The Annals of Statistics
1998, Vol. 26, No. 4, 1522–1539

TWO-LEVEL FACTORIAL DESIGNS WITH EXTREME NUMBERS OF LEVEL CHANGES

BY CHING-SHUI CHENG,[1] R. J. MARTIN AND BOXIN TANG

University of California, Berkeley, University of Sheffield and University of Memphis

The construction of run orders of two-level factorial designs with extreme (minimum and maximum) numbers of level changes is considered. Minimizing the number of level changes is mainly due to economic considerations, while the problem of maximizing the number of level changes arises from some recent results on trend robust designs. The construction is based on the fact that the 2^k runs of a saturated regular fractional factorial design for $2^k - 1$ factors can be ordered in such a way that the numbers of level changes of the factors consist of each integer between 1 and $2^k - 1$. Among other results, we give a systematic method of constructing designs with minimum and maximum numbers of level changes among all designs of resolution at least three and among those of resolution at least four. It is also shown that among regular fractional factorial designs of resolution at least four, the number of level changes can be maximized and minimized by different run orders of the same fraction.

1. Introduction. This paper considers the construction of run orders of two-level factorial designs with extreme numbers of level changes when the experiments are to be conducted sequentially Here "extreme" means both "minimum" and "maximum." The problem of minimizing the number of level changes arises naturally from economic considerations when it is expensive, time-consuming or difficult to change factor levels [Draper and Stoneman (1968), Joiner and Campbell (1976)]. On the other hand, one-dimensional dependence is to be expected in many factorial field trials, where units are usually long and thin, and adjoining along the long edge, and temporal dependence is at least a strong possibility in many industrial factorial experiments—the phrase "run order" suggests observations are taken over time. Such dependence can be modeled using fixed or random trends. Cheng and Steinberg (1991) determined trend robust run orders of two-level factorial designs under first-order autoregressive and other more complex time series models for the time trend effects. Run orders with a maximum number of level changes are found to be nearly optimal for the AR(1), and highly efficient for some other models.

The problem of minimizing the total number of level changes in a regular two-level factorial design was solved in Cheng (1985). With obvious modifica-

Received June 1996; revised December 1997.
[1]Supported by NSF Grant DMS-94-04477 and NSA Grant MDA904-95-1-1064.
AMS 1991 *subject classification*. Primary 62K15.
Key words and phrases. Orthogonal array, regular fractional factorial design, resolution, run order.

tions, it can also be applied to determine run orders with a maximum number of level changes The work of Cheng (1985) was to construct run orders with minimum numbers of level changes for a *given* defining relation. Similarly, Cheng and Steinberg (1991) found efficient run orders (under time trends or dependence) of a regular fractional factorial design with a given defining relation, but other defining relations may yield designs with more efficient run orders. In this paper, the selection of defining relation and run order will be considered at the same time. Some results along this line have been reported in Wang and Jan (1995). In particular, they have given rules for constructing designs with minimum numbers of level changes in several different situations. However, these rules are not adequately justified. The proof is incomplete (see Remark 3.1) and their rule for constructing resolution-four designs with the minimum number of level changes is not correct.

We shall first present some preliminary results concerning saturated fractional factorial designs of resolution three in Section 2. These results provide the basis for the construction in this paper. Designs with minimum numbers of level changes are then considered in Section 3. In particular, a systematic method is given for constructing designs which have minimum numbers of level changes among all the designs of resolution at least three and among those of resolution at least four. Section 4 is concerned with maximizing the number of level changes. It is interesting to note that among fractional factorial designs of resolution at least four, the number of level changes can be maximized and minimized by two different run orders of the *same* fraction. The proof of the main theorem in Section 3 is presented in Section 5.

Now we review some background material and notation that will be used throughout this paper. The two levels of each factor are denoted by 0 and 1. For any two $(0,1)$-vectors $\mathbf{a} = (a_1, \dots, a_n)^T$ and $\mathbf{b} = (b_1, \dots, b_m)^T$, $\mathbf{a} \oplus \mathbf{b}$ denotes their Kronecker sum $(a_1 + b_1, \dots, a_1 + b_m, \dots, a_n + b_1, \dots, a_n + b_m)^T$, where the arithmetic is carried out $\bmod 2$, and when $n = m$, $\mathbf{a} + \mathbf{b}$ denotes the vector whose ith component is $a_i + b_i \pmod 2$. Each combination of n two-level factors is denoted by a row vector $\mathbf{x} = (x_1, x_2, \dots, x_n)$, where $x_i = 0$ or 1. An N-run design (together with a run order) can be represented by an $N \times n$ matrix. Such a design is called an orthogonal array with strength t, denoted $OA(N, 2^n, t)$, if in any $N \times t$ submatrix, all the 2^t $1 \times t$ vectors of 0's and 1's appear equally often. Orthogonal arrays with strength 2 can be used as orthogonal *main-effect plans* since such designs allow the estimation of all the main effects when the interactions are negligible. A main-effect plan with $N = n + 1$ is called *saturated*.

Important examples of orthogonal arrays are the classical *regular* fractional factorial designs constructed by using defining relations as discussed in many textbooks on experimental design. Recall that a regular 2^{n-p} fractional factorial design, which has n two-level factors and 2^{n-p} runs, is determined by p independent defining effects (also called defining words.) The *resolution* of such a design is defined as the length of the shortest word in its defining relation [Box and Hunter (1961)]. It is well known that a regular fractional factorial design of resolution R is an orthogonal array with strength $R - 1$.

Since a 2^{n-p} fractional factorial design is a group under the componentwise addition $\mathbf{x}+\mathbf{y}$, it contains $n-p$ independent generators. These are $n-p$ factor-level combinations such that all their possible sums produce all the combinations in the fraction. Cheng and Steinberg (1991) describe a *reverse foldover algorithm*, useful for constructing run orders with extreme numbers of level changes. Let $k = n - p$ and suppose $\mathbf{x}_1, \dots, \mathbf{x}_k$ is a sequence of independent generators. The run order obtained by the reverse foldover algorithm starts with $\mathbf{0}$, the combination in which all the factors are at level 0. The subsequent runs can be constructed by induction as follows. Suppose the first 2^s runs are $\mathbf{z}_1, \dots, \mathbf{z}_{2^s}$, $0 \le s \le k-1$. Then the next 2^s runs are $\mathbf{z}_{2^s} + \mathbf{x}_{s+1}$, $\mathbf{z}_{2^s-1}+\mathbf{x}_{s+1}, \dots, \mathbf{z}_1+\mathbf{x}_{s+1}$. It is clear that in the resulting run order, the number of level changes of the ith factor, $1 \le i \le n$, is equal to $\sum_{j=1}^{k}$ (the ith component of $\mathbf{x}_j)2^{k-j}$. The generators $\mathbf{x}_1, \dots, \mathbf{x}_k$can be selected carefully to produce an extreme number of level changes. In fact, from the results in Cheng (1985), the following can be established.

LEMMA 1.1. *For any given regular 2^{n-p} fractional factorial design d, let $k = n - p$ independent generators $\mathbf{x}_1, \dots, \mathbf{x}_k$ be constructed as follows: $\mathbf{x}_1$ has the smallest number of components equal to 1 among all the combinations in d, and for each $2 \le i \le k$, $\mathbf{x}_i$ has the smallest number of components equal to 1 among all the combinations in d which are not linear combinations of $\mathbf{x}_1, \dots, \mathbf{x}_{i-1}$. Then the run order of d obtained by applying the reverse foldover algorithm to $\mathbf{x}_1, \dots, \mathbf{x}_k$ has the minimum number of level changes among all the $(2^{n-p})!$ run orders of d. In the above, if "smallest" is changed to "largest," then a run order with a maximum number of level changes is obtained.*

An important consequence of Lemma 1.1 is that extreme numbers of level changes can always be achieved by applying the reverse foldover algorithm to appropriate sequences of independent generators.

2. Saturated orthogonal arrays with strength two. We first prove that in a saturated two-level orthogonal array with strength 2, the number of level changes between any two runs is a constant.

THEOREM 2.1. *In any run order of a saturated orthogonal array $OA(N, 2^{N-1}, 2)$, there are $N/2$ level changes between any two consecutive runs.*

PROOF. Denote the two levels by 1 and -1. Represent any run order of a saturated $OA(N, 2^{N-1}, 2)$ by an $N \times (N-1)$ matrix $\mathbf{X}$. Then the matrix $\mathbf{H} = [\mathbf{1}_N \,\vdots\, \mathbf{X}]$ is a Hadamard matrix, where $\mathbf{1}_N$ is the $N \times 1$ vector of ones. It follows that $\mathbf{H}\mathbf{H}' = N\mathbf{I}_N$, that is, the rows of $\mathbf{H}$ are mutually orthogonal. Therefore for any two rows of $\mathbf{X}$, $N/2-1$ corresponding entries have the same sign and $N/2$ have opposite signs. □

An interesting consequence of Theorem 2.1 is that *all* the run orders of a saturated $OA(N, 2^{N-1}, 2)$ have the same total number of level changes

$N(N-1)/2$. In this case, there is no need to consider the minimization or maximization of the total number of level changes. If such an orthogonal array is also a *regular* fractional factorial design, then run orders can be constructed so that the numbers of level changes for the $N-1$ factors consist of each integer from 1 to $N-1$ [Wang and Jan (1995), but also discovered by us independently]. Before describing this interesting and useful fact in more detail, we note that it is not true for nonregular saturated designs.

