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A GENERAL THEORY OF MINIMUM ABERRATION AND ITS APPLICATIONS[1]

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Minimum aberration is an increasingly popular criterion for comparing and assessing fractional factorial designs, and few would question its importance and usefulness nowadays. In the past decade or so, a great deal of work has been done on minimum aberration and its various extensions. This paper develops a general theory of minimum aberration based on a sound statistical principle. Our theory provides a unified framework for minimum aberration and further extends the existing work in the area. More importantly, the theory offers a systematic method that enables experimenters to derive their own aberration criteria. Our general theory also brings together two seemingly separate research areas: one on minimum aberration designs and the other on designs with requirement sets. To facilitate the design construction, we develop a complementary design theory for quite a general class of aberration criteria. As an immediate application, we present some construction results on a weak version of this class of criteria.

1. Introduction. The general problem considered in this paper is how to select the "best" fractional factorial designs. In situations where we have little or no knowledge about the effects that are potentially important, it is appropriate to select designs using the minimum aberration criterion [Fries and Hunter (1980)]. Wu and Hamada (2000) contains tables of many known minimum aberration designs. Minimum aberration designs enjoy some attractive robust properties [Cheng, Steinberg and Sun (1999) and Tang and Deng (1999)]. Much work has been done on the construction of minimum aberration designs. For details, we refer to Franklin (1984), Chen and Wu (1991), Chen (1992), Chen and Hedayat (1996), Tang and Wu (1996), Suen, Chen and Wu (1997) and many others. Sitter, Chen and Feder (1997), Chen and Cheng (1999) and Cheng and Wu (2002) developed aberration criteria for blocked fractional factorials. A projective geometric approach to blocking fractional factorials is considered in Mukerjee and Wu (1999), and blocked fractional factorials with maximum estimation capacity are studied by Cheng and Mukerjee (2001). Wu and Zhu (2003) examined the use of a minimum aberration criterion for design selection in robust parameter design.

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Developing a general theory of minimum aberration is motivated by the desire to unify various versions of minimum aberration that have recently appeared in the literature. Based on a sound statistical principle, this paper develops a general theory of minimum aberration and discusses its various applications. In addition to building a unified framework for many of the existing aberration criteria, the theory provides a method for deriving other aberration criteria that may be more appropriate for given design situations. A minimum aberration design can be called a model robust design because of its robust properties. A design with a requirement set [Greenfield (1976)] is a model specific design since such a design specifies a set of effects to be estimated. Our general theory is capable of bringing together these seemingly unrelated two classes of designs.

We will focus our discussion on two-level regular fractional factorial designs. However, most of our arguments are quite general. Section 2 motivates, introduces and studies a general criterion of minimum aberration and discusses its application to blocked fractional factorials, and to fractional factorials when some 2-factor interactions are important. Section 3 is devoted to developing a theory of complementary designs for quite a general class of aberration criteria, and presents some construction results on weak aberration.

In what follows, we introduce some notation and definitions to set the stage for the later development. A regular 2^{m-p} design has m factors each at two levels and $n = 2^{m-p}$ runs, and is completely determined by p independent defining words. The two levels are denoted by $+1$ and -1, so the design matrix D of such a design is an $n \times m$ matrix of ± 1. The defining relation of a 2^{m-p} design is the complete set of defining words. Labels of factors are referred to as letters. A defining word specifies a set of letters that has the property that the product of the corresponding columns of D is a column of all plus ones. Including I, the column of all ones, the defining relation of a 2^{m-p} design has 2^p defining words. Let $A_i(D)$ be the number of defining words of length i in the defining relation of design D, where the length of a word is the number of letters in the word. The resolution of design D is the integer R such that $A_i(D) = 0$ for $i = 1, \dots, R-1$ and $A_R(D) > 0$. The minimum aberration criterion selects designs that sequentially minimize $A_1(D), \dots, A_m(D)$. For designs of resolution at least III, we have $A_1 = A_2 = 0$, so the minimum aberration criterion selects designs that sequentially minimize $A_3(D), \dots, A_m(D)$.

2. General theory of minimum aberration and its applications.

2.1. *A general criterion of minimum aberration.* Besides the grand mean γ_0, there are in all $2^m - 1$ factorial effects in a 2^{m-p} design. Suppose that out of the $2^m - 1$ effects, we are interested in estimating a set of effects γ_1. Then the fitted model is given by

$$Y = \gamma_0 I + W_1 \gamma_1 + \varepsilon, \tag{1}$$

where Y denotes the vector of n observations, γ_1 the vector of the effects to be estimated, W_1 the model matrix corresponding to γ_1 and ε the vector of uncorrelated random errors, assumed to have a zero mean and a constant variance. Because the remaining effects may not be negligible, we should choose a design that minimizes their contamination on the estimation of γ_1, from among all designs allowing estimation of the model in (1). Suppose that prior knowledge enables us to divide these remaining effects into $J-1$ groups, denoted by $\gamma_2, \dots, \gamma_J$, in such a way that the effects in γ_j are more important than those in γ_{j+1}, for $j = 2, \dots, J-1$. Then the true model can be written as

