Minimum Cost Trend-Free Run Orders of Fractional Factorial Designs

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Summary

Minimum Cost Trend-Free Run Orders

of Fractional Factorial Designs

Run orders of fractional factorial designs which minimize a cost function based on the number of times the factors change levels during the time sequence in which the runs are performed and which simultaneously have all factor main effects components orthogonal to a polynomial time trend are found for a wide variety of factorial plans. A construction technique based on a generalized foldover scheme is presented.

1. Introduction. Suppose an experiment is to be performed according to a given fractional factorial plan. In some cases, the time order in which the runs or treatment combinations are performed need not be randomized. Instead, certain systematic run orders may be preferred. For example, if the runs are made in some time or space sequence, each observation may be affected by a trend which is a function of time or position. In the presence of a time trend, a non-randomized run order may improve the efficiency with which factor effects are estimated. A design objective of full efficiency is attained when the factor effects are orthogonal to the time trend effects.

The cost of conducting an experiment is often of practical importance. A second design criterion is a cost function based on the number of times each factor changes levels. The practical interpretation is that it costs a certain amount to change the levels of each factor, for example, to reset a measurement instrument, change the fertilizer on a field trial, restart an industrial plant and so on. If all level changes are equally expensive, run orders that minimize the total number of factor level changes are optimal with respect to this second criterion.

Cox (1951) began the study of systematic designs, for replicated variety trials, with the single criterion of efficient estimation of treatment effects in the presence of a smooth polynomial trend. Certain 2ⁿ factorial designs robust to both linear and quadratic trends were found by Daniel and Wilcoxon (1966). The cost criterion was introduced by Draper and Stoneman (1968) in their exhaustive searches of some eight-run factorial plans. Dickinson (1974) extended the work of Draper and Stoneman to 2⁴ and 25 complete factorial plans with the search restricted to minimum cost run orders. Joiner and Campbell (1976) took an approach in which each factor changed levels from one run to the next with a given probability. More expensive factors were assigned smaller probabilities of changing levels. In an unpublished report, P.W.M. John extended the method of Daniel and Wilcoxon to certain designs for factors at two and three levels and discussed the foldover properties of such systematic run orders. Cheng (1985) gave a theoretical description of the cost structure in two-level factorial designs and

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provided some examples of run orders optimal with respect to both our design criteria. The theory presented in Section 4 extends Cheng's results and provides an algorithm for constructing optimal orders for many fractional factorial designs. In particular, our results may be applied to the designs listed in two National Bureau of Standards tables (1957, 1959). A majority of these designs can be optimally ordered with respect to both our design criteria.

In Section 2, we briefly summarize the definition and group properties of fractional factorial designs and the notation we use to describe these designs. The design criteria are defined in Section 3 while the main results are presented in Section 4. Proofs are left until the Appendix. Section 5 contains applications of the construction results of Section 4. A summary discussion appears in Section 6.

2. Fractional Factorial Designs. Attention is restricted to designs in which all factors are at the same number of levels. Consider n factors, each at s levels where s is a prime power. Let the s levels of each factor be the s elements of the Galois field of order s, GF(s). We denote the s factor levels by $0, 1, \ldots, s-1$, with 0 the additive identity and 1 the multiplicative identity in GF(s).

A complete factorial design in all n factors requires s^n runs. Let $G = (s_r^{n-p})$ denote a s^{-p} fraction of the complete factorial, blocked in s^r blocks each of size s^{n-p-r} . Let $N = s^{n-p}$ be the number of runs in the design G. Let $R = s^{n-p-r}$ be the size of each block.

DEFINITION 1. A design G is defined by a set of (p+r) linearly independent vectors whose elements are in GF(s), say $\alpha_{ij} \in GF(s)$, $i=1,\ldots,p+r$, $j=1,\ldots,n$. If $\alpha_i=(\alpha_{i1},\ldots,\alpha_{in})^T$, the treatment combinations in the initial or principal block are the R solutions $\mathbf{z}=(\zeta_1,\ldots,\zeta_n)^T$, where $\zeta_j \in GF(s)$, $j=1,\ldots,n$, to the system of equations:

$$\alpha_i^T \mathbf{z} = 0, \quad i = 1, \dots, p+r$$
 (2.1)

The remaining $s^r - 1$ blocks, each of size R, are cosets of the initial block and correspond to solutions z of the first p equations only in system (2.1).

The n-tuples $\alpha_1, \ldots, \alpha_p$ represent the p independent defining effects of the fraction while $\alpha_{p+1}, \ldots, \alpha_{p+r}$ are the blocking effects. The group operations involved in solving system (2.1) are

those of addition and multiplication in the field GF(s). To find the R solutions to system (2.1), it is sufficient to find h = n-p-r independent solutions $\mathbf{z}_1, \ldots, \mathbf{z}_h$ and from them form all linear combinations

$$b_1 \mathbf{z}_1 + \cdots + b_h \mathbf{z}_h$$
, for all $b_j \in GF(s)$, $j = 1,...,h$ (2.2)

If $\mathbf{z}_{h+1}, \ldots, \mathbf{z}_{n-p}$ are r independent solutions of the first p equations of system (2.1), but not of all (p+r) equations, they may be used to find the cosets of the principal block by forming the s^r treatment combinations

$$b_{h+1}\mathbf{z}_{h+1} + \cdots + b_{n-p}\mathbf{z}_{n-p}$$
, for all $b_j \in GF(s)$, $j = h+1,...,n-p$ (2.3)

and adding each result to all R treatment combinations in the principal block.

