	+1	+1	+1	-1	1	0	0	0	0	0	0	0
+1	+1	-1	-1	-1	-1	+1	+1	1	1	0	0	0	0	0	0
+1	-1	+1	-1	-1	+1	-1	+1	1	0	1	0	0	0	0	0
+1	+1	+1	-1	+1	-1	-1	-1	1	1	1	0	1	0	0	0
+1	-1	-1	+1	+1	-1	-1	+1	1	0	0	1	0	0	0	0
+1	+1	-1	+1	-1	+1	-1	-1	1	1	0	1	0	1	0	0
+1	-1	+1	+1	-1	-1	+1	-1	1	0	1	1	0	0	1	0
+1	+1	+1	+1	+1	+1	+1	+1	1	1	1	1	1	1	1	1

baseline designs that are optimal or nearly optimal in terms of K -aberration. Concluding remarks are given in Section 5.

2. Notation and Background

Consider an N -run baseline design for m factors represented as an $N \times m$ (0, 1)-matrix \mathcal{D} where 0 denotes the baseline level and 1 denotes the test level. Let $\Omega^s(\mathcal{D})$ represent the collection of all $N \times s$ submatrices of \mathcal{D} – when the design being referred to is obvious, Ω^s is used. Further let $\alpha(\omega)$ denote the number of rows of $\omega \in \Omega^s$ that consist entirely of ones.

Mukerjee and Tang (2012) proved the following for $s = 2, \dots, m - 1$:

$$K_s = \frac{4}{N^2} (sT_1 + T_2), \tag{2.1}$$

where $T_1 = \sum_{\omega \in \Omega^s} (\alpha(\omega))^2$ and $T_2 = \sum_{\omega^* \in \Omega^{s+1}} \sum_{\omega^\circ \in \Omega^s(\omega^*)} (2\alpha(\omega^*) - \alpha(\omega^\circ))^2$.

This paper utilizes (2.1) to establish relationships between the word length pattern of a 2^{m-p} design and the sequence of K -values for a baseline design that is created from it.

In the literature, 2-level designs are most often represented by $(-1, +1)$ -arrays as this allows the model matrix (for the orthogonal parameterization) to be readily generated from the design matrix. A similar advantage is realized for the baseline parameterization if a baseline design matrix is represented by a (0, 1)-array. Table 1 contains the model matrices under both parameterizations for a 2^3 design. In each case, the design matrix is the submatrix formed by the main effect columns (shaded). For either design matrix, the interaction columns can be generated by multiplying together main effect columns – e.g. $AB = A \odot B$ where \odot denotes component-wise multiplication. Clearly the (0, 1)-design matrix

Table 2. The $(-1, +1)$ -design matrix and the corresponding $(0, 1)$ -design matrix for a 2^{5-2} design with defining relation $I = ABD = BCE = ACDE$.

A	B	C	D	E	A	B	C	D	E
-1	-1	-1	+1	+1	0	0	0	1	1
+1	-1	-1	-1	+1	1	0	0	0	1
-1	+1	-1	-1	-1	0	1	0	0	0
+1	+1	-1	+1	-1	1	1	0	1	0
-1	-1	+1	+1	-1	0	0	1	1	0
+1	-1	+1	-1	-1	1	0	1	0	0
-1	+1	+1	-1	+1	0	1	1	0	1
+1	+1	+1	+1	+1	1	1	1	1	1

can be created from the $(-1, +1)$ -design matrix by replacing -1 's with 0 's. However, this procedure does not generate the $(0, 1)$ -model matrix from the $(-1, +1)$ -model matrix as it fails to produce the correct interaction columns. This causes some minor complications when 2^{m-p} design matrices are converted to baseline designs by replacing -1 's with 0 's. Consider a 2^{5-2} design with full defining relation $I = ABD = BCE = ACDE$: Table 2 gives both forms of the design matrix. For the $(-1, +1)$ -array, the defining relation indicates that $A \odot B \odot D = B \odot C \odot E = A \odot C \odot D \odot E = 1_8$ (where 1_8 is a vector of ones) which is equivalent to saying that the ABD , BCE and $ACDE$ interactions are completely aliased with the grand mean. Note that the equivalent statement is not true for the $(0, 1)$ -array since, for example, $A \odot B \odot D = (0, 0, 0, 1, 0, 0, 0, 1)^t$. However, an analogous relationship exists for the $(0, 1)$ -array: the sum (mod 2) of any defining word set (a set of columns that corresponds to a word in the defining relation) is either 1_N or 0_N . For the example in Table 2, it can be readily verified that $A + B + D = B + C + E = 1_8 \pmod{2}$ and $A + C + D + E = 0_8 \pmod{2}$.