$$Y = \gamma_0 I + W_1\gamma_1 + W_2\gamma_2 + \cdots + W_J\gamma_J + \varepsilon, \tag{2}$$

where W_j is the model matrix corresponding to γ_j for $j = 1, \dots, J$. The least-squares solution $\hat{\gamma}_1 = (W_1^T W_1)^{-1} W_1^T Y = n^{-1} W_1^T Y$ from the fitted model in (1) has expectation, taken under the true model in (2), $E(\hat{\gamma}_1) = \gamma_1 + C_2\gamma_2 + \cdots + C_J\gamma_J$, where $C_j = n^{-1} W_1^T W_j$ for $j \geq 2$. So the bias of $\hat{\gamma}_1$ in estimating γ_1 is $C_2\gamma_2 + \cdots + C_J\gamma_J$. Note that $C_j\gamma_j$ represents the contribution of γ_j to the bias. As γ_j is unknown, we will have to work with C_j. One size measure for a matrix $C = (c_{ij})$ is given by $\|C\|^2 \stackrel{\text{def}}{=} \operatorname{trace}(C^T C) = \sum_{i,j} c_{ij}^2$. Since the effects in γ_j are more important than those in γ_{j+1}, to minimize the bias of $\hat{\gamma}_1$, heuristically we can sequentially minimize $\|C_2\|^2, \dots, \|C_J\|^2$. For regular designs, the entries of C_j are either 0 or 1, and therefore $N_j = \|C_j\|^2$ is simply the number of effects in γ_j that are aliased with those in γ_1, for $j = 2, \dots, J$. Two effects are aliased (or confounded) with each other if their corresponding columns in the model matrix are identical.

DEFINITION 1. The general criterion of aberration is defined as the one that selects designs by sequentially minimizing $N_2, \dots, N_J$, where N_j is the number of effects in γ_j that are aliased with those in γ_1, for $j = 2, \dots, J$.

For convenience, the vector $(N_2, \dots, N_J)$ is called the word length pattern with respect to $(\gamma_1, \gamma_2, \dots, \gamma_J)$. An immediate application is to the situation where γ_1 are the main effects and γ_j are the j-factor interactions. In this case, we have

$$N_j = (j+1)A_{j+1} + (m-j+1)A_{j-1} \tag{3}$$

for $2 \leq j \leq m-1$, and $N_m = A_{m-1}$, where A_j is the number of defining words of length j as introduced in Section 1. The relationship in (3) leads to the conclusion that sequentially minimizing $N_2, N_3, \dots$ is equivalent to sequentially minimizing $A_3, A_4, \dots$.

LEMMA 1. *If γ_1 are the main effects and γ_j are the j-factor interactions, then the general criterion of aberration, given in Definition 1, is equivalent to the usual criterion of aberration.*

The essential result in Lemma 1 was first given by Tang and Deng (1999), who in fact presented their result under a more general framework, where both regular and nonregular designs are considered. Superficially, Lemma 1 provides a statistical justification for the usual criterion of aberration, which was originally defined from the combinatorial point of view. A message running a bit deeper here is that the usual minimum aberration criterion of combinatorial nature can in fact be *derived* from a general theory based on a sound statistical principle.

A more general result than Lemma 1 can easily be obtained. Let γ_1 be the main effects and all the interactions involving up to q factors. For the model in (1) to be estimable, a design of resolution $2q+1$ must exist, which implies that $A_i = 0$ for $i = 1, \dots, 2q$. Now let γ_j be the $(q-1+j)$-factor interactions for $j \geq 2$. We can easily show that

$$\begin{aligned} N_j = {} & \sum_{i=1}^{q} \binom{q-1+j+i}{i} A_{q-1+j+i} \\ & + \sum_{i=1}^{q} \binom{q-3+j+i}{i-1} \binom{m-(q-3+j+i)}{1} A_{q-3+j+i} \\ & + \sum_{i=2}^{q} \binom{q-5+j+i}{i-2} \binom{m-(q-5+j+i)}{2} A_{q-5+j+i} + \cdots. \end{aligned} \tag{4}$$

Since $A_i = 0$ for $i = 1, \dots, 2q$, we have

$$N_2 = \binom{2q+1}{q} A_{2q+1}, \qquad N_3 = \binom{2q+2}{q} A_{2q+2} + \binom{2q+1}{q-1} A_{2q+1},$$

and so on. Noting that the leading term for N_j in (4) is given by $\binom{2q-1+j}{q} A_{2q-1+j}$, we conclude that sequentially minimizing $N_2, N_3, \dots$ is equivalent to sequentially minimizing $A_{2q+1}, A_{2q+2}, \dots$. This establishes the following result.