For each $i = 1, \dots, k$, let

$$\mathbf{A}_i = \mathbf{a}_1^i \oplus \cdots \oplus \mathbf{a}_k^i, \tag{2.1}$$

where $\mathbf{a}_i^i = (0, 1)^T$, and all the other $\mathbf{a}_j^i$'s are equal to $(0, 0)^T$. Then the rows of the $2^k \times k$ matrix $[\mathbf{A}_1, \dots, \mathbf{A}_k]$ are all the 2^k combinations of k two-level factors in the standard (Yates) order. Each $\mathbf{A}_i$ can be thought of as representing the main effect of the ith factor; then for any $1 \le i_1 < \cdots < i_t \le k$, the componentwise sum $\mathbf{A}_{i_1} + \cdots + \mathbf{A}_{i_t}$ represents the interaction of factors $i_1, \dots, i_t$. There are $2^k - k - 1$ such interaction columns. Let $\mathbf{M}$ be the $2^k \times (2^k - 1)$ matrix consisting of $\mathbf{A}_1, \dots, \mathbf{A}_k$ and all the interaction columns such that the $2^k - 1$ columns are ordered as follows: the first column is $\mathbf{A}_1$, and for each $1 \le s < k$, if the first $2^s - 1$ columns are $\mathbf{a}_1, \dots, \mathbf{a}_{2^s-1}$, then the next 2^s columns are $\mathbf{A}_{s+1} + \mathbf{a}_{2^s-1}$, $\mathbf{A}_{s+1} + \mathbf{a}_{2^s-2}, \dots, \mathbf{A}_{s+1} + \mathbf{a}_1$, $\mathbf{A}_{s+1}$, where $\mathbf{A}_1, \dots, \mathbf{A}_k$ are as defined in (2.1). Now, use each column of $\mathbf{M}$ to define the levels of a factor in 2^k runs; then $\mathbf{M}$ gives a run order of a saturated design of size 2^k. For any n such that $k < n \le 2^k - 1$, a regular $2^{n-(n-k)}$ design together with a run order can be obtained by choosing n columns of $\mathbf{M}$. Furthermore, it is easy to see that the numbers of level changes of the $2^k - 1$ factors in $\mathbf{M}$ are the increasing sequence $1, 2, \dots, 2^k - 1$. This fact is useful for constructing designs with extreme numbers of level changes; see Wang and Jan (1995) and later discussions in this paper.

For example, when $k = 3$, $\mathbf{M}$ consists of the seven columns $\mathbf{A}_1$, $\mathbf{A}_1 + \mathbf{A}_2$, $\mathbf{A}_2$, $\mathbf{A}_2 + \mathbf{A}_3$, $\mathbf{A}_1 + \mathbf{A}_2 + \mathbf{A}_3$, $\mathbf{A}_1 + \mathbf{A}_3$, $\mathbf{A}_3$,

$$\begin{matrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1. \end{matrix} \tag{2.2}$$

Any n $(3 < n \le 7)$ columns of (2.2) define a run order of a $2^{n-(n-3)}$ fractional factorial design. For example, the first five columns define a 2^{5-2} design with 15 $(= 1 + 2 + 3 + 4 + 5)$ level changes. Label the five corresponding factors by A, B, C, D and E, respectively. Then since the second column is the sum of the first and the third, and the fifth column is the sum of the first and the fourth, this design has two independent defining effects ABC and ADE, and the defining relation is $I = ABC = ADE = BCDE$.

The matrix $\mathbf{M}$ can also be constructed as follows. For each integer $1 \le i \le 2^k - 1$, let $\tilde{\mathbf{b}}_i$ be the $k \times 1$ vector which gives the binary representation of i, with the digit corresponding to 2^{j-1} appearing at the $(k-j+1)$th component of $\tilde{\mathbf{b}}_i$, $1 \le j \le k$, that is, $i = \sum_{j=1}^{k}$ [the $(k-j+1)$th component of $\tilde{\mathbf{b}}_i] \cdot 2^{j-1}$. Form the matrix

$$\tilde{\mathbf{B}} = [\tilde{\mathbf{b}}_1 \quad \tilde{\mathbf{b}}_2 \ \cdots \ \tilde{\mathbf{b}}_{2^k-1}]. \tag{2.3}$$

Let the rows of $\tilde{\mathbf{B}}$ be $\tilde{\mathbf{x}}_1, \dots, \tilde{\mathbf{x}}_k$. Since $\tilde{\mathbf{b}}_1, \ \tilde{\mathbf{b}}_2, \dots, \tilde{\mathbf{b}}_{2^k-1}$ are all the $2^k - 1$ nonzero $k \times 1$ vectors of 1's and 0's, the rank of $\tilde{\mathbf{B}}$ is equal to k. Therefore $\tilde{\mathbf{x}}_1, \dots, \tilde{\mathbf{x}}_k$ are a set of independent generators of a saturated regular fractional factorial design of size 2^k. Applying the reverse foldover algorithm to this generator sequence yields the matrix $\mathbf{M}$. Indeed, the number of level changes in the ith column is equal to $\sum_{j=1}^{k}$ (the ith component of $\tilde{\mathbf{x}}_j) \cdot 2^{k-j} = \sum_{j=1}^{k}$ (the jth component of $\tilde{\mathbf{b}}_i) \cdot 2^{k-j} = \sum_{j=1}^{k}$ [the $(k-j+1)$th component of $\tilde{\mathbf{b}}_i]2^{j-1} = i$. For example, when $k = 3$, the binary representations of $1, 2, \dots, 7$ are

$$\begin{matrix} 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 0 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1. \end{matrix}$$

Run order (2.2) can be obtained by applying the reverse foldover algorithm to these three row vectors.

We conclude this section with a useful lemma.

LEMMA 2.1. *In the run order of a regular 2^{n-p} fractional factorial design obtained by applying the reverse foldover algorithm to an arbitrary sequence of independent generators, the resulting n columns of factor levels must be among the columns of* $\mathbf{M}$.

PROOF. Suppose $\mathbf{u}_1, \dots, \mathbf{u}_k$ is the sequence of independent generators used in the construction. Then since $\tilde{\mathbf{b}}_1, \ \tilde{\mathbf{b}}_2, \dots, \tilde{\mathbf{b}}_{2^k-1}$ are all the $2^k - 1$ nonzero $k \times 1$ vectors of 1's and 0's, the columns of $[\mathbf{u}_1^T, \dots, \mathbf{u}_k^T]^T$ are among those of $[\tilde{\mathbf{b}}_1 \ \tilde{\mathbf{b}}_2 \cdots \tilde{\mathbf{b}}_{2^k-1}]$. $\square$

3. Designs with minimum numbers of level changes. The fact that the columns of $\mathbf{M}$ are in a strictly increasing order with respect to the numbers of level changes suggests that a design with the minimum number of level changes can be obtained by successively choosing columns of $\mathbf{M}$ [Wang and Jan (1995)].

THEOREM 3.1. *Among the regular fractional factorial designs with n two-level factors in $N = 2^k$ runs, where $2^{k-1} \le n \le 2^k - 1$, a design with the minimum number of level changes can be obtained by selecting the first n*

columns of $\mathbf{M}$. *An equivalent method is to apply the reverse foldover algorithm to the row vectors of the submatrix* $[\tilde{\mathbf{b}}_1\ \tilde{\mathbf{b}}_2 \cdots \tilde{\mathbf{b}}_n]$ *of* (2.3). *The resulting design is of resolution at least three*.

PROOF. It is obvious that the design constructed is of resolution at least three. We now show that it has the minimum number of level changes among all the regular fractional factorial designs.

By Lemma 1.1, for a regular fractional factorial design with any given defining relation, a minimum number of level changes can always be achieved by applying the reverse foldover algorithm to an appropriate sequence of independent generators. It follows from Lemma 2.1 that in such a run order, the n columns of factor levels must be among the columns of $\mathbf{M}$. Since the columns of $\mathbf{M}$ are ordered so that the numbers of level changes of the factors are strictly increasing, the method described in this theorem obviously produces a design with the minimum number of level changes. $\square$

REMARK 3.1. In general, not all the run orders of a regular fractional factorial design can be constructed by the reverse foldover algorithm. For such run orders, the columns of factor levels are not necessarily drawn from those of $\mathbf{M}$. Therefore it is necessary to invoke Lemma 1.1 [which goes back to Cheng (1985)] to show that it is enough to restrict attention to the columns of $\mathbf{M}$, as Wang and Jan (1995) did. In this sense, Wang and Jan's (1995) arguments are incomplete.

