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A note on generalized aberration in factorial designs

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Abstract. In this paper we extend the wordlength pattern and minimum aberration for non-regular factorials. The new concepts, the generalized wordlength pattern and minimum generalized aberration, are proposed. Some connections between the generalized wordlength pattern and uniformity are given. Some applications of the new concepts in the Blackett and Burman's designs are discussed.

Key words: code theory, discrepancy, minimum aberration, orthogonal fractional factorial designs, uniformity, uniform design, wordlength pattern, generalized wordlength pattern.

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1. Introduction

Fractional factorial designs are the most popular experimental designs used in various fields. There are many useful criteria for comparing fractional factorial designs, such as resolution (Box, Hunter and Hunter (1978)), minimum aberration (Fries and Hunter (1980)), estimation capacity (Cheng and Mukerjee (1998)) and uniformity (Fang and Mukerjee (2000)). Among them the minimum aberration (MA) is the most popular used measure. However, the MA can compare only for regular factorials. There is no similar criterion for non-regular designs. In this note we extend the concept of wordlength pattern and minimum aberration criterion for non-regular factorials. The generalized wordlength pattern and the minimum generalized aberration

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(MGA) are defined based on the code theory. Furthermore, we give an analytic formula that links the uniformity and the generalized wordlength pattern of a factorial design with two or three levels. These results give an extension of Fang and Mukerjee (2000) for non-regular factorial designs. The concepts and basic knowledge in factorial experiments can refer to Dey and Mukerjee (1999).

The generalized wordlength pattern and aberration are defined in Section 2. Their applications of the new criteria to the Plackett and Burman's designs $L_{12}(2^{11})$ and $L_{20}(2^{19})$ are discussed in Section 3. Section 4 shows connections between the generalized wordlength pattern and uniformity in the sense of discrepancy. The last section gives discuss.

2. Generalized wordlength pattern and aberration

It is well known that the concept of aberration can be used in only regular factorial designs. But sometimes we need to compare non-regular designs. The geometric properties and hidden projections of a factorial can sometimes provide a justification for comparisons of non-regular factorials (Lin and Draper (1992) and Wang and Wu (1995)). However, these methods do not provide a unified way for all non-regular factorials. Therefore, we in this section propose the concepts of generalized wordlength pattern and generalized aberration that can be used for both regular and non-regular factorials.

It is well known that the mathematical equivalence between fractional factorial designs and linear codes (Cf, e.g., Suen, Chen and Wu (1997)). The concepts proposed in this paper are based on this equivalence.

Let us review some basic knowledge in the coding theory. The reader can refer to Roman (1992) for details. An $[s,k]$ linear code C is a k-dimensional linear subspace of $V(s,q)$. The $(s-k)$-dimensional orthogonal subspace of C is also a linear code $[s,s-k]$, called the *dual code* of C and denoted by $C^{\perp}$. The elements of C are called *codewords*. The *weight* of a codeword of C is defined as the number of nonzero components of the codeword and $B_i(C)$ denotes the number of vectors in C with weight i. The sequence $W_d(C) = (B_1(C),\ldots,B_s(C))$ is called the *weight distribution* of the code. For any n-run design D, let

$$E_i(D) = \frac{1}{n}\#\{(\boldsymbol{c},\boldsymbol{d})|\boldsymbol{c},\boldsymbol{d}\in D, d_H(\boldsymbol{c},\boldsymbol{d}) = i\},$$

where $d_H(\boldsymbol{c},\boldsymbol{d})$ is the *Hamming distance* between two runs $\boldsymbol{c}$ and $\boldsymbol{d}$, which is the number of places where they differ. The sequence $(E_0(D),\ldots,E_s(D))$ is called the *distance distribution of* D. The MacWilliams identities in coding theory give a fundamental relationship between the weight (distance) distribution of a linear code and its dual code.

Lemma 1 (MacWilliams)**.** *If $C\subset V(s,q)$ is a $[s,k]$ linear code and $C^{\perp}$ is its dual, $\{B_i(C)\}$ and $\{B_i(C^{\perp})\}$ are the weight distribution, $\{E_i(C)\}$ and $\{E_i(C^{\perp})\}$ are the distance distribution, respectively. Then*

$$B_i(C^\perp) = q^{-k}\sum_{j=0}^{s} P_i(j;s)B_j(C),$$

$$E_i(C^\perp) = q^{-k}\sum_{j=0}^{s} P_i(j;s)E_j(C), \quad i = 0, 1, \ldots, s, \tag{1}$$

where $P_i(j;s) = \sum_{r=0}^{i}(-1)^r(q-1)^{i-r}\binom{j}{r}\binom{s-j}{i-r}$ *is the Krawtchouk polynomial* $\left(\binom{y}{z} = 0 \text{ for } y < z\right)$.