The notation we use to describe the treatment combinations or runs of the design G is as follows. Let the n factors be named a_1, \ldots, a_n . If z is in design G, we write run z equivalently as:

$$\mathbf{g} = \mathbf{a}_1^{\zeta_1} \mathbf{a}_2^{\zeta_2} \cdot \cdot \cdot \mathbf{a}_n^{\zeta_n} \tag{2.4}$$

Design G is the group $\{\mathbf{g}_1,\ldots,\mathbf{g}_N\}$. Without loss of generality, G is generated by $\{\mathbf{g}_1,\ldots,\mathbf{g}_{n-p}\}$, the first h of which are independent solutions to all p+r equations of system (2.1) and generate the principal block. From expression (2.4), these h principal block generators are in one-to-one correspondence with the independent solutions $\mathbf{z}_1,\ldots,\mathbf{z}_h$ of (2.2). We call $\{\mathbf{g}_1,\ldots,\mathbf{g}_h\}$ the within block generators. The between block generators $\mathbf{g}_{h+1},\ldots,\mathbf{g}_{n-p}$ correspond to solutions $\mathbf{z}_{h+1},\ldots,\mathbf{z}_{n-p}$ of (2.3). Then, any treatment combination in G is of the form

$$\mathbf{g} = \mathbf{g}_1^{b_1} \mathbf{g}_2^{b_2} \cdot \cdot \cdot \mathbf{g}_{n-p}^{b_{n-p}}, \quad b_j \in GF(s), \quad j = 1,...,n-p$$
 (2.5)

We write g = 1 to denote the treatment combination corresponding to all factors at level 0. Note that we assume that any design G is at least a main effects plan, that is, the p+r n-tuples $\{\alpha_i\}$ of Definition 1 are chosen to ensure that no main effect is aliased with another main effect nor confounded with any block effect.

3. Optimal Design Criteria. Both the polynomial time trends and the values taken by the main effects components of the n factors in the design matrix are defined in terms of systems of orthogonal polynomials. We begin with a definition.

DEFINITION 2. The system of orthogonal polynomials on m equally spaced points $i=0,\ldots,m-1$ is the set $\{P_{km},\,k=0,1,2,...,m-1\}$ of polynomials satisfying

$$\sum_{i=0}^{m-1} P_{km}(i) = 0 \quad \text{for all } k \ge 1$$
 (3.1)

$$\sum_{i=0}^{m-1} P_{km}(i) P_{k'm}(i) = 0 \quad \text{for all } k \neq k'$$
(3.2)

where $P_{0m}(i) = 1$ and $P_{km}(i)$ is a polnomial of degree k. We assume that each polynomial in the system is scaled so that its values are always integers.

Note that if Q_{km} is any polynomial of degree $k \le m-1$ on m equally spaced points $i=0,\ldots,m-1$, then, for some $\{w_0,\ldots,w_k\},\,Q_{km}$ may be expressed as:

$$Q_{km}(i) = \sum_{j=0}^{k} w_j P_{jm}(i)$$
 (3.3)

DEFINITION 3. Factor Effects - The s coefficients of the j^{th} main effects component of each factor, $1 \le j \le s-1$, are P_{js} (i), $0 \le i \le s-1$, the values of the orthogonal polynomial of degree j on s equally spaced points.

DEFINITION 4. Trend Effects - The R values of a polynomial trend of degree j, $1 \le j \le R-1$, in a block of size R are $P_{jR}(i)$, $0 \le i \le R-1$, the values of the orthogonal polynomial of degree j on R equally spaced points.

The linear model for the N observations is:

$$Y = X \beta + \varepsilon \tag{3.4}$$

where ε is an N-vector of zero mean, uncorrelated random errors. Let $X=(x_1,\ldots,x_\tau)=(x_{ij}),\ i=1,\ldots,N,\ j=1,\ldots,\tau$. Each column x_j of the N x τ design matrix X is either a factor, trend or block effect. The first R rows of X correspond to the R treatment combinations in the principal block, the next R rows to the runs in the second block, and so on. There is one column in X for each block of G. Without loss of generality, these are the last s^r columns of X. For any block column x_j , $\tau-s^r+1\le j\le \tau,\ x_{ij}=1$ if run i is in block $j-(\tau-s^r)$, otherwise $x_{ij}=0$.

Let the first q_1 columns of X correspond to the factor effects in the model. Unless otherwise stated, we assume that the interactions are negligible. Then $q_1 = n(s-1)$. By Definitions 1 and 3, if column x_j represents the m^{th} main effects component of factor a_t and if factor a_t is at level $u \in GF(s)$ in run i of G, then

$$x_{ij} = P_{ms}(u) \tag{3.5}$$

We assume that the same polynomial time trend of degree k is present in each block. Let columns $\mathbf{x}_{q_1+1},\ldots,\mathbf{x}_{q_1+k}$ of X represent such a time trend, that is, the coefficients in column q_1+m , $1 \le m \le k$, are given by the polynomial of degree m from the orthogonal system defined in Definition 2 for the R equally spaced positions in each block. By Definition 4, for $j=q_1+m$, if run position $i \equiv i_0 \pmod{R}$, then $x_{ij} = P_{mR}(i_0)$

Partition the design matrix X into two parts, (X_1, X_2) , where X_1 is the N x q_1 matrix of factor effects and X_2 the N x q_2 , $(q_2=k+s^r)$, matrix of trend and block effects. Partition the parameter vector β similarly into two vectors β_1 and β_2 of dimensions q_1 and q_2 respectively. The following facts are immediate: the q_1 columns of X_1 are orthogonal; the q_2 columns of X_2 are orthogonal; the q_1 columns of X_1 are orthogonal to the s^r block effects columns of X_2 .