Our first result applies to all two-level designs (regular or non-regular) that are orthogonal arrays of strength 2 or greater. It uses the generalized word length pattern for G_2 -aberration as defined by Tang and Deng (1999). As their definition is for $(-1, +1)$ -arrays, we present an equivalent definition for $(0, 1)$ -arrays. Consider the set Ω^k of a $(0, 1)$ -matrix \mathcal{D} . For $\omega \in \Omega^k$, let $\psi(\omega)$ be the vector of row sums (mod 2) of ω and let $\Psi(\omega)$ be the sum of the elements of $\psi(\omega)$. Then define the J -characteristic of ω as

$$J_k(\omega) = |2\Psi(\omega) - N|.$$

If $\psi(\omega) = 0_N$ or 1_N then $\Psi(\omega) = 0$ or N and $J_k(\omega) = N$; if $\Psi(\omega) = N/2$ ($\psi(\omega)$ contains half zeros and half ones) then $J_k(\omega) = 0$. These are the only possibilities for a regular design. In fact for a regular design, if ω corresponds to

a defining word set, then $\psi(\omega) = 0_N$ or 1_N resulting in its J -characteristic being N , and it is 0 otherwise. For a non-regular design, $0 \leq J_k \leq N$ and there must be some (but not necessarily all) J_k such that $0 < J_k < N$.

Let the elements of the generalized word length pattern (B_3, B_4, \dots) for \mathcal{D} be

$$B_k(\mathcal{D}) = \sum_{\omega \in \Omega^k} \left(\frac{J_k(\omega)}{N} \right)^2.$$

It is clear that if \mathcal{D} is a regular design then $B_k(\mathcal{D})$ represents the number of words of length k in its defining relation and thus its generalized word length pattern is identical to its word length pattern.

3. Baseline Designs Created from Orthogonal Arrays

In this section we present three theorems that are useful when creating 2-level baseline designs from 2-level orthogonal arrays of strength ≥ 2 . Proofs are given in the Appendix.

Theorem 1. *Consider a (regular or non-regular) design \mathcal{D} that is an orthogonal array of strength $t - 1 \geq 2$. If this design is used to create a baseline design, then the (K_2, K_3, \dots) sequence satisfies:*

- (a) for $2 \leq v \leq t - 2$, $K_v = v \binom{m}{v} (1/2^{2v-2})$;
- (b) $K_{t-1} = (1/2^{2t-4}) \left[(t - 1) \binom{m}{t-1} + tB_t \right]$.

This is a useful connection between the generalized word length pattern and the sequence of K -values for baseline designs. For designs \mathcal{D}_1 and \mathcal{D}_2 that are orthogonal arrays of strength ≥ 2 , if \mathcal{D}_1 has more leading zeros in its generalized word length pattern than does \mathcal{D}_2 , then it has greater strength. Thus Theorem 1(a) indicates a baseline design based on \mathcal{D}_1 must have less K -aberration than one based on \mathcal{D}_2 . This is also true if \mathcal{D}_1 and \mathcal{D}_2 have the same number of leading zeros but the first non-zero term is smaller for \mathcal{D}_1 . Further it follows that the sequence

$$K_v = v \binom{m}{v} \frac{1}{2^{2v-2}} \quad \text{for } v = 2, 3, \dots$$

provides sequential lower bounds for the K -values of a minimum K -aberration design.

Now consider using 2^{m-p} designs to generate baseline designs. The runs in a 2^{m-p} design are uniquely determined by a set of p signed generators. These generators and their generalized interactions form the set of words that occur in the defining relation for the design. The aliasing in such a design is captured by the word length pattern denoted as (A_3, A_4, \dots) where A_j represents the number

of words of length j in the defining relation. There are 2^p possible combinations of signs for the generators and each combination produces a different design matrix – the different fractions from the same family of designs. Under the orthogonal parameterization these different fractions are equivalent in terms of aliasing in that they all have the same word length pattern. Once these fractions are converted to baseline designs, however, they are not necessarily equivalent in terms of aliasing under the baseline parameterization. However, the sequences of K -values are identical up to a certain term and only differ beyond that point.

A 2^{m-p} design of resolution t is an orthogonal array of strength $t - 1$. Thus Theorem 1 can be used ($A_t = B_t$) to find K_v for $v = 2, 3, \dots, t - 1$. As 2^{m-p} designs have more structure than non-regular designs we can extend the results to cover K_t . For a baseline design based on a 2^{m-p} design matrix, $\psi(\omega) = 1_N$ or 0_N for any submatrix ω that is a defining word set. To distinguish these cases, we let A_j^0 and A_j^1 represent the number of j -factor defining word sets for which $\psi(\omega) = 0_N$ and $\psi(\omega) = 1_N$ respectively. Hence $A_j^0 + A_j^1 = A_j$.