A factorial design is *full* if its all level-combinations appear equally often. The q^s *factorial design* is a full design with $n = q^s$ runs. The q^s factorial design can be considered as an n-dimensional linear vector space over the Galois field $GF(q)$. A q^{s-k} regular fractional factorial design D is an $(s-k)$-dimensional linear subspace of q^s. The k-dimensional orthogonal subspace, denoted by $D^\perp$, of D is the *defining contrasts subgroup* of D. The elements of $D^\perp$ are called *words*. A word and its nonzero multiples are considered to be the same in the defining relations. The *length* of a word is the number of its nonzero components. Let $A_i(D)$ be the number of distinct words of length i in the defining relation of D. Then the sequence $W(D) = \{A_1(D), \ldots, A_s(D)\}$ is called the *word length pattern* of D. A q^{s-k} regular fractional factorial design D is also an $[s, s-k]$-code. Its defining contrasts subgroup $D^\perp$ of D is also an $[s, k]$-code. Design D is the dual code of $D^\perp$ and vice-versa. And the word length pattern of D and the weight distribution of $D^\perp$ have the relation,

$$B_i(D^\perp) = (q-1)A_i(D). \tag{2}$$

In this paper all the designs we mentioned are of n runs and s q-level factors. By cording theory, for regular q^{s-k} design D, the distance distribution is the same as the weight distribution of D, i.e. $E_i(D) = B_i(D)$. Therefore, the wordlength pattern of D is the same as one-$(q-1)$th weight distribution of $D^\perp$ and is the same as one-$(q-1)$th distance distribution of $D^\perp$. From Lemma 1,

$$\begin{aligned} W(D) &= (E_1(D^\perp), \ldots, E_s(D^\perp))/(q-1) \\ &= \left(\frac{1}{n}\sum_{j=0}^{s} P_1(j;s)E_j(D), \ldots, \frac{1}{n}\sum_{j=0}^{s} P_s(j;s)E_j(D)\right)/(q-1). \end{aligned} \tag{3}$$

We can calculate the wordlength pattern of D by (3) without calculating dual design of D. Obviously, non-regular design is not linear code and so has not the wordlength pattern. Anyway, any design has the distance distribution and so we also can obtain a vector by (3). The vector is the wordlength pattern for regular design and defined as generalized wordlength pattern (Definition 1).

Definition 1. The *generalized wordlength pattern* of a design D is defined by $W^g(D) = \{A_1^g(D), \ldots, A_s^g(D)\}$, where

$$A_i^g(D) = \frac{1}{n(q-1)} \sum_{j=0}^{s} P_i(j;s) E_j(D), \quad i = 1, \ldots, s, \tag{4}$$

and $P_i(j;s)$'s are the Krawtchouk polynomials. The *resolution* of D is the smallest i with positive $A_i^g(D)$ in $W^g(D)$. Let D_1 and D_2 be two designs. Let t be the smallest integer such that $A_t^g(D_1) \neq A_t^g(D_2)$ in their generalized wordlength patterns. Then D_1 is said to have less generalized aberration than D_2 if $A_t^g(D_1) < A_t^g(D_2)$. A design D has *minimum generalized aberration* (MGA) if no other q-level design has less generalized aberration than it.

The concepts defined above can for both regular or non-regular designs. When the design is regular, the generalized wordlength pattern reduces to the original wordlength pattern $W(D) = \{A_1(D), \cdots, A_s(D)\}$ from (3).

Theorem 1. *For regular q^{s-p} factorials, the generalized wordlength pattern $W^g(D)$ reduces to their wordlength pattern $W(D)$.*

Two factorial designs are called *isomorphic* if one can be obtained from the other by relabeling factors, reordering the runs, or switching the levels of factors. It is known that a design that is isomorphic with a regular design may become non-regular one. The latter does not have the wordlength pattern in the past. Obviously, two isomorphic designs have the same distance distribution. Therefore, we have the following theorem.

Theorem 2. *Two isomorphic designs have the same generalized wordlength pattern.*

Let D be a design and r be the largest integer such that any subdesign of D with r factors is full. We said that the design D has *strength* r. Obviously, a design with strength r must be an orthogonal array of strength r. From Section 5.5 and 7 of MacWilliams and Sloane (1977), we have

Theorem 3. *The strength of a design D is t if and only if the resolution of D is* $t+1$.