For any main effect column \mathbf{x}_1 of \mathbf{X}_1 and trend column \mathbf{x}_2 of \mathbf{X}_2 , we define the time count between factor effect \mathbf{x}_1 and trend component \mathbf{x}_2 as $\mathbf{x}_1^T\mathbf{x}_2$. The design criterion based on efficient factor effect estimation in the presence of a smooth polynomial time trend may now be defined using the orthogonal polynomial structure of the linear model described above. The objective is to eliminate the effect of the time trend by finding run orders for which all the main effects components of all n factors

are orthogonal to the k trend columns of the design matrix. Such run orders are said to be k-trend free. If the time counts between all factor effects and trend effects are zero, the run order is optimal with repect to our first design criterion. If this is achieved, X_1 will be orthogonal to X_2 and the factor effects will be estimated with full efficiency.

As stated in Section 1, our second optimality criterion is a cost function based on the number of times each factor changes levels. We assume that all factor level changes are equally expensive. Then a run order is optimal if it minimizes the total number of level changes. The compatibility of this cost function with the group structure of a fractional factorial design is used in Section 4 to produce a construction method that generates run orders optimal with respect to both design criteria.

4. Construction of optimal run orders. We present conditions under which the main effects components of each factor become or remain orthogonal to a polynomial time trend during a stepwise construction of a run order of a design. We begin by assuming that design G is run in a single block of size N. Later in this section, we present results that allow this restriction to be dropped. In addition, the construction method is adapted to produce run orders that are optimal with respect to our second design criterion. Proofs of all the results in this section are in Appendix A.

Consider a single factor, a_1 say. Let $U = (u_{\xi+1}, \ldots, u_{\xi+sv})$, $u_i \in GF(s)$, $i = \xi+1, \ldots, \xi+sv$ be a sequence of sv consecutive levels of a_1 in rows $\xi+1, \ldots, \xi+sv$ of design matrix X. Usually, v is a power of s. Let x be the column of X_1 representing the main effects component of degree q of a_1 . By (3.5), $x_i = P_{qs}(u_i)$.

DEFINITION 5. Factor a_1 is k-trend free over U if

- (a) each of the s levels of a_1 appears v times in U
- (b) all (s-1) main effects components of a_1 are orthogonal to trend components P_{0N}, \ldots, P_{kN} over the sv runs of U.

Let i_{tm} , m = 1,...,v be the v run positions in U at which a_1 is at level t, for each t = 0,...,s-1. Suppose a_1 is k-trend free over U, for some $k \ge 0$. For each main effects component of degree $q = 1, \ldots, s-1$ and each trend of degree $j = 0, \ldots, k$, we have by Definition 5:

$$0 = \sum_{t=0}^{s-1} \sum_{m=1}^{v} P_{qs}(t) P_{jN}(i_{tm}) = \sum_{t=0}^{s-1} \left[P_{qs}(t) \sum_{m=1}^{v} P_{jN}(i_{tm}) \right]$$

$$= \sum_{t=0}^{s-1} P_{qs}(t) W(t;j,N)$$
(4.1)

where W(t;j,N) is the sum of the values of the j^{th} trend over the v runs of U in which a_1 is at level t. The term W(t;j,N) is simplified by Lemma 1 below. Then with Definition 6, Theorem 1 below is true. LEMMA 1. If a_1 is k-trend free over U, then W(t;j,N) = W(j,N) is independent of the level t, for $j = 1, \ldots, k$.

DEFINITION 6. For sequence of levels U as above and for some $e \in GF(s)$, let U(e) be another sequence of sv levels of factor a_1 located at run positions $\xi'+1, \ldots, \xi'+sv$, where the level of factor a_1 at position $\xi'+i$ is given by $u_{\xi+i}+e$.

THEOREM 1. Let a_1 be k-trend free over U, for some $k \ge 0$. Then a_1 is also k-trend free over U(e).

We may now define the generalized foldover of U in terms of some non-zero element e e GF(s). Then Theorem 2 which follows Definition 7 below provides the main method for constructing trend free orders optimal with respect to the first design criterion.

DEFINITION 7. Generalized Foldover of U: For U as above, the generalized foldover of U is the sequence of s^2v levels of a_1 given by

$$U^*(e) = (U, U(e), U(2e), \dots, U((s-1)e))$$

THEOREM 2. Suppose a_1 is k-trend free over U. Let $U^*(e)$ be the generalized foldover of U with respect to $e \neq 0$ ϵ GF(s). Then a_1 is (k+1)-trend free over U^* .

We give below a scheme that allows k-trend free run orders of G to be constructed. We assume that any run order of G begins with the run 1 in which all factors are at level 0. We employ the notation of expression (2.4) and write the runs of G as $\{g_1, \ldots, g_N\}$. Recall that by g^t for $t = 0, \ldots, s-1$ we mean the multiplication of each exponent of a factor name by t according to the operation of group multiplication in GF(s).