Theorem 2. *If a 2^{m-p} design of resolution t is used to create a baseline design, the value of K_t can be calculated as follows. For t odd:*

$$K_t = \frac{1}{2^{2t-2}} \left[t \binom{m}{t} + (t+1)A_{t+1} + t(m-t-1)A_t^0 + t(m-t+3)A_t^1 \right].$$

For t even:

$$K_t = \frac{1}{2^{2t-2}} \left[t \binom{m}{t} + (t+1)A_{t+1} + t(m-t+3)A_t^0 + t(m-t-1)A_t^1 \right].$$

Theorem 2 provides information on how to choose the particular fraction of a given family of 2^{m-p} designs to achieve the least possible K -aberration. If A_t is the first non-zero entry in the word length pattern, then the K -aberration depends on the values of A_t^0 and A_t^1 . Thus the selected fraction should maximise A_t^0 for t odd and A_t^1 for t even. For t odd, the fraction that contains a row of zeros will always have $A_t^0 = A_t$ (and consequently $A_t^1 = 0$) since it has $\psi = 0$ for all defining word sets of size t .

Consider using a resolution III 2^{m-p} design to create a baseline design. Theorems 1(b) and 2 can be applied to give expressions for K_2 and K_3 . It is also possible to extend the results to cover the value of K_4 .

Theorem 3. *Consider a 2^{m-p} design of resolution III. If a fraction of this design that has $A_3^0 = A_3$ is used to create a baseline design, then*

$$K_4 = \frac{1}{64} \left[4 \binom{m}{4} + 5A_5 + 4(m-1)A_4^0 + 4(m-5)A_4^1 + \frac{(m-3)(3m-20)}{2} A_3 - 6A_* \right],$$

where A_* is the number of pairs of 3-column defining word sets that have one column in common.

For a resolution III 2^{m-p} design used to create a baseline design, a design with the smallest possible value of A_3 should be used to minimize K_2 . If more than one such design exists, then the one that has the smallest value of A_4 should be used and a fraction selected such that $A_3^0 = A_3$ as this will minimize K_3 . If more than one optimal choice still exists, then Theorem 3 can be used to identify the option with the smaller value of K_4 . In this case, it is best to minimize $5A_5 - 6A_*$ and then select a fraction that has as many 4-column defining word sets as possible with row sums equal to 1 (mod 2) given that all 3-column defining word sets have row sums equal to 0 (mod 2).

4. Application

To demonstrate the application of our results, we consider the creation of a baseline design for 9 factors in 16 runs. Our procedure starts by looking at tables of non-isomorphic 2^{m-p} designs such as those given in Chen, Sun, and Wu (1993). They identify the different isomorphism classes and give one 2^{m-p} design from each class. The term isomorphic when applied to 2^{m-p} designs has the standard definition: two designs are isomorphic if the design matrix of one can be obtained from that of the other through a combination of row permutations, column permutations, and interchanging the levels for one or more factors. However, Mukerjee and Tang (2012) pointed out that interchanging levels can affect the properties (including the sequence of K -values) of baseline designs. For baseline designs a more suitable definition is: *two designs are isomorphic if the design matrix of one can be obtained from that of the other through a combination of row permutations and column permutations*. We use the terms combinatorially isomorphic (for the standard definition) and baseline isomorphic. If a single 2^{m-p} design from an isomorphism class is considered, not all of the possible baseline designs in that class are covered. Our approach considers all of the fractions in the family of designs defined by the set of generators and thus does cover the baseline isomorphism classes contained in the combinatorial isomorphism class. Consider two 2^{m-p} designs \mathcal{D}_1 and \mathcal{D}_2 that are in the same isomorphism class. Although \mathcal{D}_2 is not necessarily baseline isomorphic to \mathcal{D}_1 it must be baseline isomorphic to a design that is in the same family as \mathcal{D}_1 . To see this, consider a sequence of row permutations, column permutations and level interchanges that transforms \mathcal{D}_1 to \mathcal{D}_2 . If all of the level interchanges are performed first, then a design that is in the same family as \mathcal{D}_1 is created as an intermediate step. Clearly, \mathcal{D}_2 can be produced from this intermediate design using just row permutations and column permutations. For the rest of this section, the term isomorphic applied to 2^{m-p} designs always has the standard definition and $\psi(ABC)$ is used to denote the vector of row sums (mod 2) of the ABC defining word set.