THEOREM 1. *If γ_1 are the main effects and all the interactions involving up to q factors, and γ_j are the $(q-1+j)$-factor interactions for $j \geq 2$, then the general criterion of aberration gives rise to the usual criterion of aberration that sequentially minimizes $A_{2q+1}, A_{2q+2}, \dots$ among all designs of resolution $2q+1$.*

2.2. *Application to blocked fractional factorials.* In addition to m treatment factors, a blocked fractional factorial contains m_1 blocking factors. The main effects of blocking factors are block effects. So are the interactions of blocking factors. Therefore, the total number of block effects produced by m_1 blocking factors is $2^{m_1} - 1$.

To avoid confusion, the terms "factor" and "effect" are carefully used in this paper. We stick to the meanings of the terms as in the following: a factor has a main effect, two factors have a 2-factor interaction (effect), three factors have a

3-factor interaction (effect) and so on. We therefore speak of m_1 blocking factors and $2^{m_1}-1$ block effects.

A basic requirement for blocked fractional factorials is that all the $2^{m_1}-1$ block effects should be included in the fitted model. In addition, interactions between treatment and blocking factors are assumed to be nonexistent, which is necessary for the effectiveness of blocking. Now consider all the treatment effects. To apply the general theory, we need to specify a set of treatment effects we want to estimate. Then the fitted model contains these treatment effects in addition to all the block effects. In what follows, we look at two important special cases.

The first case is that the main effects of the m treatment factors are in the fitted model. Then γ_1 in model (1) consists of the main effects of all the m treatment factors and all the $2^{m_1}-1$ block effects. For the remaining treatment effects, we assume as usual that the hierarchical ordering principle applies [Wu and Hamada (2000)], and therefore γ_j in model (2) represents the vector of all the j-factor interactions of treatment factors, where $j=2,\dots,m$.

A defining word in a blocked fractional factorial is a subset of $m+m_1$ letters among which m letters represent treatment factors and m_1 letters represent blocking factors. Let A_j be the number of defining words of length j that contain no blocking factors, and let B_j be the number of defining words that contain j treatment factors and at least one blocking factor. Note that we must have $A_1=A_2=B_0=B_1=0$ for the fitted model to be estimable.

PROPOSITION 1. *Let γ_1 denote all main effects of treatment factors and all block effects, and let γ_j denote all the j-factor interactions of treatment factors. Then the word length pattern $(N_2,\dots,N_m)$ is given by $N_2=3A_3+B_2$, $N_3=4A_4+B_3$, and in general*

$$N_j=(j+1)A_{j+1}+(m-j+1)A_{j-1}+B_j, \tag{5}$$

where A_j and B_j are defined in the preceding paragraph.

The proof is straightforward. Our general criterion of aberration for blocked fractional factorials therefore selects designs by sequentially minimizing $N_2=3A_3+B_2$, $N_3=4A_4+B_3$ and so on. Chen and Cheng (1999) proposed a criterion of aberration, and using our notation, their word length pattern is given by $(3A_3+B_2, A_4, 10A_5+B_3, A_6,\dots)$. We see that the leading component in their criterion is identical to the leading component N_2 in our general criterion of aberration. Sitter, Chen and Feder (1997) also proposed a criterion that sequentially minimizes A_3, B_2, A_4, B_3, A_5, B_4, and so on. If the magnitude of A_{j+1} is about the same as or larger than that of B_j, the criterion of Sitter, Chen and Feder (1997) provides a reasonably good approximation to our general criterion. We give an illustration using a simple example.

EXAMPLE 1. Suppose that we want to study nine factors in 16 runs, which are to be arranged in two blocks. We use $1, \ldots, 9$ to denote the nine factors, and b to denote the single blocking factor. Consider the following two designs. Design D_1 is given by $5 = 123$, $6 = 124$, $7 = 134$, $8 = 234$, $9 = 12$, and $b = 13$, and design D_2 given by $5 = 123$, $6 = 124$, $7 = 134$, $8 = 13$, $9 = 12$, and $b = 234$. One can easily verify that $A_3(D_1) = 4$ and $B_2(D_1) = 4$, and $A_3(D_2) = 6$ and $B_2(D_2) = 2$. The criterion of Sitter, Chen and Feder (1997) selects D_1 as a better design because D_1 has a smaller value of A_3. Now applying our criterion, we see that $N_2(D_1) = 16$ and $N_2(D_2) = 20$, and again D_1 is better. Note that design D_1 in fact has a larger value of B_2 but its smaller value of A_3 plays a dominant role here.

The other important special case is that we are interested in estimating all main effects and all 2-factor interactions of treatment factors. So γ_1 consists of all the main effects and all the 2-factor interactions of treatment factors, as well as all the block effects. For $j \geq 2$, γ_j is the vector of all the $(j+1)$-factor interactions of the treatment factors. For the fitted model to be estimable, we must have $A_1 = A_2 = A_3 = A_4 = B_0 = B_1 = B_2 = 0$. Applying our general theory, we obtain the following.