The condition $2^{k-1} \le n \le 2^k - 1$ is to ensure that the rank of $[\tilde{\mathbf{b}}_1\ \tilde{\mathbf{b}}_2 \cdots \tilde{\mathbf{b}}_n]$ is equal to k, and therefore the design constructed is a genuine unreplicated fractional factorial design. If $k \le n < 2^{k-1}$, then the design obtained by applying the reverse foldover algorithm to the row vectors of $[\tilde{\mathbf{b}}_1\ \tilde{\mathbf{b}}_2 \cdots \tilde{\mathbf{b}}_n]$ is a replicated fractional factorial design. Such a design has a minimum number of level changes when replicated fractional factorial designs are allowed. If one insists on using unreplicated fractional factorial designs, then a design with the minimum number of level changes can be constructed by choosing the k columns $\{\tilde{\mathbf{b}}_{2^s}\}_{0 \le s \le k-1}$ together with the first $n-k$ columns in the matrix obtained by deleting $\tilde{\mathbf{b}}_{2^s}$, $0 \le s \le k-1$, from $[\tilde{\mathbf{b}}_1\ \tilde{\mathbf{b}}_2 \cdots \tilde{\mathbf{b}}_{2^k-1}]$. Note that $\{\tilde{\mathbf{b}}_{2^s}\}_{0 \le s \le k-1}$ are the first k linearly independent columns of $[\tilde{\mathbf{b}}_1\ \tilde{\mathbf{b}}_2 \cdots \tilde{\mathbf{b}}_{2^k-1}]$.

When additional properties besides resolution three are desired, the selection of columns from $\mathbf{M}$ or (2.3) must be subject to some constraints. For instance, Cheng and Jacroux (1988) showed that for any $1 \le i_1 < \cdots < i_t \le n$, the t-factor interaction column $\mathbf{A}_{i_1} + \cdots + \mathbf{A}_{i_t}$ is orthogonal to a polynomial time trend with degree $t-1$, and suggested the method of selecting appropriate interaction columns to construct trend-free run orders. This and the same argument as in the proof of Theorem 3.1 can be used to justify Wang and Jan's (1995) rule that a design with the minimum number of level changes among those of resolution at least three in which all the main-effect contrasts are linear-trend free can be obtained by selecting the first n non-main-effect columns of $\mathbf{M}$. Wang and Jan (1995) also gave selection rules subject to other constraints. If a design of resolution at least four is required, then the sum of any two selected columns cannot be selected. This makes the construction of run orders with minimum numbers of level changes among all the designs of resolution at least four a nontrivial problem. In fact, as we shall see later in Example 3.1, Wang and Jan's (1995) rule for constructing such designs is not correct.

The rest of this section is devoted to a correct method of constructing designs with minimum numbers of level changes among those of resolution at least four. We shall present our construction and proof in terms of the selection of columns from $\tilde{\mathbf{B}}$ in (2.3). For convenience, we shall let $\mathbf{y}_1 = \mathbf{0}$, and define $\mathbf{y}_i = \tilde{\mathbf{b}}_{i-1}$, $2 \le i \le 2^k$. If we think of each $\mathbf{y}_i$ as a factor-level combination in a 2^k design, then $\mathbf{y}_1, \dots, \mathbf{y}_{2^k}$ are the 2^k combinations in the standard (Yates) order. A design with n factors can be constructed by selecting n columns from $\mathbf{y}_2, \dots, \mathbf{y}_{2^k}$. Then each $\mathbf{y}_i$ defines a factor with $i-1$ level changes.

It is well known that an n-factor design of resolution at least four must have at least $2n$ runs. Therefore for a regular fractional factorial design of size 2^k to be of resolution at least four, the number of factors is at most 2^{k-1}. The following describes a solution for designs of resolution at least four for n factors in 2^k runs, where $2^{k-2}+1 \le n \le 2^{k-1}$.

THEOREM 3.2. (i) *When* $2^{k-2}+1 \le n \le 2^{k-2}+2^{k-3}$, *a design with n factors in* 2^k *runs which minimizes the number of level changes among those of resolution at least four can be constructed by selecting the* 2^{k-2} *columns* $\mathbf{y}_{2^{k-3}+1}, \dots, \mathbf{y}_{2^{k-3}+2^{k-2}}$ *and the* $n-2^{k-2}$ *columns* $\mathbf{y}_{2^{k-1}+1}, \dots, \mathbf{y}_{2^{k-1}+n-2^{k-2}}$;

(ii) *When* $2^{k-2}+2^{k-3}+1 \le n \le 2^{k-1}$, *a solution can be obtained by selecting the* 2^{k-2} *columns* $\mathbf{y}_{2^{k-3}+1}, \dots, \mathbf{y}_{2^{k-3}+2^{k-2}}$, *the* 2^{k-3} *columns* $\mathbf{y}_{2^{k-1}+1}, \dots, \mathbf{y}_{2^{k-1}+2^{k-3}}$ *and the* $n-2^{k-2}-2^{k-3}$ *columns* $\mathbf{y}_{2^k-2^{k-3}+1}, \dots, \mathbf{y}_{2^{k-1}+n}$.

It is clear that in Theorem 3.2, the sum of any two selected columns is not selected. Therefore the design obtained is of resolution at least four. The proof that this method does produce designs with minimum numbers of level changes among those of resolution at least four will be presented in Section 5.

Applying the method of Theorem 3.2, we obtain the following selection of columns from $\mathbf{y}_2, \dots, \mathbf{y}_{2^k}$:

2^{4-1}: select columns 2, 3, 5, 8
2^{5-1}: select columns 3, 4, 5, 6, 9
2^{6-2}: select columns 3, 4, 5, 6, 9, 10
2^{7-3}: select columns 3, 4, 5, 6, 9, 10, 15
2^{8-4}: select columns 3, 4, 5, 6, 9, 10, 15, 16
2^{9-4}: select columns 5, 6, 7, 8, 9, 10, 11, 12, 17
2^{10-5}: select columns 5, 6, 7, 8, 9, 10, 11, 12, 17, 18
$\cdots$.

Note that for 2^{n-p} designs, the columns referred to in the above are $(n-p) \times 1$ vectors. For example, both column five's used in constructing 2^{8-4} and 2^{9-4} designs are binary representations of 4, but the former is the 4×1 vector $(0,1,0,0)^T$, and the latter is the 5×1 vector $(0,0,1,0,0)^T$. We also note that the designs constructed by the method of Theorem 3.2 are not the only possible solutions.

EXAMPLE 3.1. Consider 2^{10-5} designs. The 10 columns given above lead to a design with 93 level changes. This is the same as to select the following ten columns of $\mathbf{M}$: $\mathbf{A}_2+\mathbf{A}_3$, $\mathbf{A}_1+\mathbf{A}_2+\mathbf{A}_3$, $\mathbf{A}_1+\mathbf{A}_3$, $\mathbf{A}_3$, $\mathbf{A}_3+\mathbf{A}_4$, $\mathbf{A}_1+\mathbf{A}_3+\mathbf{A}_4$, $\mathbf{A}_1+\mathbf{A}_2+\mathbf{A}_3+\mathbf{A}_4$, $\mathbf{A}_2+\mathbf{A}_3+\mathbf{A}_4$, $\mathbf{A}_4+\mathbf{A}_5$, $\mathbf{A}_1+\mathbf{A}_4+\mathbf{A}_5$. Wang and Jan's (1995) solution is to select the first five linearly independent columns $\mathbf{A}_1$, $\mathbf{A}_1+\mathbf{A}_2$, $\mathbf{A}_2+\mathbf{A}_3$, $\mathbf{A}_3+\mathbf{A}_4$, $\mathbf{A}_4+\mathbf{A}_5$ of $\mathbf{M}$ and then successively select five additional columns subject to the constraint that the sum of any two selected columns cannot be selected: $\mathbf{A}_3$, $\mathbf{A}_2+\mathbf{A}_3+\mathbf{A}_4$, $\mathbf{A}_1+\mathbf{A}_2+\mathbf{A}_4$, $\mathbf{A}_1+\mathbf{A}_4$, $\mathbf{A}_2+\mathbf{A}_4+\mathbf{A}_5$. These correspond to $\mathbf{y}_2$, $\mathbf{y}_3$, $\mathbf{y}_5$, $\mathbf{y}_9$, $\mathbf{y}_{17}$ and $\mathbf{y}_8$, $\mathbf{y}_{12}$, $\mathbf{y}_{14}$, $\mathbf{y}_{15}$, $\mathbf{y}_{20}$, with 95 level changes.