Consider using the minimum aberration 2^{9-5} design to produce a baseline design. This design can be found in Chen, Sun, and Wu (1993) and has word length pattern $(4, 14, 8, 0, 4, 1, 0)$. There is no need to consider any other (non-isomorphic) 2^{9-5} design since all such designs have larger values of A_3 and thus, by Theorem 1(b), produce baseline designs with larger values of K_2 .

For the minimum aberration 2^{9-5} design $A_3 = 4$ and so applying Theorem 1(b) gives:

$$K_2 = \frac{1}{4}m(m-1) + \frac{3}{4}A_3 = \frac{1}{4}9 \times 8 + \frac{3}{4}4 = 21.$$

This value of K_2 applies to any baseline design created using one of the 32 possible fractions for this 2^{9-5} design. The expression for K_3 in Theorem 2 depends on A_3^0 and A_3^1 which depend on the specific fraction that is chosen. A fraction that has $A_3^0 = A_3$ and $A_3^1 = 0$ should be used – as noted previously at least one such fraction always exists. For our example, one possible set of generators is $\{ABE, ACF, ADG, AHJ, BCDH\}$ and only the two fractions that have $\psi(ABE) = \psi(ACF) = \psi(ADG) = \psi(AHJ) = 0_N$ have the desired property. One of these has $\psi(BCDH) = 0_N$ and the other one has $\psi(BCDH) = 1_N$. For both $A_3^0 = 4$ and $A_3^1 = 0$ and, from Theorem 2,

$$K_3 = \frac{1}{16} \left[3 \binom{m}{3} + 4A_4 + 3(m-4)A_3^0 + 3mA_3^1 \right] = 23.$$

The choice has been narrowed to two specific fractions. Values of A_5, A_*, A_4^0 and A_4^1 are needed to apply Theorem 3. Clearly $A_5 = 8$ for both fractions. As the generalized interaction of any pair of the 3-column generators gives a 4-column effect, it follows that $A_* = 6$ for both fractions. The values of A_4^0 and A_4^1 differ for the two fractions. If the fraction with $\psi(BCDH) = 0_N$ is used, then all generalized interactions between the generators must have row sums equal to 0 (mod 2) and thus $A_4^0 = 14$ and $A_4^1 = 0$. If the $\psi(BCDH) = 1_N$ fraction is used, then $A_4^0 = 6$ and $A_4^1 = 8$. Applying Theorem 3 reveals that this second fraction has the smaller value of K_4 :

$$K_4 = \frac{1}{64} \left[4 \binom{m}{4} + 5A_5 + 4(m-1)A_4^0 + 4(m-5)A_4^1 + \frac{(m-3)(3m-20)}{2}A_3 - 6A_* \right] = 14.25.$$

For the $\psi(BCDH) = 0_N$ fraction $K_4 = 16.25$.

Thus the best (smallest K -aberration) baseline design is obtained by setting the generators for the minimum aberration 2^{9-5} design as

$$\psi(ABE) = \psi(ACF) = \psi(ADG) = \psi(AHJ) = 0_N, \quad \psi(BCDH) = 1_N.$$

Table 3. For N -run m -factor designs, the baseline design created using the minimum aberration regular design has a K -sequence that is identical to that for the minimum K -aberration design, up to and including term K_{r-1} .

$N = 32$ runs		$N = 64$ runs	
m	K_{t-1}	m	K_{r-1}
6	K_5	7	K_6
7-16	K_3	8	K_4
17-29	K_2	9-32	K_3
		33-61	K_2

The full sequence of K -values for this design is 21, 23, 14.25, 4.5, 0.5625, 0, 0, 0.

5. Concluding Remarks

The question arises of how the designs produced using our results compare to the minimum K -aberration design over all possible baseline designs. Mukerjee and Tang (2012) identified minimum K -aberration designs for all 16-run m -factor scenarios. The minimum K -aberration design that they found for 9 factors is isomorphic to the design generated in the previous section. Thus our approach found an optimal 9-factor 16-run baseline design – there are other non-isomorphic 9-factor 16-run designs that can be created using non-regular designs that are also minimum K -aberration designs. All the other minimum K -aberration m -factor 16-run designs reported in Mukerjee and Tang (2012) can also be created from 2^{m-p} designs using our approach. Thus we conclude that, for 16-run designs, the proposed method always finds a minimum K -aberration design.