PROPOSITION 2. *Suppose that γ_1 consists of all main effects and all 2-factor interactions of treatment factors, as well as all block effects. Let γ_j be the vector of all the $(j+1)$-factor interactions of the treatment factors for $j \geq 2$. Then the word length pattern $(N_2, N_3, \ldots)$ is given by $N_2 = 10A_5 + B_3$, $N_3 = 15A_6 + 5A_5 + B_4$, and in general*

$$
\begin{aligned}
N_j = {} & (j+2)A_{j+2} + \binom{j+3}{2} A_{j+3} + B_{j+2} \\
& + (m-j)A_j + (m-j-1)(j+1)A_{j+1} + \binom{m-j+1}{2} A_{j-1},
\end{aligned}
\tag{6}
$$

where A_j and B_j are defined as before.

Proposition 2 is easily established by a simple combinatorial argument. Comparing our criterion with that of Chen and Cheng (1999), we find that the leading component in their criterion becomes $10A_5 + B_3$, which is precisely the N_2 given by our general theory. In fact, we have verified that the leading component in the word length pattern of Chen and Cheng (1999) is also correct if in addition to all block effects, the true model consists of all main effects and all interactions involving up to q factors with $q \geq 3$. One can therefore appropriately regard the aberration criterion of Chen and Cheng (1999) as a robust version of our general aberration criterion when applied to blocked fractional factorials.

Before moving on, we remark that like other work in the area, block effects are treated as fixed effects in this paper. Our discussion in this section focuses on the situation where we are interested in estimating these block effects. If the block effects are not of interest, the contamination on their estimation due to nonnegligible treatment effects will not be a concern. Our general criterion can easily be modified to accommodate this situation. In the meantime, many new issues arise and they will be looked into in the future.

2.3. *Fractional factorials when some* 2*-factor interactions are important.* Suppose that a set of 2-factor interactions (2fi's) is postulated to be important, and in addition to the main effects, we are also interested in estimating these important 2fi's. In this situation the fitted model in (1) consists of all main effects and these important 2fi's. For the remaining effects, we assume as usual that the hierarchical ordering principle applies. Using the notation in Section 2.1, we have that γ_1 represents the main effects and the important 2fi's, γ_2 represents the remaining 2fi's and γ_j represents the j-factor interactions for $j \geq 3$.

A 2fi of a fractional factorial D can be represented by an unordered pair (c, d), where c and d are two columns of D. Let $(c_1, d_1), \dots, (c_S, d_S)$ denote the important 2fi's. For each 2fi (c_s, d_s) where $s = 1, \dots, S$, let $A_j(c_s, d_s)$ be the number of length-j words containing both letters c_s and d_s, let $A_j(c_s, \bar{d}_s)$ be the number of length-j words containing c_s but not d_s, let $A_j(\bar{c}_s, d_s)$ be the number of length-j words containing d_s but not c_s, and let $A_j(\bar{c}_s, \bar{d}_s)$ be the number of length-j words containing neither c_s nor d_s. Obviously, $A_j = A_j(c_s, d_s) + A_j(c_s, \bar{d}_s) + A_j(\bar{c}_s, d_s) + A_j(\bar{c}_s, \bar{d}_s)$. Let

$$A_j^{(2)} = \sum_{s=1}^{S} A_j(c_s, d_s), \qquad A_j^{(1)} = \sum_{s=1}^{S} [A_j(c_s, \bar{d}_s) + A_j(\bar{c}_s, d_s)],$$
$$A_j^{(0)} = \sum_{s=1}^{S} A_j(\bar{c}_s, \bar{d}_s). \tag{7}$$

If a defining word of length j contains more than one pair of letters in the list of the important 2fi's $(c_1, d_1), \dots, (c_S, d_S)$, it is counted more than once in calculating $A_j^{(2)}$. So $A_j^{(2)}$ in fact represents the total number of times that a defining word of length j contains an important 2fi (c_s, d_s). Interpretation of $A_j^{(1)}$ and $A_j^{(0)}$ is similar.

PROPOSITION 3. *When some 2fi's are important, the word length pattern* $(N_2, N_3, \dots, N_m)$ *is given by* $N_2 = 3A_3 + A_4^{(2)}$, $N_3 = 4A_4 + A_5^{(2)} + A_3^{(1)}$ *and in general*

$$N_j = (j+1)A_{j+1} + (m-j+1)A_{j-1} + A_{j+2}^{(2)} + A_j^{(1)} + A_{j-2}^{(0)}, \tag{8}$$

where $A_{j+2}^{(2)}$, $A_j^{(1)}$ *and* $A_{j-2}^{(0)}$ *are defined in* (7).

The above version of the word length pattern is given in terms of the defining words of the original design matrix D. We now present another version in terms of the defining words of the augmented design given by the model matrix $W_1 = (D, D_2)$, where W_1 is as in model (1) and D_2 corresponds to the important 2fi's in the fitted model. This latter version is convenient for developing a general complementary design theory in Section 3.