At the beginning of this section, we assumed that design G would be run in a single block of size s^{n-p} . We now reinstate the block structure. There are s^r blocks of size $R=s^h$, where h=n-p-r. Recall that by a within block generator we mean a run g that is in the principal block and is used, along with h-1 other independent principal block runs, to generate the principal block by (2.2) while a between block generator is one of the r independent runs from r distinct blocks, other than the principal block, used to generate the s^r-1 cosets of the principal block by (2.3).

Let $\{g_1, \ldots, g_{n-p}\}$ be n-p independent generators of G, the first h of which generate the principal block. Suppose G is generated as follows: set $U_0=1$ then let

$$U_i = U_{i-1}^*(\mathbf{g}_i)$$
 $i = 1, ..., n-p$ (4.2)

where if $\mathbf{g}_i = a_1^{e_1} \cdot \cdot \cdot \cdot a_n^{e_n}$ then factor a_j is folded over according to Definition 7 with respect to level e_j .

Theorem 3 below shows how k-trend free orders may be constructed. We preced Theorem 3 by a result that exploits the block structure of the design and the assumption that the trend components in every block of G are identical.

LEMMA 2. Using generalized foldover scheme (4.2), if a factor is at a nonzero level in at least one between block generator $\{g_{h+1}, \ldots, g_{n-p}\}$, that factor is orthogonal to all the polynomial trend components present in linear model (3.4).

THEOREM 3. For G generated according to system (4.2), G is k-trend free if each factor appears at least (k+1) times at non-zero levels in the sequence of generators or, for any factor appearing fewer than (k+1) times at a nonzero level, that factor is at a nonzero level in at least one between block generator. Note that these (k+1) appearances at non-zero levels do not have to be at the same level.

EXAMPLE 1. Consider the design $G=2_0^{3-0}$, a complete 2^3 factorial in factors a, b and c run in one block of eight runs. Then $G=\{1, a, b, c, ab, ac, bc, abc\}$ and if we choose $\mathbf{g}_1=ab$, $\mathbf{g}_2=abc$, $\mathbf{g}_3=ac$ each non-zero factor level appears at least twice and the resulting run order constructed according to the scheme (4.2) is linear trend free or 1-trend free. This order is $G=\{1, ab, abc, c, ac, bc, b, a\}$ and was found by Draper and Stoneman in their exhaustive search of all 8! run orders.

Note that with the generalized foldover scheme (4.2), the last run of the first s^i runs, $i=1,\ldots,n$ -p, is given by

$$\mathbf{g}_{1}^{s-1}\mathbf{g}_{2}^{s-1}\cdots\mathbf{g}_{i}^{s-1}$$
 (4.3)

We turn now to the second design criterion: a cost function given by the number of factor level changes. Recall the assumption that all factor level changes are equally expensive. Cheng (1985) gives a method for constructing minimum cost run orders of two-level fractional factorial designs. Presented below is a generalization of Cheng's arguments to fractional factorial designs at s levels, where s is a prime power. A method based on the generalized foldover scheme defined above is shown to produce minimum cost run orders of designs G. For convenience, we employ the same notation as Cheng. The reader is referred to Cheng (1985) for details.

Define a cost or distance function between any two subsets A and B of G by

$$d(A, B) = \min_{\omega \in A, \mathbf{v} \in B} d(\omega, \mathbf{v})$$

where $d(\omega, \mathbf{v})$ is the number of factor level changes between runs ω and \mathbf{v} . In the notation of (2.4), if $\omega = a_1^{\omega_1} \cdots a_n^{\omega_n}$ and $\mathbf{v} = a_1^{\mathbf{v}_1} \cdots a_n^{\mathbf{v}_n}$, $\omega_i, \mathbf{v}_i \in GF(s)$, then $d(\omega, \mathbf{v}) = \sum I(\omega_i \neq \mathbf{v}_i)$. In particular, $d(\mathbf{1}, \omega)$

is the number of level changes between run 1 and run ω . In what follows, assume that the first block of G is the principal block, denoted by B_1 , a subgroup of G. Blocks B_2, \ldots, B_{s^r} are cosets of B_1 in G.

LEMMA 3. Let $\{g_1, \ldots, g_{n-p}\}$ generate G by the generalized foldover scheme of Theorem 3. Let

$$d_i = d (g_i, \prod_{j=0}^{i-1} g_j^{s-1}), \quad i = 1, \dots, n-p$$
 (4.4)

Then the cost of the run order so generated is

$$C = \sum_{i=1}^{n-p} (s-1) s^{n-p-i} d_i$$
 (4.5)

Consider the following group structured decomposition of the principal block, B_1 . Beginning with $H_1^{(0)} = \{1\}$, iteratively define the following quotient groups, subgroups, the set of minimum within-block costs $\{c_i\}$ and coset structure of B_1 .

$$G_{i} = B_{1}/H_{1}^{(i)}, \quad i = 0, 1, \dots, t-1$$

$$c_{i+1} = \min_{H, K \in G_{i}, H \neq K} d(H, K)$$

$$S_{1}^{(i)} = \text{subgroup of } G_{i} \text{ generated by } \{H : d(H_{1}^{(i)}, H) = c_{i+1}\}$$

$$H_{1}^{(i+1)} = \bigcup_{H \in S_{1}^{(i)}} H$$

$$m_{i} = |S_{1}^{(i-1)}| = s^{r_{i}}$$

$$N_{i} = N_{i-1}/m_{i}, \quad N_{0} = s^{n-p-r}$$

The N_i are the number of cosets of $H_1^{(i)}$ in B_1 , where for convenience we count $H_1^{(i)}$ as a coset of itself, each coset being of size $m_1m_2\cdots m_i$, while r_{i+1} is the number of independent generators of $S_1^{(i)}$, the subgroup of the quotient group G_i generated by those elements of G_i distance c_{i+1} from the current subgroup $H_1^{(i)}$ of B_1 . The elements of $S_1^{(i)}$ are cosets of $H_1^{(i)}$. The $H_1^{(i)}$'s form a nested sequence of subgroups, of strictly increasing size, of B_1 . The sequence of costs $\{c_i, i=1, \ldots, t\}$ is

strictly increasing. The iterations terminate when $N_t = 1$ for some t at which time $H_1^{(t)} = B_1$. Note that $r_1 + \cdots + r_t = n - p - r$.