REMARK 3.2. When $k \le n \le 2^{k-2}$, the rules given in Theorem 3.2 need to be modified. We first give a solution for the easier case where replicated fractional factorial designs are allowed. In this case, let k' be an integer such that $2^{k'-2}+1 \le n \le 2^{k'-1}$. Then apply the same rule as in Theorem 3.2 (with k replaced by k') to select n columns from the $2^{k'}-1$ columns $\{\mathbf{y}_2, \mathbf{y}_3, \dots, \mathbf{y}_{2^{k'}}\}$, where each $\mathbf{y}_i$ is $k \times 1$. Since $k' < k$, these n columns do not have full rank. Therefore the design obtained is a replicated fractional factorial design. If one insists on using an unreplicated fractional factorial design, then there must be k linearly independent columns among those which are selected. This can be achieved by the following method: let n' be the largest integer such that $n \ge n' \ge 2^{k-(n-n')-2}+1$. Then a design with the minimum number of level changes among the unreplicated fractional factorial designs of resolution at least four can be obtained by selecting the $n-n'$ columns $\bigcup_{m=1}^{n-n'}\{\mathbf{y}_{2^{k-m}+1}\}$ and n' additional columns from $\{\mathbf{y}_2, \mathbf{y}_3, \dots, \mathbf{y}_{2^{k'}}\}$ by using the rules of Theorem 3.2, where $k' = k-(n-n')$. For example, consider 2^{8-3} designs. If replicated fractions are allowed, then one solution is obtained by choosing the eight columns $\mathbf{y}_3$, $\mathbf{y}_4$, $\mathbf{y}_5$, $\mathbf{y}_6$, $\mathbf{y}_9$, $\mathbf{y}_{10}$, $\mathbf{y}_{15}$, $\mathbf{y}_{16}$, where each $\mathbf{y}_i$ is a 5×1 vector. On the other hand, if only unreplicated fractions are allowed, then one needs to include $\mathbf{y}_{17}$. To choose seven additional columns, since $7 \ge 2^{4-2}+1$, one can apply the same rules as in Theorem 3.2 to choose seven columns from $\mathbf{y}_2, \mathbf{y}_3, \dots, \mathbf{y}_{16}$. This results in the eight columns $\mathbf{y}_3$, $\mathbf{y}_4$, $\mathbf{y}_5$, $\mathbf{y}_6$, $\mathbf{y}_9$, $\mathbf{y}_{10}$, $\mathbf{y}_{15}$, $\mathbf{y}_{17}$.

The following alternative description of a design constructed by the method of Theorem 3.2 is useful for determining its defining relation. Let

$$\mathbf{a}_j = \tilde{\mathbf{b}}_{2^{j-1}}, \quad j = 1, \dots, k. \tag{3.1}$$

Then $\tilde{\mathbf{b}}_1$, $\tilde{\mathbf{b}}_2, \dots, \tilde{\mathbf{b}}_{2^k-1}$ are in the Yates order for the independent columns $\mathbf{a}_1, \dots, \mathbf{a}_k$; that is, $[\tilde{\mathbf{b}}_1,\ \tilde{\mathbf{b}}_2, \dots, \tilde{\mathbf{b}}_{2^k-1}] = [\mathbf{a}_1,\ \mathbf{a}_2, \mathbf{a}_1+\mathbf{a}_2, \mathbf{a}_3, \mathbf{a}_1+\mathbf{a}_3, \mathbf{a}_2+\mathbf{a}_3, \mathbf{a}_1+\mathbf{a}_2+\mathbf{a}_3, \mathbf{a}_4, \mathbf{a}_1+\mathbf{a}_4, \mathbf{a}_2+\mathbf{a}_4, \dots]$. Now let $\mathbf{c}_1 = \mathbf{a}_{k-2}$, $\mathbf{c}_j = \mathbf{a}_{k-2}+\mathbf{a}_{j-1}$ for $j = 2, \dots, k-2$, $\mathbf{c}_{k-1} = \mathbf{a}_{k-1}$ and $\mathbf{c}_k = \mathbf{a}_k$. Obviously $\mathbf{c}_1, \dots, \mathbf{c}_k$ are k independent columns. Furthermore, it can be seen that the design with a minimum number of level changes among those of resolution at least four constructed by the method of Theorem 3.2 *takes the odd-order interaction* *columns* (*including main effect columns*) *successively* in the Yates order for the independent columns $\mathbf{c}_1, \dots, \mathbf{c}_k$. That is, it is given by

$$\begin{aligned}
&\mathbf{c}_1,\ \mathbf{c}_2,\ \mathbf{c}_3,\ \mathbf{c}_1+\mathbf{c}_2+\mathbf{c}_3,\ \mathbf{c}_4,\ \mathbf{c}_1+\mathbf{c}_2+\mathbf{c}_4,\ \mathbf{c}_1+\mathbf{c}_3+\mathbf{c}_4,\\
&\quad \mathbf{c}_2+\mathbf{c}_3+\mathbf{c}_4,\ \mathbf{c}_5,\ \mathbf{c}_1+\mathbf{c}_2+\mathbf{c}_5,\ \mathbf{c}_1+\mathbf{c}_3+\mathbf{c}_5,\ \mathbf{c}_2+\mathbf{c}_3+\mathbf{c}_5,\\
&\quad \mathbf{c}_1+\mathbf{c}_4+\mathbf{c}_5,\ \mathbf{c}_2+\mathbf{c}_4+\mathbf{c}_5,\ \mathbf{c}_3+\mathbf{c}_4+\mathbf{c}_5,\ \mathbf{c}_1+\mathbf{c}_2+\mathbf{c}_3+\mathbf{c}_4+\mathbf{c}_5,\\
&\quad \mathbf{c}_6,\ \mathbf{c}_1+\mathbf{c}_2+\mathbf{c}_6,\ \mathbf{c}_1+\mathbf{c}_3+\mathbf{c}_6,\ \mathbf{c}_2+\mathbf{c}_3+\mathbf{c}_6,\ \mathbf{c}_1+\mathbf{c}_4+\mathbf{c}_6,\\
&\quad \mathbf{c}_2+\mathbf{c}_4+\mathbf{c}_6,\ \mathbf{c}_3+\mathbf{c}_4+\mathbf{c}_6,\ \mathbf{c}_1+\mathbf{c}_2+\mathbf{c}_3+\mathbf{c}_4+\mathbf{c}_6,\dots.
\end{aligned} \tag{3.2}$$

This can be verified by comparing the two sequences and noting that $\mathbf{y}_1, \dots, \mathbf{y}_{2^k}$ are in the Yates order. From the pattern of the columns in (3.2), one can easily determine the defining relation of the resulting design.

EXAMPLE 3.2. Consider 2^{8-4} designs. The binary representations of 2, 3, 4, 5, 8, 9, 14 and 15 give the following 4×8 matrix:

$$\begin{matrix}
0 & 0 & 0 & 0 & 1 & 1 & 1 & 1\\
0 & 0 & 1 & 1 & 0 & 0 & 1 & 1\\
1 & 1 & 0 & 0 & 0 & 0 & 1 & 1\\
0 & 1 & 0 & 1 & 0 & 1 & 0 & 1.
\end{matrix}$$

Applying the reverse foldover algorithm to the four rows of the above matrix, we obtain a run order of a 2^{8-4} design with the minimum number of level changes among all 2^{8-4} designs of resolution at least four. Label the eight factors (columns) by A, B, C, D, E, F, G and H. Then by the remark in the previous paragraph, these eight columns correspond to $\mathbf{c}_1$, $\mathbf{c}_2$, $\mathbf{c}_3$, $\mathbf{c}_1+\mathbf{c}_2+\mathbf{c}_3$, $\mathbf{c}_4$, $\mathbf{c}_1+\mathbf{c}_2+\mathbf{c}_4$, $\mathbf{c}_1+\mathbf{c}_3+\mathbf{c}_4$ and $\mathbf{c}_2+\mathbf{c}_3+\mathbf{c}_4$. Clearly this design is defined by $D = ABC$, $F = ABE$, $G = ACE$ and $H = BCE$ and therefore has independent defining effects $ABCD$, $ABEF$, $ACEG$ and $BCEH$.