3. Applications of the generalized aberration in factorials

For factorials, generally speaking, the less generalized aberration the design is, the less confounding has it. The following examples studied by Lin and Draper (1992) and Wang and Wu (1995) show the usefulness of the generalized aberration. The notation $L_n(q^s)$ gives an orthogonal design of n runs with s q-level factors.

Example 1. Suppose that there are 5 2-level factors in an experiment and the experimenter wants to arrange this experiment by the Plackett and Burman design $L_{12}(2^{11})$. We need to choose a subdesign of 5 columns from $L_{12}(2^{11})$ such that it has the best statistical property in a certain sense. Unfortunately, the Plackett and Burman design is non-regular and we can not use the MA criterion to choose such a design. Therefore, Lin and Draper (1992) sorted the

$\binom{12}{5} = 462$ subdesigns into two non-isomorphic subclass, denoted by D12-5.1 and D12-5.2, respectively, one with a repeat-run pair and the other without any repeat-run pair. From geometric viewpoint, they prefer the D12-5.1 as it has one more degree of freedom than the D12-5.2. Wang and Wu (1995) further found that D12-5.1 has a better estimable capacity than that of D12-5.2. By definition 1, the generalize wordlength patterns of the designs D12-5.1 and D12-5.2 are

$$(0, 0, 10/9, 5/9, 0) \quad \text{and} \quad (0, 0, 10/9, 5/9, 4/9),$$

respectively. Both the designs have the resolution III, but D12-5.1 has less generalized aberration than D12-5.2. The new criterion gives an additional justification that D12-5.1 is better than D12-5.2. As there are only two non-isomorphic $L_{12}(2^5)$ (Draper (1985)), D12-5.1 has minimum generalized aberration.

Example 2. Let us consider the 20-run Plackett and Burman (1946)'s design which is a cyclic design with the first row $(++--++++-+-+----++-)$ and the final row of minus signs. The generalized wordlength patterns of all 3876 4-dimensional subdesigns are sorted into three groups:

a. 2726 subdesigns have generalized wordlength pattern $(0, 0, 0.16, 0.04)$.
b. 228 subdesigns have $(0, 0, 0.16, 0.36)$.
c. 912 subdesigns have $(0, 0, 0.48, 0.04)$.

The 3 class designs are denoted by D20-4.1, D20-4.2, D20-4.3, respectively. Lin and Draper (1991) and Wang and Wu (1995) indicated that D20-4.1 is better than D20-4.2 and D20-4.2 is better than D20-4.3 in the sense of geometric properties or estimable capacity. This is also true in the sense of generalized aberration.

Obviously, from these two examples we can see that the generalized wordlength pattern and MGA criterion can be applied to all regular and non-regular factorials. This gives a unified criterion to compare all factorials.

Example 3. In this example, we construct two non-regular designs 2^{14-7} and 2^{13-6} that have higher resolution than the respective MA designs.

A non-regular $L_{256}(2^{16})$, denoted by D_0, has generalized word-length pattern

$$(0, 0, 0, 0, 0, 112, 0, 30, 0, 112, 0, 0, 0, 0, 0, 1)$$

and so has resolution VI (Roman (1992) p259, pp 263–264). Deleting the 128 rows of D_0 with level 1 in the first column of D_0 and then deleting the first column of the remaining design, we obtain a design $L_{128}(2^{15})$, denoted by D_1. It can be shown that D_1 has generalized wordlength pattern

$$[0, 0, 0, 0, 42, 70, 15, 15, 70, 42, 0, 0, 0, 0, 1]$$

and has resolution V. After deleting the last column of D_1 we obtain an $L_{128}(2^{14})$, denoted by D_2, with generalized wordlength pattern

$$[0, 0, 0, 0, 28, 42, 8, 7, 28, 14, 0, 0, 0, 0]$$

and resolution V. It is known that the minimum aberration design 2^{14-7}, denoted by D_2^*, has wordlength pattern

$$[0, 0, 0, 3, 24, 36, 16, 11, 24, 12, 0, 1, 0, 0]$$

and has resolution IV (Chen (1998)). Obviously, the design D_2 has a higher resolution than of the MA design D_2^*.

Furthermore, an $L_{128}(2^{13})$ is obtained by deleting the last two columns of D_1 and this design has

$$[0, 0, 0, 0, 18, 24, 4, 3, 10, 4, 0, 0, 0]$$

and resolution V. The minimum aberration 2^{13-6} has wordlength pattern

$$[0, 0, 0, 2, 16, 18, 10, 9, 4, 2, 0, 0]$$

and has only resolution IV (Chen (1998)).