At each stage $i=0,\ldots,t-1$, there is an arrangement of the $s^{r_{i+1}}$ elements of $S_1^{(i)}$ that has cost c_{i+1} between any two adjacent elements in the arrangement. This produces a minimum cost ordering of the elements of $S_1^{(i)}$. We show below how to construct one such minimum cost arrangement and thereby minimally order the principal block. When the principal block has been minimally ordered, we repeat the above induction starting with $H_1^{(t)} = B_1$, G replacing B_1 and $N_t = s^r$ until some $N_{t+t'} = 1$ and $H_1^{(t+t')} = G$. The between block minimum costs $\{c_{t+1}, \ldots, c_{t+t'}\}$ found from this second iterative procedure, although strictly increasing, may be less than the within block costs found when ordering B_1 .

When performing the iterations described above, the following sequence of steps is most useful. Given subgroup $H_1^{(i)}$ of B_1 , find the next minimum cost c_{i+1} by finding a run g not in $H_1^{(i)}$ with the fewest factors at a nonzero level, that is, having the shortest distance from starting run 1. There will be $r_{i+1} \ge 1$ runs not in $H_1^{(i)}$ this same distance c_{i+1} from run 1, some r_{i+1} of which are in distinct, independent elements of $S^{(i)}$. These r_{i+1} runs of cost c_{i+1} may be used to generate $H_1^{(i+1)}$ by forming the $s^{r_{i+1}}$ products of all s distinct powers of each of the r_{i+1} runs chosen and multiplying every run in $H_1^{(i)}$ by each such product. A similar procedure works for the between block generators. Cheng (1985) contains examples of this iterative procedure for designs with factors at two levels.

To construct minimum cost trend-free run orders, we combine Theorem 3 and the cost structured group decompostion of G detailed above with the generalized foldover scheme (4.2). To begin, suppose $S_1^{(i-1)}$ is generated by $\{K_{i1},\ldots,K_{ir_i}\}$ \in G_{i-1} , for each $i=1,\ldots,t+t'$. By definition of $S_1^{(i-1)}$, there must exist independent runs $\mathbf{z}_{ij} \in K_{ij}$, $j=1,\ldots,r_i$ each distance \mathbf{c}_i from run 1. From now on, we assume that all runs of design G are written in the form of expression (2.4). Setting $\mathbf{r}_0=1$ and $\mathbf{z}_{01}=1$, define a set of n-p independent generators of G as follows:

$$\mathbf{g}_{ij} = \left(\prod_{i_1=1}^{i-1} \prod_{j_1=1}^{r_{i_1}} \mathbf{g}_{i_1 j_1}^{s-1}\right) \left(\prod_{j_1=1}^{j-1} \mathbf{g}_{i j_1}^{s-1}\right) \mathbf{z}_{ij}, \quad j = 1, \dots, r_i, \quad i = 1, \dots, t+t'$$

$$(4.6)$$

Note that \mathbf{g}_{ij} is \mathbf{z}_{ij} multiplied by the product of all previous generators raised to the power (s-1). Since

the \mathbf{z}_{ij} are independent in $H_{1}^{(i)}$, the collection

$$\{g_{ij}, j=1,\ldots,r_i, i=1,\ldots,t+t'\}$$
 (4.7)

are n-p independent generators of G. With the help of Lemma 2, the following theorem is true.

THEOREM 4. If a run order of G is constructed by the generalized foldover scheme (4.2) applied to the sequence of generators (4.7), the resulting run order has minimum cost given by

$$C_{\min} = \sum_{i=1}^{t+t'} (N_{i-1} - N_i) c_i$$
 (4.8)

Including the between block costs $\{c_{t+1}, \ldots, c_{t+t'}\}$ in the cost decomposition described above implies that the the observations for treatment combinations in each block are made before the next block's observations are begun. In reality, observations for runs in each block may be made concurrently and there will be no between block costs. If this is the case, a run order will have minimum cost of level changes if each block is minimally ordered according to the within block costs found above and any r independent between block generators may be used in the generalized foldover scheme (4.2). With this added freedom, minimum cost run orders that satisify the orthogonality design criterion above are more readily found. An examples is provided in Section 5. Note that expression (4.8) for the minimum cost for design G becomes:

$$C_{\min} = s^{r} \sum_{i=1}^{t} (N_{i-1} - N_{i}) c_{i}$$
(4.9)

The results above provide a sufficient condition under which a run order of G is optimal with respect to both design criteria: trend elimination and minimum cost of level changes. Assume that there are k trend effects in the linear model in the sense that the trend is of degree k and is represented by k columns in design matrix X as described in Section 3. Usually, k will be small: values of 1 and 2 are most common. Let the cost structure of G be given by

$$\{(c_1, r_1), (c_2, r_2), \dots, (c_{t+t'}, r_{t+t'})\}$$
 where $\sum_{j=1}^{t+t'} r_j = n-p$

Let $\{z_{ij}, j=1, \ldots, r_i, i=1, \ldots, t+t'\}$ be some choice of n-p independent minimum distance runs with respect to this cost structure. Let $\{g_{ij}\}$ be formed from these as in expression (4.6). All preceding results may be combined to give:

THEOREM 5. If each factor appears at some non-zero level at least (k+1) times in the sequence of runs $\{g_{ij}\}$ which generate G by the generalized foldover scheme (4.2), or at least once in a between block generator, the resulting run order, having minimum cost (4.8), or (4.9) if the between block costs are zero, and being k-trend free by Theorem 3, is optimal with respect to both design criteria.