For larger run sizes, we cannot guarantee that this is necessarily the case. To our knowledge for $N = 32$, no non-regular designs have yet been identified that have either more leading 0's, or the same number of leading 0's and a smaller first non-zero term in their generalized word length patterns than that for the minimum aberration regular designs. A similar statement is true for $N = 64$ with the exception of the 13-factor and the 14-factor cases (see below). Under these circumstances Theorem 1 guarantees that if the minimum aberration regular design is of resolution t , then its K -sequence is identical to that for the minimum K -aberration design up to and including term K_{t-1} . Table 3 contains the values of K_{t-1} for 32 and 64 run designs.

It is always the case that K_2 is optimal and, for $m \leq N/2$, both K_2 and K_3 are always optimal (except for the 13-factor and the 14-factor 64-run designs). For $m = N - 1$ and $m = N - 2$ Mukerjee and Tang (2012) described a method of producing minimum K -aberration designs starting with any saturated orthogonal array of strength 2 (including saturated regular designs).

For the 13-factor and the 14-factor 64-run case Xu and Wong (2007) report nonregular designs that have less G_2 -aberration than the minimum aberration

regular designs. For the 13-factor case the generalized word length pattern for the nonregular design is $(0, 10, 36, \dots)$, whereas that for the minimum aberration regular design is $(0, 14, 28, \dots)$. Using Theorem 1, a baseline design created from the nonregular design has $K_2 = 39$ and $K_3 = 56.125$ compared to $K_2 = 39$ and $K_3 = 57.125$ for one created from the regular design. For the 14-factor case the generalized word length pattern is $(0, 14, 56, \dots)$ for the nonregular design and $(0, 22, 40, \dots)$ for the minimum aberration regular design. As a result $K_2 = 45.5$ and $K_3 = 71.75$ for the nonregular design, and $K_2 = 45.5$ and $K_3 = 73.75$ for the regular design.

In general Theorem 1 indicates that in searching for good baseline designs, it is advisable to start with designs that are optimal (or nearly optimal) in terms of G_2 -aberration. The minimum aberration regular designs usually fall into this category especially for moderate run sizes ($N \leq 64$). As run size increases, there may be more of an advantage to using a nonregular design. For many cases, the optimal G_2 -aberration design is not known so it makes sense to use the “current best known design.” For example, for designs with $N = 128$ or 256 runs Xu and Wong (2007) report a number of cases where non-regular designs exist that have less G_2 -aberration than the minimum aberration regular design.

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Appendix

Preliminary Results

The following results are essential for the proofs that follow. Their proofs are omitted as straight forward.

PR1 Consider any two-level design and let ω be a submatrix formed by c of its columns. If ω is an OA (orthogonal array) of strength c then $\alpha(\omega) = N/2^c$.

PR2 When applying (2.1), if a design forms an OA of strength c and $s \leq c$, then $T_1 = \binom{m}{s}(N^2/2^{2s})$.

PR3 In the calculation of T_2 it is only necessary to consider those ω^* in Ω^{s+1} that are not OA’s of strength $s + 1$. Further if the design being considered is an OA of strength $s + 1$ then $T_2 = 0$.

Proof of Theorem 1(a). Consider (2.1), $K_v = (4/N^2)(vT_1 + T_2)$. Since $B_j = 0$ for all $j < t$, \mathcal{D} must be an OA of strength $t - 1$. Thus for $v \leq t - 2$ we have $T_1 = \binom{m}{v}N^2/2^{2v}$ from PR2 and $T_2 = 0$ from PR3. Substituting these expressions into the equation gives the result.

Proof of Theorem 1(b). Since the design is an OA of strength $t - 1$, for equation (2.1) we have $T_1 = \binom{m}{t-1} N^2 / 2^{2t-2}$ by PR2.

To find T_2 , PR3 indicates that we need only consider those $\omega^* \in \Omega^t$ that are not OA's of strength t . Since the design is an OA of strength $t - 1$, Proposition 2 from Deng and Tang (1999) applies – this proposition is a refinement of a result in Cheng (1995). The first part of this proposition establishes that ω^* is an OA of strength t if and only if $J_t(\omega^*) = 0$ (and thus any such ω^* does not contribute to T_2). The second part of the proposition indicates that if $J_t(\omega^*) \neq 0$ then the rows of ω^* must consist of $(N - J_t(\omega^*)) / 2^t$ copies of the complete 2^t factorial plus $J_t(\omega^*) / 2^{t-1}$ copies of a (resolution t) half replicate of the 2^t factorial. For those ω^* with $J_t(\omega^*) \neq 0$ divide the rows into two parts with ω_1^* being the rows that consist of the copies of the complete 2^t factorial and ω_2^* being the rows that consist of the copies of the half replicate. As ω_1^* is an OA of strength t , the net contribution of these rows to T_2 is zero. For the rows in ω_2^* there are four possible cases created by $\psi(\omega_2^*) = 0_N$ or $\psi(\omega_2^*) = 1_N$ and t being odd or even. Consider the case where $\psi(\omega_2^*) = 0_N$ and t is odd. As there are no rows that contain all ones $\alpha(\omega_2^*) = 0$. Further, each row that contains one zero and $t - 1$ ones occurs $J_t(\omega^*) / 2^{t-1}$ times which means that $\alpha(\omega^\circ) = J_t(\omega^*) / 2^{t-1}$ for each $\omega^\circ \in \Omega^{t-1}(\omega_2^*)$. Thus $2\alpha(\omega^*) - \alpha(\omega^\circ) = -J_t(\omega^*) / 2^{t-1}$. The other three cases can be similarly dealt giving the following results:

Case	$\alpha(\omega^*)$	$\alpha(\omega^\circ)$	$2\alpha(\omega^*) - \alpha(\omega^\circ)$
$\psi(\omega_2^*) = 0_N$ for t odd	0	$J_t(\omega^*) / 2^{t-1}$	$-J_t(\omega^*) / 2^{t-1}$
$\psi(\omega_2^*) = 0_N$ for t even	$J_t(\omega^*) / 2^{t-1}$	$J_t(\omega^*) / 2^{t-1}$	$J_t(\omega^*) / 2^{t-1}$
$\psi(\omega_2^*) = 1_N$ for t odd	$J_t(\omega^*) / 2^{t-1}$	$J_t(\omega^*) / 2^{t-1}$	$J_t(\omega^*) / 2^{t-1}$
$\psi(\omega_2^*) = 1_N$ for t even	0	$J_t(\omega^*) / 2^{t-1}$	$-J_t(\omega^*) / 2^{t-1}$

All four cases end up making the same contribution to T_2 and thus we get:

$$\begin{aligned}
 T_2 &= \sum_{\omega^* \in \Omega^t} \sum_{\omega^\circ \in \Omega^{t-1}(\omega^*)} \left(2\alpha(\omega^*) - \alpha(\omega^\circ) \right)^2 \\
 &= \sum_{\omega^* \in \Omega^t} t \left(\frac{J_t(\omega^*)}{2^{t-1}} \right)^2 \\
 &= t \left(\frac{N^2}{2^{2t-2}} \right) \sum_{\omega^* \in \Omega^t} \left(\frac{J_t(\omega^*)}{N} \right)^2 \\
 &= t \left(\frac{N^2}{2^{2t-2}} \right) B_t.
 \end{aligned}$$

Plugging in the derived expressions for T_1 and T_2 into the expression for K_{t-1} gives the result.

Proof of Theorem 2. First consider the calculation of T_1 in (2.1). Any set of c columns from a 2^{m-p} design forms an OA of strength c if and only if it does not contain a defining word set – see Cheng (2014, pp. 147-151). As A_t is the first non-zero term in the word length pattern there are three possible cases for $\omega \in \Omega^t$: (i) the columns of ω are not a defining word set and thus ω is an OA of strength t , (ii) the columns of ω are a defining word set and $\psi = 0_N$ and (iii) the columns of ω are a defining word set and $\psi = 1_N$. There is a total of $\binom{m}{t}$ elements in Ω^t of which A_t^0 fall under (ii), A_t^1 fall under (iii), and the rest under (i). For (i), PR1 gives $\alpha(\omega) = N/2^t$. For cases (ii) and (iii), ω is a half fraction of a 2^t design and thus $\alpha(\omega) = 0$ or $N/2^{t-1}$ depending on whether or not ω contains a row of ones. The following table summarizes the results.

	$\alpha(\omega)$ for t odd	$\alpha(\omega)$ for t even	number
(i)	$N/2^t$	$N/2^t$	$\binom{m}{t} - A_t^0 - A_t^1$
(ii)	0	$N/2^{t-1}$	A_t^0
(iii)	$N/2^{t-1}$	0	A_t^1

Thus we get

$$\begin{aligned} \text{For } t \text{ odd} \quad T_1 &= \frac{N^2}{2^{2t}} \left(\binom{m}{t} - A_t^0 + 3A_t^1 \right), \\ \text{For } t \text{ even} \quad T_1 &= \frac{N^2}{2^{2t}} \left(\binom{m}{t} + 3A_t^0 - A_t^1 \right). \end{aligned}$$