From the above example, we can obtain non-regular designs that has higher resolution or less generalized aberration than that of the corresponding MA designs. Therefore, we should search MGA designs.

4. Connections between generalized aberration and uniformity

The uniformity is the most important criterion in designs of computer experiments (Bates, et al. (1996)), especially in the uniform design (Fang and Wang (1994)). Recently, Fang and Mukerjee (2000) obtained connections between uniformity in sense of the centered L_2-discrepancy and the original wordlength pattern in regular 2-level factorials. They obtained an analytic formula to link the discrepancy and the wordlength pattern of a regular 2-level design. In this section we extend their result to non-regular factorials.

Let $\mathscr{P} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n\}$ be a set of n points in the s-dimensional unit cube $C^s = [0, 1)^s$. Many different measures of uniformity of $\mathscr{P}$ have been proposed but many authors (cf. Fang and Wang (1994)). A good review for up-to-date development can refer to Hickernell (1998a,b) who in these papers also proposed several new measures such as symmetric L_2-discrepancy (SD), centered L_2-discrepancy (CD) and wrap-around L_2-discrepancy (WD). Their definitions and computation formulas can refer to his papers. The following theorem gives connections between the discrepancies WD, CD and SD and the generalized wordlength pattern.

Theorem 4. *Let D be a two-level factorial with n runs and s factors. Then its following discrepancies can be expressed in terms of its generalized wordlength pattern $A^g(D)$ as follows*

$$[WD(D)]^2 = \left(\frac{11}{8}\right)^s \sum_{r=1}^{s} \frac{A_r^g(D)}{11^r} + \left(\frac{11}{8}\right)^s - \left(\frac{4}{3}\right)^s, \tag{5}$$

$$[(CD(D))]^2 = \left(\frac{9}{8}\right)^s \left(1 + \sum_{r=1}^{s} \frac{A_r^g(D)}{9^r}\right) - 2\left(\frac{35}{32}\right)^s + \left(\frac{13}{12}\right)^s, \tag{6}$$

and

$$[(SD(D))]^2 = \left(\frac{4}{3}\right)^s - 2\left(\frac{11}{8}\right)^s + \left(\frac{3}{2}\right)^s \left(1 + \sum_{r=1}^{s} \frac{A_r^g(D)}{3^r}\right). \tag{7}$$

For any three-level factorial D with n runs and s factors, we have

$$[WD(D)]^2 = \left(\frac{73}{54}\right)^s \left[1 + 2\sum_{j=1}^{s} \left(\frac{4}{73}\right)^j A_j^g(D)\right] - \left(\frac{4}{3}\right)^s. \tag{8}$$

5. Conclusion and discussion

The generalized aberration defined in this note can be used for compare both regular and non-regular factorials. There are close relationships between the discrepancies WD, CD and SD and the generalized aberration of a fractional with two-levels or three-levels. Therefore, the uniformity in the sense of WD, CD or SD can be used as a criterion of comparing factorials with two-levels and three-levels. It can be expected that the uniformity may be considered a criterion for assessing factorials with high levels. This is an open problem. On other hand, two factorial designs that have the same generalized aberration may have different uniformity. Are there any differences in statistical inference between these two designs? This is another open problem. The study on the problems above may suggest an approach to construct MGA designs.

Appendix

Proof of Theorem 1. By cording theory, for regular q^{s-p} design D, the distance distribution is the same as the weight distribution of D, i.e. $E_i(D) = B_i(D)$. From (4) and MacWilliams identities in Lemma 1, the $A_i(D)$ is the weight distribution of the dual of D and so is also wordlength pattern of D. The proof is completed. □

The following analytical expression of the WD can be easily derived (Hickernell (1998b)).

Lemma 2. *For a set of points $\mathscr{P} = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$ its square WD is given by*

$$(WD(\mathscr{P}))^2 = -\left(\frac{4}{3}\right)^s + \frac{1}{n^2}\sum_{k=1}^{n}\sum_{j=1}^{n}\prod_{i=1}^{s}\left[\frac{3}{2} - |x_{ki} - x_{ji}|(1 - |x_{ki} - x_{ji}|)\right], \tag{9}$$

where $\mathbf{x}_k = (x_{k1}, \ldots, x_{ks})$.