4. Designs with maximum numbers of level changes. To construct designs with maximum numbers of level changes, we start from $\mathbf{y}_{2^k}$ and move down the list. For example, the maximum number of level changes for n factors in $N = 2^k$ runs is $Nn - n(n+1)/2$, which results from choosing columns $\mathbf{y}_{2^k}, \dots, \mathbf{y}_{2^k-n+1}$. Designs constructed in this manner have resolution at least three, and the resolution is at least four when $n \le N/2$. The latter holds because $\mathbf{y}_{N-i} + \mathbf{y}_{N-j} = \mathbf{y}_i + \mathbf{y}_j$, for all i, j and $\mathbf{y}_i + \mathbf{y}_j = \mathbf{y}_r$, $i, j \le 2^{k-1} \Rightarrow r \le 2^{k-1}$; therefore if $n \le N/2$, then the sum of any two selected columns is not selected. However, since $\mathbf{y}_N + \mathbf{y}_{N-1} + \mathbf{y}_{N-2} + \mathbf{y}_{N-3} = \mathbf{0}$, the resolution is at most four when $n > 3$. Furthermore, since $\{\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_{2^{k-1}}\}$ is a subgroup, increasingly many words in the defining relation will have length 4 for $n > 3$. The implications of these results are that for $n > 3$, designs which maximize the number of level changes over all designs (including replicated fractional factorials) do not have maximum resolution if there exist designs of resolution higher than four, and even if the maximum resolution is four, resolution-four designs with maximum numbers of level changes may have more words of length four [higher aberration in the sense of Fries and Hunter (1980)]. In other words, maximum resolution and minimum aberration designs tend not to produce maximum numbers of level changes.

For example, among all unreplicated 2^{7-2} designs, the maximum number of level changes (194) is achieved by the resolution-four design with defining relation $I = ABCD = CDEF = ABEF$. For the minimum aberration design, which has one word of length four and two words of length five, the maximum number of level changes is only 183. These numbers of level changes can be verified by using Lemma 1.1. A third design with two words of length four and one word of length six can produce 187 level changes. On the other hand, if replicated designs are allowed, then the maximum of 196 is achieved. Note that the large increase possible in the maximum number of level changes over the usual unreplicated designs can appreciably increase the design efficiency under dependence.

It can be seen that $\mathbf{y}_{2^k} = \sum_{i=1}^{k} \mathbf{a}_i$, and for $m = 0, 1, \dots, k-2$, $\mathbf{y}_{2^k-2^m} = \sum_{1\le i\le k,\, i\ne m+1} \mathbf{a}_i$, where $\mathbf{a}_1, \dots, \mathbf{a}_k$ are as defined in (3.1). The k columns $\mathbf{y}_{2^k}, \mathbf{y}_{2^k-1}, \mathbf{y}_{2^k-2}, \dots, \mathbf{y}_{2^k-2^{k-2}}$ are clearly linearly independent. In fact, they maximize the total number of level changes among all choices of k linearly independent columns from $\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_{2^k}$. Therefore a run order of the complete 2^k design with a maximum number of level changes can be obtained by using columns $\mathbf{y}_{2^k}, \mathbf{y}_{2^k-1}, \mathbf{y}_{2^k-2}, \dots, \mathbf{y}_{2^k-2^{k-2}}$. Another consequence of this is that when $2^{k-2}+1 \le n \le 2^{k-1}$, the resolution-four design obtained by selecting the n columns $\mathbf{y}_{2^k}$, $\mathbf{y}_{2^k-1}$, $\mathbf{y}_{2^k-2}, \dots, \mathbf{y}_{2^k-n+1}$ is an unreplicated fractional factorial design because they include all the k linearly independent columns $\mathbf{y}_{2^k}$, $\mathbf{y}_{2^k-1}$, $\mathbf{y}_{2^k-2}, \dots, \mathbf{y}_{2^k-2^{k-2}}$. Now let $\mathbf{c}_1 = \mathbf{y}_{2^k}$ and $\mathbf{c}_i = \mathbf{y}_{2^k-2^{i-2}}$ for $i = 2, \dots, k$. Then $\mathbf{y}_{2^k}, \mathbf{y}_{2^k-1}, \mathbf{y}_{2^k-2}, \dots, \mathbf{y}_{2^k-n+1}$ can also be obtained by taking the odd-order interaction columns (including main effect columns) successively in the Yates order for $\mathbf{c}_1, \dots, \mathbf{c}_k$ as in (3.2), except that we have a different definition of $\mathbf{c}_i$ here. This shows that when $2^{k-2}+1 \le n \le 2^{k-1}$, the resolution-four designs with maximum and minimum numbers of level changes constructed here and in Section 3, respectively, have the same defining relation. In fact, it can be seen that this is also true for unreplicated fractions when $k \le n \le 2^{k-2}$.

EXAMPLE 4.1. Consider 2^{8-4} designs. The binary representations of 15, 14, 13, 12, 11, 10, 9 and 8 give the following 4×8 matrix:

$$\begin{matrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 & 0. \end{matrix}$$

Applying the reverse foldover algorithm to the four rows of the above matrix, we obtain a run order of a 2^{8-4} design with the maximum number of level changes among all 2^{8-4} designs of resolution at least four. Label these eight columns by A, B, C, D, E, F, G and H. Then, as in Example 3.2, this design has independent defining effects $ABCD$, $ABEF$, $ACEG$ and $BCEH$.

The following is a list of 4-, 8-, 16- and 32-run designs with maximum numbers of level changes. When more than one design of the same size is given, the first is a usual unreplicated design. If this design is not of the highest possible resolution for the given size, it is followed by an unreplicated design of the highest resolution, which has fewer level changes. A replicated fractional factorial design is also given if it has a larger number of level changes. The notation 2^{n-p+1} means two identical replicates of a 2^{n-p} design. The components of $\mathbf{s} = (s_1, \ldots, s_n)$ are the numbers of level changes of the n factors, and $S = \sum_{i=1}^{n} s_i$ is the total number of level changes. The designs are obtained by selecting columns $\mathbf{y}_{s_1+1}, \ldots, \mathbf{y}_{s_n+1}$.

$N = 4$

$n = 2$: $\mathbf{s} = (3, 2)$, $S = 5$, (complete 2^2)

$n = 3$: $\mathbf{s} = (3, 2, 1)$, $S = 6$. (2_{III}^{3-1}, $I = ABC$)

$N = 8$

$n = 3$: $\mathbf{s} = (7, 6, 5)$, $S = 18$, (complete 2^3)

$n = 4$: $\mathbf{s} = (7, 6, 5, 4)$, $S = 22$, (2_{IV}^{4-1}, $I = ABCD$)

$n = 5$: $\mathbf{s} = (7, 6, 5, 4, 3)$, $S = 25$, (2_{III}^{5-2}, $I = ABCD = ADE = BCE$)

2_{III}^{6-3}, 2_{III}^{7-4} similar.

$N = 16$

$n = 4$: $\mathbf{s} = (15, 14, 13, 11)$, $S = 53$, (complete 2^4)

$\mathbf{s} = (15, 14, 13, 12)$, $S = 54$, (2_{IV}^{4-1+1}, $I = ABCD$)

$n = 5$: $\mathbf{s} = (15, 14, 13, 12, 11)$, $S = 65$, (2_{IV}^{5-1}, $I = ABCD$)

$\mathbf{s} = (15, 14, 13, 11, 7)$, $S = 60$, (2_{V}^{5-1}, $I = ABCDE$)

$n = 6$: $\mathbf{s} = (15, 14, 13, 12, 11, 10)$, $S = 75$, (2_{IV}^{6-2}, $I = ABCD = CDEF = ABEF$)

2_{IV}^{7-3}, 2_{IV}^{8-4}, $2_{III}^{9-5}, \ldots, 2_{III}^{15-11}$ similar.

$N = 32$

$n = 5$: $\mathbf{s} = (31, 30, 29, 27, 23)$, $S = 140$, (complete 2^5)

$\mathbf{s} = (31, 30, 29, 28, 27)$, $S = 145$, (2_{IV}^{5-1+1}, $I = ABCD$)

$n = 6$: $\mathbf{s} = (31, 30, 29, 28, 27, 23)$, $S = 168$, (2_{IV}^{6-1}, $I = ABCD$)

$\mathbf{s} = (31, 30, 29, 27, 23, 16)$, $S = 156$, (2_{VI}^{6-1}, $I = ABCDEF$)

$\mathbf{s} = (31, 30, 29, 28, 27, 26)$, $S = 171$, (2_{IV}^{6-2+1}, $I = ABCD = ABEF = CDEF$)

$n = 7$: $\mathbf{s} = (31, 30, 29, 28, 27, 26, 23)$, $S = 194$, (2_{IV}^{7-2}, $I = ABCD = CDEF = ABEF$)

$\mathbf{s} = (31, 30, 29, 28, 27, 26, 25)$, $S = 196$, (2_{IV}^{7-3+1}, $I = ABCD = ABEF = ACEG = \cdots$)

$n = 8$: $\mathbf{s} = (31, 30, 29, 28, 27, 26, 25, 23)$, $S = 219$, (2_{IV}^{8-3} $I = ABCD = ABEF = ACEG = \cdots$)

$\mathbf{s} = (31, 30, 29, 28, 27, 26, 25, 24)$, $S = 220$, (2_{IV}^{8-4+1}, $I = ABCD = ABEF = ACEG = ABGH = \cdots$)

$n = 9$: $\mathbf{s} = (31, 30, 29, 28, 27, 26, 25, 24, 23)$, $S = 243$, (2_{IV}^{9-4}, $I = ABCD = ABEF = ACEG = ABGH = \cdots$)

2_{IV}^{10-5}, $2_{IV}^{11-6}, \ldots, 2_{IV}^{16-11}$, $2_{III}^{17-12}, \ldots, 2_{III}^{31-26}$ similar.