5. Examples of optimal run orders. In this section, we present some examples of series of fractional factorial designs with factors at two or three levels for which optimal orders may be found by the construction techniques of Section 4. Throughout this section, unless otherwise stated, a run order is optimal if it is *linear trend free*, that is 1-trend free, and has minimum cost of level changes. We add one further result which leads to linear trend free two-factor interactions for designs with factors at two levels but requires more than the minimum number of factor level changes.

Before presenting specific examples, we make the following observation: when s is a prime number, group operations in GF(s) are addition and multiplication modulo s. Thus, if $\{\omega_1, \ldots, \omega_{n-p}\}$ is the ordered series of minimum cost runs, in one-to-one correspondence with the runs $\{\mathbf{z}_{ij}, j=1, \ldots, r_i, i=1, \ldots, t+t'\}$ used in (4.6) to find the set of generators that construct an optimal run order of G by the generalized foldover scheme, then

$$\mathbf{g}_{i} = \mathbf{\omega}_{i-1}^{(s-1)} \mathbf{\omega}_{i} \tag{5.1}$$

since $(s-1)^2+(s-1)\equiv 0 \pmod s$. Only the current and previous members of $\{\omega_i\}$ are needed to find the next generator in (4.6). With this simplification of (4.6), whenever a sequence of generators for a particular design is presented below, only the set of minimum cost runs $\{\omega_i, i=1,\ldots,n-p\}$ is shown.

By Theorem 3, for a two-level factor to be linear trend free it must be at its high level, level 1, in at least two of the generators in sequence (4.7). An equivalent form of this requirement is: following the first appearance of the factor at its high level in, say, run ω_i it must be at its low level, 0, in some

subsequent minimum cost run ω_j , j > i. It is this condition that is most easily checked for some choice of $\{\omega_i\}$.

Cheng gives an example of a series of fractional factorial designs that have an optimal order. The series he proves can be optimally ordered is $\{G=2_0^{n-1},\ n\geq 5\}$, with defining relation $I=A_1\cdots A_n$. This is the series of 1/2 replicates of a complete 2^n in one block of size 2^{n-1} with the highest order interaction confounded. All (n-1) independent minimum cost runs have cost 2 so a minimum cost run order requires $2(2^{n-1}-1)$ level changes, by (4.8). We may reproduce Cheng's result by using the sequence of minimum cost runs:

$$a_{1}a_{2}\text{, }a_{3}a_{4}\text{ ,}\dots\text{, }a_{n-3}a_{n-2}\text{ }a_{n-1}a_{n}\text{, }a_{1}a_{3}\text{ }\cdots$$

if n is even, where the remaining (n/2-1) minimum cost runs may be any other independent cost 2 runs, and if n is odd the slight modification:

$$a_1a_2$$
, a_3a_4 , . . . , $a_{n-4}a_{n-3}$, $a_{n-2}a_{n-1}$, a_na_1 , a_2a_3 · · ·

where any ((n-1)/2-3) other independent cost 2 runs may be used after a_2a_3 .

We give two other examples of series of designs, each member of which may be optimally ordered, to illustrate how readily Theorem 5 may be used.

The first example is the series of 1/4 replicates of a complete 2^n for $n \ge 7$ defined by $I = A_1A_2S = A_3A_4S$ where the common stem $S = A_5 \cdots A_n$. A minimum cost run sequence that produces optimal run orders is:

$$a_1a_2$$
, a_3a_4 , a_5a_6 , a_6a_7 , a_7a_8 , . . . , $a_{n-1}a_n$, $a_1a_3a_5$

The cost structure is $\{(2, n-3), (3, 1)\}$, for the (c_i, r_i) , and the minimum cost is $2^{n-1}-1$ level changes by (4.8).

The next example of this section is the series of 1/8 replicates of a complete 2^n factorial in one block of size 2^{n-3} defined by $I = A_1A_4A_5S = A_2A_4A_6S = A_3A_5A_6S$ where the common stem $S = A_7 \cdots A_n$. The cost structure is $\{(2, n-7), (3, 4)\}$ so the minimum number of level changes becomes $2(2^{n-3}-2^4)+3(2^4-1)=2^{n-2}+13$. For $n \ge 8$, an optimal set of minimum cost runs is:

 $a_{n-1}a_n$, $a_{n-2}a_n$, $a_1a_2a_4$, $a_1a_3a_5$, $a_4a_5a_6$, $a_1a_2a_7$

As stated in the introduction, the construction techniques of Section 4 were applied to the designs tabled in two National Bureau of Standards publications. Of the 125 plans for factors at two levels in Applied Mathematics Series 48 (1957), 96 may be optimally ordered by the generalized foldover scheme. Furthermore, for 63 of these 96 plans, not only a linear but also a quadratic trend free run order with minimum cost is obtainable. Similarly, all 41 plans for factors at three levels in Applied Mathematics Series 54 (1959) may be optimally ordered. Tables of minimum cost linear trend free run sequences for all the designs with optimal orders may be obtained from the authors.