Consider the words in the defining relation of the augmented design $W_1 = (D, D_2)$. Let A_j be the number of length-j words having all their j letters from D, and let B_j be the number of length-$(j+1)$ words having j letters from D and one letter from D_2.

PROPOSITION 4. *When some 2fi's are important, the word length pattern* $(N_2, N_3, \dots, N_m)$ *is given by* $N_2 = 3A_3 + B_2 - S$, *and*

$$N_j = (j+1)A_{j+1} + (m-j+1)A_{j-1} + B_j \tag{9}$$

for $j \geq 3$.

In Proposition 4, dependence of N_j on the important 2fi's is expressed through B_j, which depends on matrix D_2, given by the columns of the important 2fi's.

The expression for N_2 in Proposition 4 needs a bit of explanation. Let (c_s, d_s) be an important 2fi, for $s = 1, \dots, S$. Then the three columns c_s, d_s and $c_s d_s$, where columns c_s and d_s are from D and column $c_s d_s$ is from D_2, form a word of length 3 that contributes to B_2 but not to N_2. This explains why we have $N_2 = 3A_3 + B_2 - S$ instead of $N_2 = 3A_3 + B_2$.

Ke and Tang (2003) examined practical issues in design selection using the general criterion of aberration when some 2fi's are important, and presented a collection of designs of 16 and 32 runs for models containing up to four important 2fi's.

2.4. *Other applications.* In robust parameter design, there are two sets of factors, control factors and noise factors. The goal of the experiment is to choose the settings of control factors so that the response variable is insensitive to noise factors. Suitable designs should therefore allow analysis of both location and dispersion effects. Wu and Zhu (2003) examined the use of an aberration criterion for robust parameter design which is mainly motivated by the analysis of location effects. It would be interesting to see how our general theory can be modified to take into account the analysis of dispersion effects. One possibility is to select designs using our criterion from among those designs allowing suitable analysis of dispersion effects as can be found in Hedayat and Stufken (1999). Our general theory is potentially useful in fractional factorial split plot designs. Huang, Chen and Voelkel (1998) and Bingham and Sitter (1999) considered aberration criteria for split plot designs. Since split plot designs have more than one error structure, some sort of modification seems necessary for our theory to be applicable to such problems. In our future research, both areas of application will be considered.

3. Theory of complementary designs. In this section, we will develop a complementary design theory for a class of aberration criteria. This class of criteria, to be introduced below, is quite broad, and in particular includes as special cases the aberration criteria for blocked fractional factorials and for designs when some 2fi's are important as discussed in Sections 2.2 and 2.3, respectively.

3.1. *A class of aberration criteria.* Suppose that besides the main effects γ_1' of m factors, we are also interested in estimating additional S effects γ_1''. For convenience, these m factors are called major factors. In addition to the m major factors, we may have m_1 minor factors, where $m_1 \geq 0$. When $m_1 = 0$, the additional S effects γ_1'' are a set of interactions only involving major factors. When $m_1 \geq 1$, the effects in γ_1'' are a subset of effects from the collection of all the following effects: the interactions only involving major factors, the main effects of minor factors, the interactions only involving minor factors and the interactions involving both major and minor factors. The γ_1 in the fitted model (1) is therefore given by $\gamma_1 = (\gamma_1', \gamma_1'')$. Let γ_j denote the j-factor interactions only involving the major factors that are not included in γ_1'', for $j = 2, \ldots, m$. We assume as earlier that the effects in γ_j are more important than those in γ_{j+1}, for $j \geq 2$. With $\gamma_1, \ldots, \gamma_m$ defined above, the true model is now given in (2). A remark on the true model is in order when there is at least one minor factor, that is, $m_1 \geq 1$. An implicit assumption made here is that all other effects involving at least one minor factor besides those in γ_1'' are assumed to be nonexistent. The above formulation is fairly general, and includes as special cases all the situations discussed in Sections 2.1–2.3. For example, for blocked fractional factorials, we take the treatment factors as the major factors and the blocking factors as the minor factors. Choices for major and minor factors are also natural for fractional factorials in the row-column setting [Cheng and Mukerjee (2003)].

We now derive the word length pattern for the above situation. Let D_1 be the design matrix corresponding to the main effects γ_1' of the m major factors and let D_2 be the matrix corresponding to the additional S effects γ_1''. Note that D_1 has m columns and D_2 has S columns. The word length pattern will be given in terms of the model matrix $W = (D_1, D_2)$, specified by its two components D_1 and D_2. Let $A_j(D_1)$ be the number of length-j defining words in design D_1. Define $B_j(D_1, D_2)$ to be the number of length-$(j+1)$ defining words in design $W = (D_1, D_2)$, which have j letters from D_1 and one letter from D_2. Then it is easily established that the word length pattern $(N_2, \ldots, N_m)$ is given by

$$N_j(D_1, D_2) = (j+1)A_{j+1}(D_1) + (m-j+1)A_{j-1}(D_1) + B_j(D_1, D_2) - S_j$$

for $j \geq 2$, where S_j is the number of the interactions of j major factors that are included in γ_1''. (For an explanation of why S_j is necessary, see the end of Section 2.3.) Note that S_j is a constant for the purpose of choosing D_1 and D_2. For simplicity, ignoring S_j, we redefine the word length pattern $(N_2, \ldots, N_m)$ as

$$N_j(D_1, D_2) = (j+1)A_{j+1}(D_1) + (m-j+1)A_{j-1}(D_1) + B_j(D_1, D_2). \qquad (10)$$