REMARK 4.1. As noted in Remark 3.1, although the method presented in this paper can be used to construct designs and run orders with maximum numbers of level changes, not all such run orders can be generated by the reverse foldover algorithm. There may be run orders with the same maximum total number of level changes S, but different $\mathbf{s}$. For example, Cheng and Steinberg (1991) presented two different run orders of a complete 2^4 design with the same maximum number of level changes, but one has $\mathbf{s} = (15, 14, 13, 11)$ and the other has $\mathbf{s} = (15, 13, 13, 12)$. In fact, $(14, 14, 13, 12)$ is possible. A more uniform distribution of level changes leads to slightly higher efficiency and more equal variances of estimated effects. For more discussions of this issue, see Saunders, Eccleston and Martin (1995).

5. Proof of Theorem 3.2. Note that in order to have resolution at least four, if two columns $\mathbf{x}$ and $\mathbf{y}$ are selected, then $\mathbf{x}+\mathbf{y}$ cannot be selected. We first state two simple lemmas which impose some constraints on the selection of columns.

LEMMA 5.1. *For any integers s and a, where $a > 0$, if $\mathbf{y} \in \{\mathbf{y}_{2^s+1}, \dots, \mathbf{y}_{2^{s+1}}\}$, $\mathbf{z} \in \{\mathbf{y}_{a\cdot 2^{s+1}+1}, \dots, \mathbf{y}_{a\cdot 2^{s+1}+2^s}\}$ and $\mathbf{u} \in \{\mathbf{y}_{a\cdot 2^{s+1}+2^s+1}, \dots, \mathbf{y}_{(a+1)\cdot 2^{s+1}}\}$, then $\mathbf{y}+\mathbf{z} \in \{\mathbf{y}_{a\cdot 2^{s+1}+2^s+1}, \dots, \mathbf{y}_{(a+1)\cdot 2^{s+1}}\}$ and $\mathbf{y}+\mathbf{u} \in \{\mathbf{y}_{a\cdot 2^{s+1}+1}, \dots, \mathbf{y}_{a\cdot 2^{s+1}+2^s}\}$.*

PROOF. As noted earlier, $\mathbf{y}_1, \mathbf{y}_2, \dots, \mathbf{y}_{2^k}$ can be viewed as the combinations of a 2^k design in the standard (Yates) order. □

LEMMA 5.2. *For any integers s and a, where $a > 0$, if at least one of the 2^s columns $\mathbf{y}_{2^s+1}, \dots, \mathbf{y}_{2^{s+1}}$ is selected, then at most 2^s columns can be selected from $\{\mathbf{y}_{a\cdot 2^{s+1}+1}, \dots, \mathbf{y}_{(a+1)\cdot 2^{s+1}}\}$.*

PROOF. Suppose $\mathbf{y} \in \{\mathbf{y}_{2^s+1}, \dots, \mathbf{y}_{2^{s+1}}\}$ is selected. It follows from Lemma 5.1 that if $\mathbf{v} \in \{\mathbf{y}_{a\cdot 2^{s+1}+1}, \dots, \mathbf{y}_{(a+1)\cdot 2^{s+1}}\}$, then $\mathbf{y}+\mathbf{v} \in \{\mathbf{y}_{a\cdot 2^{s+1}+1}, \dots, \mathbf{y}_{(a+1)\cdot 2^{s+1}}\}$. Only one of $\mathbf{v}$ and $\mathbf{y}+\mathbf{v}$ can be selected. □

For an arbitrary design d of resolution at least four, we shall show that the method of Theorem 3.2 produces a design with the number of level changes no more than that of d. Lemma 5.2 holds for any s, but in the following we shall let s be the *smallest* integer such that at least one of $\mathbf{y}_2, \dots, \mathbf{y}_{2^{s+1}}$ is selected by d (so *none* of the columns $\mathbf{y}_i$ with $i \le 2^s$ is selected). The proof of Theorem 3.2 is now presented in four steps.

STEP 1. Show that it is sufficient to consider the case $s \le k-3$.

Divide the 2^k columns $\mathbf{y}_1, \dots, \mathbf{y}_{2^k}$ into 2^{k-s-2} sets of size 2^{s+2}, each of which is further divided into four sets of size 2^s. Specifically, for any nonnegative integer m such that $(m+1)2^{s+2} \le 2^k$, let $A_0^m = \{\mathbf{y}_{m2^{s+2}+1}, \dots, \mathbf{y}_{m2^{s+2}+2^s}\}$, $A_1^m = \{\mathbf{y}_{m2^{s+2}+2^s+1}, \dots, \mathbf{y}_{m2^{s+2}+2^{s+1}}\}$, $A_2^m = \{\mathbf{y}_{m2^{s+2}+2^{s+1}+1}, \dots, \mathbf{y}_{m2^{s+2}+3\cdot 2^s}\}$ and $A_3^m = \{\mathbf{y}_{m2^{s+2}+3\cdot 2^s+1}, \dots, \mathbf{y}_{(m+1)2^{s+2}}\}$.

STEP 2. For $s \le k-3$, show that it is enough to consider the case where at least one column is selected from $A_0^m \cup A_2^m$ for a certain m with $0 \le m \le 2^{k-s-3}-1$.

Let g be the smallest m as in Step 2. If $g = 0$, let $r = 0$; otherwise, let r be such that $2^{r-1} \le g \le 2^r - 1$. Now write n as $n = t \cdot 2^{r+s+1} + u$, where $0 \le u < 2^{r+s+1}$ and

$$u = e2^{s+1} + q, \tag{5.1}$$

$0 \le q < 2^{s+1}$. Let

$$w = t2^r + e. \tag{5.2}$$

Then $n = w2^{s+1} + q$. Now $2^{r-1} \le g \le 2^{k-s-3} - 1 \Rightarrow r - 1 < k - s - 3 \Rightarrow 2^{r+s+1} \le 2^{k-2}$. Since $n > 2^{k-2}$, $n > 2^{r+s+1}$; therefore,

$$t \ge 1. \tag{5.3}$$

STEP 3. Show that when $u \le 2^{r+s}$, the total number of level changes under d is at least as large as that of the n columns $\{\bigcup_{m=0}^{t2^r-1}(A_1^m \cup A_2^m)\} \cup \{\mathbf{y}_{t2^r\cdot 2^{s+2}+1}, \mathbf{y}_{t2^r\cdot 2^{s+2}+2}, \dots, \mathbf{y}_{t2^r\cdot 2^{s+2}+u}\}$, while for $u > 2^{r+s}$, it is at least as large as the total number of level changes in $\{\bigcup_{m=0}^{t2^r-1}(A_1^m \cup A_2^m)\} \cup \{\mathbf{y}_{t2^r\cdot 2^{s+2}+1}, \mathbf{y}_{t2^r\cdot 2^{s+2}+2}, \dots, \mathbf{y}_{t2^r\cdot 2^{s+2}+2^{r+s}}\} \cup \{\mathbf{y}_{t2^r\cdot 2^{s+2}+3\cdot 2^{r+s}+1}, \dots, \mathbf{y}_{t2^r\cdot 2^{s+2}+2^{r+s+1}+u}\}$. Since $n = t2^{r+s+1} + u \le 2^{k-1}$, we do have $t2^r \cdot 2^{s+2} + 2^{r+s+1} + u \le 2^k$. Therefore the selection of these columns is possible. Note that these columns may not produce resolution-four designs; they are merely used to provide lower bounds.

STEP 4. Show that the total number of level changes of the columns in Step 3 is at least as large as that under a design constructed by the method of Theorem 3.2.

PROOF OF STEP 1. If $s > k - 3$, then none of the 2^{k-2} columns $\mathbf{y}_1, \dots, \mathbf{y}_{2^{k-2}}$ is selected. Divide all the 2^k columns successively into eight sets of equal size, say $B_1, B_2, \dots, B_8$, where B_1 consists of the first 2^{k-3} columns, B_2 consists of the next 2^{k-3} columns, and so on. Then the design of Theorem 3.2 successively selects columns from B_2, B_3, B_5 and B_8, while d skips B_1 and B_2, and draws its first column from B_3. It is clear that the excessive numbers of level changes of columns from B_3 cannot be compensated by any possible savings provided by later columns.

PROOF OF STEP 2. We first state the following simple lemma.