Expression (4.9) gives the minimum cost for a run order under the often realistic assumption that between block costs are zero. To illustrate how this modification may be beneficial, consider the design $G = 2_2^{8-3}$ defined by I = ABEGH = ACFG = ABCD with blocking effects ABEF and ACE. This is plan 8.8.8 in Applied Mathematics Series 48 (1957). For this design, the generalized foldover scheme does not find a minimum cost run sequence that has all eight factor main effects linear trend free. However, if between block costs are zero, the run sequence

bdfg acfg adegh bdh abcdefg

has minimum cost by (4.9) and all eight factors are both linear and quadratic trend free. Of the 29 plans in AMS 48 that cannot be optimally ordered when costs are given by (4.8), there are 12 with an optimal order using (4.9).

Draper and Stoneman (1968) found a run order of a complete 2³ factorial with all three main effects linear trend free and requiring eleven level changes, four more than the minimum of seven level changes. No 1-trend free run order had fewer than 11 level changes. By an exhaustive search, we confirmed that at least four extra level changes are required for any 1-trend free run order of a complete 2⁴.

Cheng (1985) proved that for any $n \ge 3$, there exists an order of a complete 2^n with all main effects linear trend free and requiring $2^n + 3$ level changes, again four more than the minimum. This result may be reproduced by constructing the sequence of generators (5.1) from the following run sequence:

$$a_1, a_2, \ldots, a_{n-3}, a_{n-2}a_{n-1}, a_n, a_{n-2}$$

and using the generalized foldover scheme (4.2). By (4.4), this run sequence has cost structure $d_1 = \cdots = d_{n-3} = d_{n-1} = d_n = 1$, $d_{n-2} = 2$ which gives the required cost by (4.5).

The generalized foldover scheme may be used to find run orders of two level fractional factorial designs for which all main effects and two factor interactions are linear trend free, although the run order is unlikely to have minimum cost. Without loss of generality, let $G = (2_0^{n-p})$ be run in a single block. We have the following construction theorem:

THEOREM 6. Suppose a run order of G, constructed by the generalized foldover scheme (4.2) with generator sequence $\{g_1, \ldots, g_{n-p}\}$, is 1-trend free. For each pair of factors a_1 and a_2 , suppose that there exist generators g_i , g_j $i \neq j$, $i, j \in \{1, \ldots, n-p\}$ in which a_1 and a_2 are at different levels (that is, one is high and the other low). Then all n(n-1)/2 two factor interactions are linear trend free.

Applying this theorem to complete 2ⁿ factorials gives the following corollary:

COROLLARY 1. For $n \ge 4$, the generalized foldover scheme (4.2) applied to run sequence $\{\omega_i, i=1,...,n\}$

$$a_n, \ldots, a_5, a_1a_2, a_1a_3, a_4, a_2$$
 (5.2)

from which generators $\{g_i, i=1,...,n\}$ may be found by (5.1), produces a run order that has all main effects and two factor interactions linear trend free and requires $2^n + 11$ level changes, twelve more than the minimum.

EXAMPLE 2. Consider the case n=4. The run order:

Daniel and Wilcoxon found a run order of a complete 2⁴ with all main effects 2-trend free. Their run order may be found by folding over with the generator sequence {abd, acd, bcd, abcd}. Each factor name appears at least three times so by Theorem 3 each factor is quadratic trend free. The cost of 37 level changes is well above the minimum of 15.

6. Discussion. Linear trend free minimum cost run orders have been found for a wide variety of two and three level fractional factorial designs. The examples of Section 5 illustrate the construction techniques detailed in Section 4. It is important to note that as the number of factor levels and/or the number of blocks increases, by Lemma 2, it becomes easier to find run orders that are k-trend free for k>1. The assumption of zero between block costs also aids in this search.

If the two factor interactions are not negligible, the double optimization problem becomes difficult or impossible in small designs as the requirements of Theorem 6 become harder to satisify. When faced with this difficulty, the experimenter must decide how to compromise between the competing criteria of efficiency and cost. Additionally, if factor level changes for a subset of the factors are expensive, for example, closing down and cleaning a chemical plant between runs at different levels, while the remaining factors are essentially free, throwing a switch to change the operating temperature say, then run orders for which the first set of factors change levels least often may be sought by finding generator sequences in which the expensive factors appear at non-zero levels in the latter generators only. The cost optimization must be attempted whenever the experimenter has a design problem with cost constraints of the type developed here. If in reality no cost minimization is required, trend elimination is even easier to achieve as a scalar optimization problem only.

In certain problems it may be necessary to *maximize* the number of factor level changes to meet some other optimality condition. For example, for n factors each at two levels, if there is a correlated error structure represented by a first order autoregression with positive correlation, a run order that maximizes the number of factor level changes may lead to a D-optimal design. Such run orders may be constructed by applying the same generalized foldover scheme (4.2) to sequences of maximum length generators.

APPENDIX

Proofs

Proofs of the results presented in Sections 4 and 5 follow.