The goal here is to choose D_1 and D_2 by sequentially minimizing $N_2, N_3, \ldots.$

3.2. *A complementary design theory.* Let $H_k = (D_1, D_2, D_3)$, where H_k denotes a saturated design of $n = 2^k$ runs and $n - 1$ factors. Obviously, it is impossible to completely characterize design pair (D_1, D_2) through D_3 alone. Our complementary design theory to be developed below characterizes design pair (D_1, D_2) through design pair (D_2, D_3). This approach is most effective when the number of columns in D_3 is smaller than that in D_1.

We need a result from Tang and Wu (1996) and Suen, Chen and Wu (1997), who developed a complementary design theory for the usual minimum aberration criterion. The explicit coefficients in Lemma 2 are due to Suen, Chen and Wu (1997).

LEMMA 2. *Let $H_k = (D, \bar{D})$, where D has m factors. Then we have*

$$A_j(D) = \sum_{i=0}^{j} c_m(i, j) A_i(\bar{D}),$$

where $c_m(1, j) = c_m(2, j) = 0$, $c_m(i, j) = (-1)^{j-[(j-i)/2]}\binom{m-2^{k-1}}{[(j-i)/2]}$ for $3 \le i \le j$, and

$$c_m(0, j) = (-1)^{j-[j/2]}\binom{m - 2^{k-1}}{[j/2]} + 2^{-k}[P_j(0; m) - P_j(2^{k-1}; m)],$$

where $P_j(x; m) = \sum_{s=0}^{j}(-1)^s\binom{x}{s}\binom{m-x}{j-s}$ is a Krawtchouk polynomial.

Note that $N_j(D_1, D_2)$ in (10) depends on design pair (D_1, D_2). The main result of our complementary design theory is contained in the following theorem, which expresses $N_j(D_1, D_2)$ in terms of design pair (D_2, D_3).

THEOREM 2. *The word length pattern in* (10) *for the class of criteria discussed in Section* 3.1 *depends on design pair (D_2, D_3) through*

$$\begin{aligned} N_j(D_1, D_2) = {} & \sum_{i=0}^{j+1}[(j + 1 - S)c_m(i, j + 1) + Sc_{m+1}(i, j + 1)]A_i(D_2 \cup D_3) \\ & - \sum_{i=0}^{j+1} c_{m+1}(i, j + 1)E_i(D_2, D_3) \\ & + (m - j + 1)\sum_{i=0}^{j-1} c_m(i, j - 1)A_i(D_2 \cup D_3), \end{aligned}$$

where $E_i(D_2, D_3) = \sum_{p=1}^{i} pE_i^{(p)}(D_2, D_3)$ with $E_i^{(p)}(D_2, D_3)$ denoting the number of length-i defining words in $D_2 \cup D_3$ that have exactly p letters from D_2.

PROOF. Applying Lemma 2 to design D_1, we have

$$A_j(D_1) = \sum_{i=0}^{j} c_m(i, j) A_i(D_2 \cup D_3). \tag{11}$$

For any $d \in D_2$, applying Lemma 2 to design $D_1 \cup \{d\}$, we obtain

$$A_j(D_1 \cup \{d\}) = \sum_{i=0}^{j} c_{m+1}(i, j) A_i\big((D_2 \setminus \{d\}) \cup D_3\big). \tag{12}$$

Let $B_{j-1}(d, D_1)$ be the number of length-j defining words in design (D_1, D_2) that contain letter d and $j-1$ letters from D_1. Clearly, we have $A_j(D_1 \cup \{d\}) = A_j(D_1) + B_{j-1}(d, D_1)$. Let

$$T_j(d, D_2, D_3) = \sum_{i=0}^{j} c_{m+1}(i, j) A_i\big((D_2 \setminus \{d\}) \cup D_3\big). \tag{13}$$

Then (12) can be rewritten as

$$A_j(D_1) + B_{j-1}(d, D_1) = T_j(d, D_2, D_3). \tag{14}$$

Taking summation over all d in D_2 on both sides of (14) gives

$$\sum_{d \in D_2} \big(A_j(D_1) + B_{j-1}(d, D_1)\big) = \sum_{d \in D_2} T_j(d, D_2, D_3).$$