Consider T_2 . Applying PR3, we only need consider those $\omega^* \in \Omega^{t+1}$ that are not OA's of strength $t + 1$. These ω^* are those whose columns contain a defining word set. For $\omega^* \in \Omega^{t+1}$ it is possible that ω^* could either be a defining word set of size $t + 1$ or contain a defining word set of size t . Since $A_j = 0$ for all $j < t$, ω^* cannot contain more than one defining word set. For the columns of ω^* that are in the defining word set ψ is either 0_N or 1_N . There are four cases to consider: (i) ω^* is a defining word set of size $t + 1$ with $\psi(\omega^*) = 0_N$, (ii) ω^* is a defining word set of size $t + 1$ with $\psi(\omega^*) = 1_N$, (iii) ω^* contains a defining word set of size t with $\psi = 0_N$ for the defining word set, and (iv) ω^* contains a defining word set of size t with $\psi = 1_N$ for the defining word set. The number of $\omega^* \in \Omega^{t+1}$ that correspond to these cases is (i) A_{t+1}^0 , (ii) A_{t+1}^1 , (iii) $(m - t)A_t^0$ and (iv) $(m - t)A_t^1$. Again, different values of $\alpha(\omega^*)$ and $\alpha(\omega^\circ)$ can occur for t odd and t even.

Consider t odd. The following table contains examples of $\omega^* \in \Omega^{t+1}$ for each of the four cases when $t = 3$ and $N = 8$. For cases (iii) and (iv) it is the first three columns of ω^* that form the defining word set.

case (i)	case (ii)	case (iii)	case (iv)
0 0 0 0	0 0 0 1	0 0 0 0	0 0 1 0
1 0 0 1	1 0 0 0	0 0 0 1	0 0 1 1
0 1 0 1	0 1 0 0	1 0 1 0	1 0 0 0
1 1 0 0	1 1 0 1	1 0 1 1	1 0 0 1
0 0 1 1	0 0 1 0	0 1 1 0	0 1 0 0
1 0 1 0	1 0 1 1	0 1 1 1	0 1 0 1
0 1 1 0	0 1 1 1	1 1 0 0	1 1 1 0
1 1 1 1	1 1 1 0	1 1 0 1	1 1 1 1

The values of $\alpha(\omega^*)$, $\alpha(\omega^\circ)$, and $2\alpha(\omega^*) - \alpha(\omega^\circ)$ needed to find T_2 for $t = 3$ and $N = 8$ can be readily deduced from these tables and it is straight forward to extend these to general odd t and N . For cases (iii) and (iv) the value of $\alpha(\omega^\circ)$ for $\omega^\circ \in \Omega^t(\omega^*)$ depends on whether ω° is the defining word set or not. In the following table we summarize the results for odd t and give the number of $\omega^\circ \in \Omega^t(\omega^*)$ that result in each value in brackets.

case	$\alpha(\omega^*)$	$\alpha(\omega^\circ)$	$2\alpha(\omega^*) - \alpha(\omega^\circ)$
(i)	$N/2^t$	$N/2^t [\times t + 1]$	$N/2^t [\times(t + 1)]$
(ii)	0	$N/2^t [\times t + 1]$	$-N/2^t [\times(t + 1)]$
(iii)	0	$0 [\times 1]$ or $N/2^t [\times t]$	$0 [\times 1]$ or $-N/2^t [\times t]$
(iv)	$N/2^t$	$N/2^{t-1} [\times 1]$ or $N/2^t [\times t]$	$0 [\times 1]$ or $N/2^t [\times t]$

Similarly, for t even we get:

case	$\alpha(\omega^*)$	$\alpha(\omega^\circ)$	$2\alpha(\omega^*) - \alpha(\omega^\circ)$
(i)	0	$N/2^t [\times(t + 1)]$	$-N/2^t [\times(t + 1)]$
(ii)	$N/2^t$	$N/2^t [\times(t + 1)]$	$N/2^t [\times(t + 1)]$
(iii)	$N/2^t$	$N/2^{t-1} [\times 1]$ or $N/2^t [\times t]$	$0 [\times 1]$ or $N/2^t [\times t]$
(iv)	0	$0 [\times 1]$ or $N/2^t [\times t]$	$0 [\times 1]$ or $-N/2^t [\times t]$

For both t odd and t even, the expression for T_2 is

$$\begin{aligned}
 T_2 &= \frac{N^2}{2^{2t}} \left((t + 1) A_{t+1}^0 + (t + 1) A_{t+1}^1 + t(m - t) A_t^0 + t(m - t) A_t^1 \right) \\
 &= \frac{N^2}{2^{2t}} \left((t + 1) A_{t+1} + t(m - t) A_t^0 + t(m - t) A_t^1 \right).
 \end{aligned}$$

Combining these expressions with those obtained for T_1 gives the result.