Proof of Theorem 4. We prove only (5) and others are similar. For any set of points $\mathscr{P} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n\}$, by the (9), we have $\frac{3}{2} - |x_{ki} - x_{ji}|(1 - |x_{ki} - x_{ji}| = 3/2$, if $x_{ki} = x_{ji}$, otherwise $5/4$ for $k, j = 1, \ldots, n, i = 1, \ldots, s$. Therefore

$$\prod_{i=1}^{s}\left[\frac{3}{2} - |x_{ki} - x_{ji}|(1 - |x_{ki} - x_{ji}|)\right]$$
$$= \left(\frac{3}{2}\right)^{s-d_H(\boldsymbol{x}_k,\boldsymbol{x}_j)}\left(\frac{5}{4}\right)^{d_H(\boldsymbol{x}_k,\boldsymbol{x}_j)} = \left(\frac{3}{2}\right)^{s}\left(\frac{5}{6}\right)^{d_H(\boldsymbol{x}_k,\boldsymbol{x}_j)}.$$

From the definition of $E_i(D)$ and (9), the WD can be expressed as in terms of the distance distribution $\{E_i(D)\}$

$$(WD(D))^2 = \frac{1}{n}\left(\frac{3}{2}\right)^{s}\sum_{i=0}^{s} E_i(D)\left(\frac{5}{6}\right)^{i} - \left(\frac{4}{3}\right)^{s}. \tag{10}$$

It is well known that the weight distribution and distance distribution coincide for regular fractional factorial designs. So

$$(WD(D))^2 = \frac{1}{n}\left(\frac{3}{2}\right)^{s}\sum_{i=0}^{s} B_i(D)\left(\frac{5}{6}\right)^{i} - \left(\frac{4}{3}\right)^{s},$$

where $B_i(D)$ is the weight distribution of D. Let $D^{\perp}$ be the defining contrasts subgroup and is also the dual of D. From MacWilliams identities in Lemma 1 and the relation of the weight distribution and word length pattern, we have

$$\begin{aligned}
&(WD(D))^2\\
&= \frac{1}{n}\left(\frac{3}{2}\right)^{s}\sum_{i=0}^{s}\left(\frac{5}{6}\right)^{i} 2^{-k}\sum_{j=0}^{s} P_i(j;s)B_j(D^{\perp}) - \left(\frac{4}{3}\right)^{s}\\
&= \frac{1}{n}\left(\frac{3}{2}\right)^{s}\sum_{i=0}^{s}\left(\frac{5}{6}\right)^{i} 2^{-k}\sum_{j=0}^{s}\sum_{r=0}^{i}(-1)^{r}(q-1)^{i-r}\binom{j}{r}\binom{s-j}{i-r}B_j(D^{\perp}) - \left(\frac{4}{3}\right)^{s}\\
&= \frac{2^{-k}}{2^{s-k}}\left(\frac{3}{2}\right)^{s}\sum_{j=0}^{s}\left[\sum_{i=0}^{s}\sum_{r=0}^{i}\left(\frac{5}{6}\right)^{i}(-1)^{r}(q-1)^{i-r}\binom{j}{r}\binom{s-j}{i-r}\right]B_j(D^{\perp}) - \left(\frac{4}{3}\right)^{s}\\
&= \left(\frac{3}{4}\right)^{s}\sum_{j=0}^{s}\left(1+\frac{5}{6}\right)^{s-j}\left(1-\frac{5}{6}\right)^{j}B_j(D^{\perp}) - \left(\frac{4}{3}\right)^{s}\\
&= \left(\frac{11}{8}\right)^{s}\sum_{j=0}^{s}\frac{B_j(D^{\perp})}{11^{j}} - \left(\frac{4}{3}\right)^{s},
\end{aligned}$$

where the last two equality is from (2) and the last second equality follows Lemma 3 below. The proof is completed. □

Lemma 3. *For any integer s,* $0 \le j \le s$, $q > 1$, *and real* $a > 0$, *we have*

$$\sum_{i=0}^{s}\sum_{r=0}^{i} a^i(-1)^r(q-1)^{i-r}\binom{j}{r}\binom{s-j}{i-r} = (a(q-1)+1)^{s-j}(1-a)^j. \quad (11)$$

Proof. Expanding the right-hand side of (11) we have

$$(a(q-1)+1)^{s-j}(1-a)^j = \sum_{t=0}^{s-j}\binom{s-j}{t}a^t(q-1)^t\sum_{r=0}^{j}\binom{j}{r}(-a)^r.$$

Its coefficient of a^i is $\sum_{r=0}^{i}(-1)^r(q-1)^{i-r}\binom{j}{r}\binom{s-j}{i-r}$ and the lemma follows. □

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