Noting that D_2 has S columns and that $B_{j-1}(D_1, D_2)$ defined in Section 3.1 is equal to $\sum_{d \in D_2} B_{j-1}(d, D_1)$, we obtain $SA_j(D_1) + B_{j-1}(D_1, D_2) = T_j(D_2, D_3)$, where

$$T_j(D_2, D_3) = \sum_{d \in D_2} T_j(d, D_2, D_3). \tag{15}$$

Therefore, $B_j(D_1, D_2) = T_{j+1}(D_2, D_3) - SA_{j+1}(D_1)$. Substituting this expression of $B_j(D_1, D_2)$ into (10), we obtain

$$\begin{aligned} &N_j(D_1, D_2) \\ &\quad = (j + 1 - S) A_{j+1}(D_1) + T_{j+1}(D_2, D_3) + (m - j + 1) A_{j-1}(D_1). \end{aligned} \tag{16}$$

Now let us calculate $T_{j+1}(D_2, D_3)$ in (15). Let $E_i(d, D_2, D_3)$ be the number of length-i defining words in (D_2, D_3) that contain letter d. We have $A_i((D_2 \setminus \{d\}) \cup D_3) = A_i(D_2 \cup D_3) - E_i(d, D_2, D_3)$. Then (13) becomes

$$T_{j+1}(d, D_2, D_3) = \sum_{i=0}^{j+1} c_{m+1}(i, j+1)[A_i(D_2 \cup D_3) - E_i(d, D_2, D_3)].$$

Summing both sides over all d in D_2, we obtain

$$
\begin{aligned}
T_{j+1}(D_2, D_3) = S \sum_{i=0}^{j+1} c_{m+1}(i, j+1) A_i(D_2 \cup D_3) \\
- \sum_{i=0}^{j+1} c_{m+1}(i, j+1) E_i(D_2, D_3),
\end{aligned}
\tag{17}
$$

where $E_i(D_2, D_3) = \sum_{d \in D_2} E_i(d, D_2, D_3)$. Note that $E_i(d, D_2, D_3)$ is the number of length-i words containing letter d in design $D_2 \cup D_3$. Thus $E_i(D_2, D_3)$ represents the total number of times length-i words in design $D_2 \cup D_3$ contain a letter in D_2. Therefore

$$
E_i(D_2, D_3) = \sum_{p=1}^{i} p E_i^{(p)}(D_2, D_3), \tag{18}
$$

where $E_i^{(p)}$ denotes the number of length-i words in $D_2 \cup D_3$ having exactly p letters from D_2. Combining (11) and (16)–(18), we obtain the result in Theorem 2. □

Chen and Cheng (1999) developed a complementary design theory for blocked fractional factorials. Our complementary design theory given in Theorem 2 is applicable to a broad class of aberration criteria including all the cases discussed in Sections 2.1–2.3. We want to mention that our theory does not include their theory as a special case, because our word length pattern when applied to blocked factorials is not exactly the same as theirs. On the other hand, one can adopt our approach to derive their complementary design theory. Our approach appears considerably simpler than theirs.

Zhu (2003) found a relationship between A_{ij0} and A_{0kl}, where A_{ij0} is the number of length-$(i + j)$ words having i letters from D_1 and j letters from D_2, and A_{0kl} is the number of length-$(k + l)$ words having k letters from D_2 and l letters from D_3. In principle, Theorem 2 is derivable from his result. On the other hand, it is not obvious how one can obtain the result in Theorem 2, which clearly shows how N_2 depends on D_2 and D_3, from Zhu's rather involved formula that connects A_{ij0} to A_{0kl}.

3.3. *Some results on weak aberration.* The general criterion of aberration sequentially minimizes $N_2(D_1, D_2), N_3(D_1, D_2), \ldots$. A weak version of the criterion is given by minimizing $N_2(D_1, D_2) = 3A_3(D_1) + B_2(D_1, D_2)$ alone. Using Theorem 2, we find that

$$
N_2(D_1, D_2) = \text{constant} - 3A_3(D_2 \cup D_3) + E_3(D_2, D_3),
$$

where the *constant* does not depend on D_2 and D_3. Noting that

$$E_3(D_2, D_3) = E_3^{(1)}(D_2, D_3) + 2E_3^{(2)}(D_2, D_3) + 3E_3^{(3)}(D_2, D_3),$$

$$A_3(D_2 \cup D_3) = A_3(D_3) + E_3^{(1)}(D_2, D_3) + E_3^{(2)}(D_2, D_3) + E_3^{(3)}(D_2, D_3),$$

we have that

$$N_2(D_1, D_2) = \text{constant} - 3A_3(D_3) - 2E_3^{(1)}(D_2, D_3) - E_3^{(2)}(D_2, D_3).$$

So minimizing $N_2(D_1, D_2)$ is equivalent to maximizing

$$g(D_2, D_3) = 3A_3(D_3) + 2E_3^{(1)}(D_2, D_3) + E_3^{(2)}(D_2, D_3). \tag{19}$$

The following lemma gives an upper bound on $g(D_2, D_3)$.