LEMMA 5.3. *If* $\mathbf{y} \in A_i^0$, $i = 0$ *or* 2 *and* $\mathbf{z} \in A_j^m$, $j = 0, 1, 2, 3$, *then* $\mathbf{y}+\mathbf{z} \in A_l^m$, *where* $l \equiv i + j (\mathrm{mod}\, 4)$. *Hence if* v *of the* 2^s *columns in* A_i^0 *are selected, and at least one column in* A_j^m *is also selected, then at most* $2^s - v$ *columns in* A_l^m *can be selected.*

Since at least one of the 2^s columns $\mathbf{y}_{2^s+1}, \dots, \mathbf{y}_{2^{s+1}}$ is selected, by Lemma 5.2 for each $m \ge 2^{k-s-3}$, at most 2^s columns can be selected from $A_0^m \cup A_1^m$. Suppose for all $0 \le m \le 2^{k-s-3} - 1$, none of the columns in $A_0^m \cup A_2^m$ is selected. Then those selected from the first 2^{k-1} columns must be from sets of the form A_1^m or A_3^m. It can easily be seen that, compared with the design constructed by the method of Theorem 3.2, the resulting excessive numbers of level changes cannot be compensated by any possible savings from those selected from the second half, which suffer from the restriction that at most 2^s columns can be selected from each $A_0^m \cup A_1^m$.

Since the proof of Step 3 is long, we present the proof of Step 4 first.

PROOF OF STEP 4. By comparing the columns selected by the method of Theorem 3.2 and those in Step 3, it can be seen that both achieve the same number of level changes for selecting 2^{k-2} columns from $\mathbf{y}_1, \dots, \mathbf{y}_{2^{k-1}}$ and also for selecting 2^{k-1} columns from $\mathbf{y}_1, \dots, \mathbf{y}_{2^k}$. For values of n between $2^{k-2}+1$ and $2^{k-2}+2^{k-3}$, the method of Theorem 3.2 successively chooses the columns with the smallest numbers of level changes, while for values of n between 2^{k-1} and $2^{k-2}+2^{k-3}+1$, it successively deletes from $\mathbf{y}_1, \dots, \mathbf{y}_{2^k}$ those with the largest numbers of level changes.

PROOF OF STEP 3. We have seen that at most 2^s columns can be selected from $\mathbf{y}_{a2^{s+1}+1}, \dots, \mathbf{y}_{(a+1)2^{s+1}}$. It follows that for each $0 \le m \le w$, at most 2^{s+1} columns can be selected from $A_0^m \cup A_1^m \cup A_2^m \cup A_3^m$. For any $0 \le m \le w-1$, if b of these columns are selected by d, where $b < 2^{s+1}$, then $2^{s+1}-b$ columns must be made up from those beyond $\mathbf{y}_{w2^{s+2}+q}$. For convenience, let $S(m)$ be the total number of level changes of these 2^{s+1} columns. Then by Lemma 5.2,

$$S(m) \ge \sum_{i=1}^{2^s}(m2^{s+2}+i-1) + \sum_{i=1}^{2^s}(m2^{s+2}+2^{s+1}+i-1). \tag{5.4}$$

We shall also use $S(w)$ to denote the total number of level changes of the q columns selected from $A_0^w \cup A_1^w \cup A_2^w \cup A_3^w$, excluding the make-up columns mentioned earlier if there are any. Let $\mathbf{y}_{i_1}, \dots, \mathbf{y}_{i_n}$, $i_1 < \cdots < i_n$, be the columns selected in Step 3. For $0 \le m \le w-1$, let $T(m)$ denote the total number of level changes of $\{\mathbf{y}_{i_{m2^{s+1}+1}}, \dots, \mathbf{y}_{i_{(m+1)2^{s+1}}}\}$, and if $q > 0$, let $T(w)$ be the total number of level changes of $\{\mathbf{y}_{i_{w2^{s+1}+1}}, \dots, \mathbf{y}_{i_{w2^{s+1}+q}}\}$. Thus, for example, when $0 \le m \le t2^r - 1$,

$$T(m) = \sum_{i=1}^{2^{s+1}}(m2^{s+2}+2^s+i-1). \tag{5.5}$$

The difference $S(m) - T(m)$, denoted $E(m)$, will be called the excess of d in $A_0^m \cup A_1^m \cup A_2^m \cup A_3^m$. It remains to show that the total excess $\sum_{m=0}^{w} E(m)$ is nonnegative. The proof requires careful calculation of a lower bound on each $S(m)$ subject to the constraints in Lemmas 5.2 and 5.3. We shall treat the cases $g = 0$ and $g \ne 0$ separately.

Case 1. $g = 0$. In this case, $r = 0$, $q = u$ and $t = w$. Let v be the number of columns selected from A_2^0. Then since none of the columns in A_0^0 is selected, by the definition of g, $v > 0$.

(i) Bounding $E(0)$: by Lemma 5.3, $\mathbf{x} \in A_2^0$ and $\mathbf{y} \in A_1^0 \Rightarrow \mathbf{x}+\mathbf{y} \in A_3^0$. Therefore at most 2^s columns can be chosen from $A_1^0 \cup A_3^0$, and hence at most 2^s+v columns are selected from $A_0^0 \cup A_1^0 \cup A_2^0 \cup A_3^0$. It follows that at least 2^s-v columns need to be chosen from those beyond $\mathbf{y}_{t2^{s+2}+u}$. Thus

$$S(0) \geq \sum_{i=1}^{2^s+v}(2^s+i-1)+\sum_{i=1}^{2^s-v}(t2^{s+2}+u+i-1). \tag{5.6}$$

From (5.5) and (5.6), a straightforward calculation shows that

$$E(0) \geq [(t-1)2^{s+2}+2^{s+1}+u-v](2^s-v). \tag{5.7}$$

(ii) Bounding $E(m)$ for each $0<m<t$: suppose at least one column is chosen from A_0^m. Then by Lemma 5.3, at most 2^s-v columns in A_2^m can be selected. As a consequence, if 2^s columns are to be selected from $A_2^m \cup A_3^m$, then at least v columns must be chosen from A_3^m. So

$$\begin{aligned} S(m) \geq {} & \sum_{i=1}^{2^s}(m2^{s+2}+i-1)+\sum_{i=1}^{2^s-v}(m2^{s+2}+2^{s+1}+i-1) \\ & +\sum_{i=1}^{v}(m2^{s+2}+3\cdot 2^s+i-1). \end{aligned} \tag{5.8}$$

It follows from (5.5) and (5.8) that

$$E(m) \geq -(2^s-v)(2^s+v). \tag{5.9}$$

On the other hand, if none of the columns of A_0^m is selected, then

$$S(m) \geq \sum_{i=1}^{2^{s+1}}(m2^{s+2}+2^s+i-1)=T(m).$$

So $E(m)\geq 0$, and (5.9) still holds for all $0<m<t$.

(iii) Bounding $E(t)$: similarly to (5.8), a lower bound on $S(t)$ can be obtained by successively choosing u columns from {the 2^s columns of A_0^t} $\cup$ {the first 2^s-v columns of A_2^t} $\cup$ {the first v columns of A_3^t} in the order they appear. Compare this with how Step 3 selects the columns beyond $\mathbf{y}_{t\cdot 2^{s+2}}$; it is easy to see that

$$\text{if } u \leq 2^s, \text{ then } E(t) \geq 0, \tag{5.10}$$

and when $u>2^s$, by the same argument as in the proof of Step 4, we may assume $u=2^{s+1}$ for bounding $E(t)$ from below. Therefore as in (5.9),

$$u>2^s \Rightarrow E(t) \geq -(2^s-v)(2^s+v). \tag{5.11}$$

Finally, from (5.7), (5.9), (5.10) and (5.11), we conclude that the total excess is at least $(2^s-v)[(t-1)2^{s+2}+2^{s+1}+u-v-(t-1)(2^s+v)]$ when $u\leq 2^s$ and is at least $(2^s-v)[(t-1)2^{s+2}+2^{s+1}+u-v-t(2^s+v)]$ when $u>2^s$. Both are nonnegative since $v\leq 2^s$ and, by (5.3), $t\geq 1$. This proves Case 1.

Case 2. $g > 0$. In this case, the above argument needs to be modified. A key point in the proof of Case 1 is that, by Lemma 5.3, $\mathbf{y} \in A_i^0$, $i = 0$ or 2, and $\mathbf{z} \in A_0^m \cup A_1^m \cup A_2^m \cup A_3^m \Rightarrow \mathbf{y} + \mathbf{z} \in A_0^m \cup A_1^m \cup A_2^m \cup A_3^m$, which implies certain constraints on the selection of columns from $A_0^m \cup A_1^m \cup A_2^m \cup A_3^m$. For $g > 0$, when $\mathbf{y} \in A_i^g$, $i = 0$ or 2 and $\mathbf{z} \in A_0^m \cup A_1^m \cup A_2^m \cup A_3^m$, $\mathbf{y} + \mathbf{z}$ may not belong to $A_0^m \cup A_1^m \cup A_2^m \cup A_3^m$. Instead, we have the following modification of Lemma 5.3.