Proof of Theorem 3. Considering T_1 in (2.1), there are four cases for $\omega \in \Omega^4$: (i) four independent columns, (ii) a 4-column defining word set with $\psi = 0_N$, (iii) a 4-column defining word set with $\psi = 1_N$ and (iv) contains a 3-column defining word set with $\psi = 0_N$. The following results can be deduced:

	$\alpha(\omega)$	number
(i)	$N/16$	$\binom{m}{4} - A_4^0 - A_4^1 - (m-3)A_3$
(ii)	$N/8$	A_4^0
(iii)	0	A_4^1
(iv)	0	$(m-3)A_3$

Thus we have

$$\begin{aligned}
 T_1 &= \left(\frac{N}{16}\right)^2 \left(\binom{m}{4} - A_4^0 - A_4^1 - (m-3)A_3 \right) + \left(\frac{N}{8}\right)^2 A_4^0 \\
 &= \left(\frac{N}{16}\right)^2 \left(\binom{m}{4} + 3A_4^0 - A_4^1 - (m-3)A_3 \right).
 \end{aligned}$$

Now consider T_2 . Again using PR3, we only need consider those $\omega^* \in \Omega^5$ that have linearly dependent columns. There are six such possible cases: (i) ω^* is a 5-column defining word set with $\psi = 0_N$, (ii) ω^* is a 5-column defining word set with $\psi = 1_N$, (iii) ω^* contains a 4-column defining word set with $\psi = 0_N$, (iv) ω^* contains a 4-column defining word set with $\psi = 1_N$, (v) ω^* contains a 3-column defining word set with $\psi = 0_N$ and (vi) ω^* contains two 3-column defining word sets and one 4-column defining word set. Note that (vi) occurs if and only if there are two 3-column defining word sets which have one column in common. For example if 123 and 345 are words in the defining relation then 1245 is also in the defining relation and the set of columns $\{1, 2, 3, 4, 5\}$ form a ω^* that satisfies case (vi). Further for (vi), since the two 3-column defining word sets both have $\psi = 0_N$, the 4-column defining word set must also have $\psi = 0_N$.

The values of $\alpha(\omega^*)$, $\alpha(\omega^\circ)$, and $2\alpha(\omega^*) - \alpha(\omega^\circ)$ for each of these cases are as follows.

	$\alpha(\omega^*)$	$\alpha(\omega^\circ)$	$2\alpha(\omega^*) - \alpha(\omega^\circ)$
(i)	0	$N/16$ [$\times 5$]	$-N/16$ [$\times 5$]
(ii)	$N/16$	$N/16$ [$\times 5$]	$N/16$ [$\times 5$]
(iii)	$N/16$	$N/8$ [$\times 1$] or $N/16$ [$\times 4$]	0 [$\times 1$] or $N/16$ [$\times 4$]
(iv)	0	0 [$\times 1$] or $N/16$ [$\times 4$]	0 [$\times 1$] or $-N/16$ [$\times 4$]
(v)	0	0 [$\times 2$] or $N/16$ [$\times 3$]	0 [$\times 2$] or $-N/16$ [$\times 3$]
(vi)	0	0 [$\times 4$] or $N/8$ [$\times 1$]	0 [$\times 4$] or $-N/8$ [$\times 1$]

Now consider the number of times each of (i) through (vi) occurs for $\omega^* \in \Omega^5$. Let A_* represent the number of times (vi) occurs. Then the results are: (i) A_5^0 , (ii) A_5^1 , (iii) $(m-4)A_4^0 - A_*$, (iv) $(m-4)A_4^1$, (v) $\binom{m-3}{2}A_3 - 2A_*$ and (vi) A_* . The results for (i), (ii) and (iv) are obvious. For (iii) consider that any 4-column defining word set occurs in $m-4$ elements of Ω^5 and that, if a particular 4-column defining word set is the product of two 3-column defining word sets, then

exactly one of these corresponds to (vi). For (v) consider that any 3-column defining word set occurs in $\binom{m-3}{2}$ elements of Ω^5 . If two of these have a column in common then at least one of them occurs in a total of $\binom{m-3}{2} - 1$ elements of Ω^5 , and of these one corresponds to (vi).

Thus we have

$$\begin{aligned} T_2 &= \left(\frac{N}{16}\right)^2 \left(5A_5 + 4[(m-4)A_4 - A_*] + 3 \left[\binom{m-3}{2} A_3 - 2A_* \right] \right) + \left(\frac{N}{8}\right)^2 A_* \\ &= \left(\frac{N}{16}\right)^2 \left(5A_5 + 4(m-4)A_4 + 3 \binom{m-3}{2} A_3 - 6A_* \right). \end{aligned}$$

Plugging the expressions for T_1 and T_2 into that for K_4 and simplifying gives the result.

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