LEMMA 3. *Let $m_2 = S$ and $m_3 = 2^k - 1 - m - S$ be the numbers of columns in D_2 and D_3, respectively. We have that*:

(i) $3A_3(D_3) + E_3^{(1)}(D_2, D_3) \le \binom{m_3}{2}$,
(ii) $E_3^{(1)}(D_2, D_3) + E_3^{(2)}(D_2, D_3) \le m_2 m_3/2$, *and*
(iii) $g(D_2, D_3) \le m_3(m_2 + m_3 - 1)/2$.

The upper bound in (iii) *is reached if and only if the bounds in* (i) *and* (ii) *are both reached*.

PROOF. For any two columns c and d in D_3, the product cd must belong to one of D_1, D_2 or D_3. Consider all the $\binom{m_3}{2}$ pairs of columns in D_3. The number of the pairs whose products are in $D_2 \cup D_3$ is given by $E_3^{(1)}(D_2, D_3) + 3A_3(D_3)$. Therefore

$$E_3^{(1)}(D_2, D_3) + 3A_3(D_3) \le \binom{m_3}{2}, \tag{20}$$

which proves part (i) of Lemma 3. Similarly, by considering all the products cd such that $cd \in D_2 \cup D_3$ where $c \in D_2$ and $d \in D_3$, we obtain

$$2E_3^{(1)}(D_2, D_3) + 2E_3^{(2)}(D_2, D_3) \le m_2 m_3, \tag{21}$$

from which Lemma 3(ii) follows. Combining (20) and (21), we obtain

$$g(D_2, D_3) \le \binom{m_3}{2} + m_2 m_3/2 = m_3(m_2 + m_3 - 1)/2.$$

This is Lemma 3(iii). The last statement in Lemma 3 is obvious. □

From the proof of Lemma 3, we see that the bound in (20) is reached if $cd \in D_2 \cup D_3$ for any two columns $c, d \in D_3$, and that the bound in (21) is reached if $cd \in D_2 \cup D_3$ for any $c \in D_2$ and any $d \in D_3$. One structure for

D_2 and D_3 to have these properties is given as follows. Let $a_1, a_2, \dots, a_k$ be a set of k independent columns that generates the saturated design H_k of $n = 2^k$ runs and $n-1$ factors. Now choose $D_2 \cup D_3$ to be $H_r = H(a_1, \dots, a_r)$, the saturated design generated by independent columns $a_1, \dots, a_r$ where $r = 1, \dots, k-1$. Note that D_2 can be any $m_2 = S$ columns from H_r.

THEOREM 3. *Let H_r be the saturated design generated by r independent columns $a_1, \dots, a_r$. Then so long as $D_2 \cup D_3 = H_r$, any design pair (D_2, D_3) maximizes $g(D_2, D_3)$ in* (19). *Therefore design pair (D_1, D_2) has minimum weak aberration, where D_1 is given by $H_k \setminus H_r$.*

Recall that in introducing the class of aberration criteria in Section 3.1, design D_1 corresponds to the main effects of m major factors and design D_2 represents $m_2 = S$ additional effects we are interested in estimating, which may involve some minor factors. In order for design pair (D_1, D_2) given in Theorem 3 to be a legitimate design, we need to specify D_2 in such a way that it indeed represents the S additional effects. We now look at two situations. The first is that D_1 represents the main effects of m treatment factors, and D_2 are all the $2^{m_1} - 1$ block effects given by m_1 blocking factors. Then choosing $D_2 = H_{m_1}$, the saturated design generated by $a_1, \dots, a_{m_1}$ where $m_1 \le r$ in Theorem 3, satisfies the requirement. This characterization for blocked designs was given in Chen and Cheng (1999). We see that it is now derived from Theorem 3. The second situation we will look at is that D_1 are the main effects of m factors, and D_2 are some 2-factor interactions of the m factors. We illustrate how to choose D_2 through an example.

EXAMPLE 2. Suppose that we want a 16-run design that allows estimation of the main effects $1, 2, 3, 4, 5, 6, 7$ and 8 of eight factors and the following 2-factor interactions: $12, 13, 24$ and 35. Let a_1, a_2, a_3, a_4 be four independent columns. Theorem 3 says that we should choose $D_2 \cup D_3 = \{a_1, a_2, a_1a_2, a_3, a_3a_1, a_3a_2, a_3a_1a_2\}$. That is, the eight factors are assigned to the columns in $D_1 = \{a_4, a_4a_1, a_4a_2, a_4a_1a_2, a_4a_3, a_4a_3a_1, a_4a_3a_2, a_4a_3a_1a_2\}$. Now assign factor 1 to a_4, factor 2 to a_4a_1, factor 3 to a_4a_2, factor 4 to a_4a_3 and factor 5 to $a_4a_3a_1$. Factors $6, 7$ and 8 can be arbitrarily assigned to the remaining three columns in D_1. We have that $12 = a_1$, $13 = a_2$, $24 = a_1a_3$ and $35 = a_1a_2a_3$. So $D_2 = \{a_1, a_2, a_1a_3, a_1a_2a_3\}$.

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