LEMMA 5.4. *For any nonnegative integer* m, *there is an* $h(m)$ *such that* $h(0) = g$ *and if* $\mathbf{y} \in A_i^g$, $i = 0$ *or* 2, *and* $\mathbf{z} \in A_j^m$, $j = 0, 1, 2, 3$, *then* $\mathbf{y}+\mathbf{z} \in A_l^{h(m)}$, *where* $l \equiv i + j \pmod 4$. *Hence if* v *of the* 2^s *columns in* A_i^g *are selected and at least one column in* A_j^m *is also selected, then at most* $2^s - v$ *columns in* $A_l^{h(m)}$ *can be selected. Write* m *as* $m = a2^r + b$, *where* $0 \leq b < 2^r$. *Then* $h(m) = a2^r + b'$ *for some* b', *where* $b < 2^{r-1} \Rightarrow 2^{r-1} \leq b' \leq 2^r - 1$ *and* $b \geq 2^{r-1} \Rightarrow 0 \leq b' < 2^{r-1}$.

Unlike the case $g = 0$, selecting columns from $A_0^m \cup A_1^m \cup A_2^m \cup A_3^m$ causes some constraints on the selection of columns from $A_0^{h(m)} \cup A_1^{h(m)} \cup A_2^{h(m)} \cup A_3^{h(m)}$. Instead of bounding each $E(m)$ separately, we shall derive lower bounds on $E(m) + E(h(m))$.

Let v be the number of columns selected from A_0^g.

(i) Bounding $E(0) + E(g) = E(0) + E(h(0))$: by the definition of g, none of the columns in $A_0^0 \cup A_2^0$ is selected. A simple application of Lemma 5.4 shows that at most $3 \cdot 2^s + v$ columns can be selected from $(A_0^0 \cup A_1^0 \cup A_2^0 \cup A_3^0) \cup (A_0^g \cup A_1^g \cup A_2^g \cup A_3^g)$. Therefore at least $2^s - v$ columns must be made up from those beyond $\mathbf{y}_{w2^{s+2}+q}$. Similarly to (5.6), $S(0) + S(h(0)) = S(0) + S(g) \geq \sum_{i=1}^{2^s}(2^s + i - 1) + \sum_{i=1}^{2^s}(3 \cdot 2^s + i - 1) + \sum_{i=1}^{v}(g2^{s+2} + i - 1) + \sum_{i=1}^{2^s}(g2^{s+2} + 2^{s+1} + i - 1) + \sum_{i=1}^{2^s - v}(w2^{s+2} + q + i - 1)$. By comparing with (5.5), we have

$$E(0) + E(g) \geq [(w - g)2^{s+2} + q - v](2^s - v). \tag{5.12}$$

(ii) Bounding $E(m)$ for $0 < m \leq 2^r - 1$, $m \neq g$: by the definition of g, when $0 \leq m \leq g - 1$, $S(m) \geq \sum_{i=1}^{2^s}(m2^{s+2} + 2^s + i - 1) + \sum_{i=1}^{2^s}(m2^{s+2} + 3 \cdot 2^s + i - 1)$. Comparing this with (5.5), we have

$$E(m) \geq 2^{2s} \quad \text{for all } 0 < m < g, \tag{5.13}$$

while from (5.4),

$$E(m) \geq -2^{2s} \quad \text{for all } g < m \leq 2^r - 1. \tag{5.14}$$

(iii) Bounding $E(m) + E(h(m))$ for $2^r \leq m \leq t2^r - 1$: it follows from Lemma 5.4 that if at least one column is selected from each of A_0^m and A_2^m, then at most $2^s - v$ columns can be selected from each of $A_0^{h(m)}$ and $A_2^{h(m)}$. As a consequence, if 2^{s+1} columns are to be chosen from $A_0^{h(m)} \cup A_1^{h(m)} \cup A_2^{h(m)} \cup A_3^{h(m)}$, then at least v columns must be chosen from each of $A_1^{h(m)}$ and $A_3^{h(m)}$. Then

$$
\begin{aligned}
&S(m)+S(h(m))\\
&\quad\geq \sum_{i=1}^{2^s}(m2^{s+2}+i-1)+\sum_{i=1}^{2^s}(m2^{s+2}+2^{s+1}+i-1)\\
&\qquad+\sum_{i=1}^{2^s-v}(h(m)2^{s+2}+i-1)+\sum_{i=1}^{v}(h(m)2^{s+2}+2^s+i-1)\\
&\qquad+\sum_{i=1}^{2^s-v}(h(m)2^{s+2}+2^{s+1}+i-1)\\
&\qquad+\sum_{i=1}^{v}(h(m)2^{s+2}+3\cdot 2^s+i-1).
\end{aligned} \tag{5.15}
$$

From (5.5) and (5.15), a straightforward calculation shows that $E(m)+E(h(m))\geq -2(2^s-v)(2^s+v)$. Similarly, if no column is selected from A_0^m or no column is selected from A_2^m, then $E(m)+E(h(m))\geq -(2^s-v)(2^s+v)$, and if no column is selected from $A_0^m\cup A_2^m$, then $E(m)+E(h(m))\geq 0$. In any case, we have

$$E(m)+E(h(m))\geq -2(2^s-v)(2^s+v)\quad \text{for all } 2^r\leq m\leq t2^r-1. \tag{5.16}$$

By Lemma 5.4, $m\leq t2^r-1 \Rightarrow h(m)\leq t2^r-1$. Thus $\sum_{m=2^r}^{t2^r-1}\{E(m)+E(h(m))\}=2\sum_{m=2^r}^{t2^r-1}E(m)$. By (5.16),

$$\sum_{m=2^r}^{t2^r-1}E(m)\geq -(t-1)2^r(2^s-v)(2^s+v). \tag{5.17}$$

(iv) Bounding $\sum_{m\geq t2^r}\{E(m)+E(h(m))\}$: since $m\geq t2^r\Rightarrow h(m)\geq t2^r$, again, by comparing with how Step 3 selects the columns beyond $\mathbf{y}_{t2^r2^{s+2}}$, it is easy to see that

$$\text{if } u\leq 2^{r+s} \text{ then } \sum_{m\geq t2^r}\{E(m)+E(h(m))\}\geq 0 \tag{5.18}$$

and when $u>2^{r+s}$, by the same argument as in the proof of Step 4, we may assume $u=2^{r+s+1}$ for bounding $\sum_{m\geq t2^r}\{E(m)+E(h(m))\}$ from below. Then since $\sum_{m=t2^r}^{(t+1)2^r-1}T(m)=\sum_{i=1}^{2^{r+s}}(t2^{r+s+2}+i-1)+\sum_{i=1}^{2^{r+s}}(t2^{r+s+2}+3\cdot 2^{r+s}+i-1)=\sum_{m=t2^r}^{(t+1)2^r-1}\{\sum_{i=1}^{2^{s+1}}(m2^{s+2}+2^s+i-1)\}$, without changing the total excess, we may replace each $T(m)$ with $\sum_{i=1}^{2^{s+1}}(m2^{s+2}+2^s+i-1)$, as in (5.5). Then (5.16) continues to hold for $m\geq t2^r$. Thus

$$\sum_{m=t2^r}^{(t+1)2^r-1}\{E(m)+E(h(m))\}\geq -2(2^s-v)(2^s+v)2^r,$$

which implies that

$$\sum_{m=t2^r}^{(t+1)2^r-1} E(m) \geq -(2^s - v)(2^s + v)2^r. \tag{5.19}$$

By (5.12), (5.13), (5.14), (5.17), (5.18) and (5.19), the total excess is at least $[(w-g)2^{s+2}+q-v](2^s-v)+(2g-2^r)2^{2s}-2^r(t-1)(2^s+v)(2^s-v)$ when $u \leq 2^{r+s}$ and is at least $[(w-g)2^{s+2}+q-v](2^s-v)+(2g-2^r)2^{2s}-t2^r(2^s+v)(2^s-v)$ when $u > 2^{r+s}$. Both are nonnegative since $v \leq 2^s$, $2^{r-1} \leq g \leq 2^r - 1$, $t \geq 1$ [by (5.3)], and when $u > 2^{r+s}$, by (5.1) and (5.2), we have $w - g \geq t2^r + e - 2^r + 1$, with $e \geq 2^{r-1}$. This completes the proof. □

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C.-S. CHENG
DEPARTMENT OF STATISTICS
UNIVERSITY OF CALIFORNIA
367 EVANS HALL #3860
BERKELEY, CALIFORNIA 94720-3860
E-MAIL: cheng@stat.berkeley.edu

R. J. MARTIN
SCHOOL OF MATHEMATICS AND STATISTICS
UNIVERSITY OF SHEFFIELD
SHEFFIELD, S3 7RH
UNITED KINGDOM
E-MAIL: r.j.martin@sheffield.ac.uk

B. TANG
DEPARTMENT OF MATHEMATICAL SCIENCES
UNIVERSITY OF MEMPHIS
CAMPUS BOX 526429
MEMPHIS, TENNESSEE 38152-6429
E-MAIL: tangb@msci.memphis.edu