LEMMA 1. Fix j and N and suppress them in the expressions that follow. A polynomial of degree at most (s-1) may be fitted exactly through the s points $\{(t, W(t)), t=0, \ldots, s-1\}$. By the remark following Definition 2 and expression (3.3), we may express this polynomial as a weighted sum of the orthogonal polynomials $P_{j_1}s$, $j_1=0,\ldots,s-1$, that is:

$$W(t) = \sum_{j_1=0}^{s-1} w_{j_1} P_{j_1 s}(t)$$

For each component $q = 1, \dots, s-1$, expression (4.1) becomes:

$$0 = \sum_{t=0}^{s-1} \left\{ P_{qs}(t) \sum_{j_1=0}^{s-1} w_{j_1} P_{j_1 s}(t) \right\}$$

$$= \sum_{j_1=0}^{s-1} \left\{ w_{j_1} \sum_{t=0}^{s-1} P_{qs}(t) P_{j_1 s}(t) \right\}$$

$$= w_q \sum_{t=0}^{s-1} (P_{qs}(t))^2$$
 by Definition 3

Hence $w_q = 0$ for $q = 1, \ldots, s-1$ and $W(t) = w_0 P_{0s}(t) = constant$ by Definition 2

THEOREM 1. By the group properties of addition in GF(s), each level of factor a_1 appears equally often in U(e). In particular, level t appears in run positions $i_{tm} - \xi + \xi' = i_{tm} + \xi_1$ say. The time count over U(e) of the q^{th} main effects component of a_1 against the j^{th} trend is:

$$\sum_{t=0}^{s-1} \sum_{m=1}^{v} P_{qs}(t+e) P_{jN}(i_{tm} + \xi_1)$$
(A.1)

Now $P_{jN}(i_{tm}+\xi_1)$ is a polynomial of degree j in i_{tm} . By (3.3), this polynomial may be written

$$P_{jN}(i_{tm} + \xi_1) = \sum_{j_1=0}^{j} w_{j_1} P_{j_1N}(i_{tm})$$

where the coefficients w_{j_1} depend on the constant ξ_1 only. Substituting this expression into (A.1) gives

a time count of:

$$\sum_{t=0}^{s-1} \sum_{m=1}^{v} \left\{ P_{qs}(t+e) \sum_{j_1=0}^{j} w_{j_1} P_{j_1 N}(i_{tm}) \right\}$$

$$= \sum_{j_1=0}^{j} \left\{ w_{j_1} \sum_{t=0}^{s-1} P_{qs}(t+e) W(t;j_1,N) \right\}$$
(A.2)

By the assumptions of the theorem and Lemma 1, $W(t;j_1,N) = W(j_1,N)$ so (A.2) becomes:

$$\sum_{j_1=0}^{j} \left\{ w_{j_1} W(j_1,N) \sum_{t=0}^{s-1} P_{qs}(t+e) \right\} = 0$$

The above is true for each $j=0, \ldots, k$ and hence a_1 is k-trend free over U(e)

THEOREM 2. Without loss of generality, U is in run positions $1, \ldots, sv$ of G. By Theorem 1, a_1 is k-trend free over U^* . As t ranges over GF(s)- $\{0\}$, so too does te, $t, e \neq 0$. As before, assume that a_1 is at level t in positions i_{tm} , $m=1,\ldots,v$ of U. Then a_1 is at level (t+qe) in these same run positions of U(qe), $q=1,\ldots,s-1$. Each level of a_1 is represented by some (t+qe) as q ranges from 0 to s-1 for fixed t and similarly as t ranges from 0 to s-1 for fixed q.

Let the level of factor a_1 be fixed at t. The contribution to the time count of the l^{th} main effects component of a_1 against a trend of degree (k+1) over the run positions $\{i_{tm}\}$ in each U(qe) of U^* is:

$$\sum_{q=0}^{s-1} \sum_{m=1}^{v} P_{ls}(t+qe) P_{k+1,N}(qsv+i_{tm})$$
(A.3)

Now

$$P_{k+1,N}(qsv + i_{tm}) = w_{k+1}P_{k+1,N}(i_{tm}) + \sum_{j_1=0}^{k} w_{j_1}(q)P_{j_1N}(i_{tm})$$

where w_{k+1} is a constant not depending on q and $w_{j_1}(q)$ is a polynomial in q of degree at most (k+1). Then (A.3) becomes :

$$\sum_{q=0}^{s-1} \left\{ P_{ls}(t+qe) \sum_{m=1}^{v} \left\{ w_{k+1} P_{k+1,N}(i_{tm}) + \sum_{j_1=0}^{k} w_{j_1}(q) P_{j_1,N}(i_{tm}) \right\} \right\}$$

In the preceeding expression, $\sum w_{k+1} P_{k+1,N}(i_{tm})$ depends on t but not q and summing $P_{ls}(t+qe)$ over q

ranging from 0 to s-1 yields zero by the discussion above so the first inner term vanishes and (A.3) simplifies to :

$$\sum_{j_1=0}^{k} \sum_{q=0}^{s-1} \left\{ w_{j_1}(q) P_{l_s}(t+qe) \sum_{m=1}^{v} P_{j_1,N}(i_{tm}) \right\}$$

$$= \sum_{j_1=0}^{k} \sum_{q=0}^{s-1} W_{j_1}(q) P_{l_s}(t+qe) W(j_1,N)$$

In this last expression, the terms $P_{ls}(t+qe)$ sum to zero over $q=0,\ldots,s-1$, for each fixed t and j_1 . So the total time count over U^* of the l^{th} component of a_1 against $P_{k+1,N}$ is zero for each $l=1,\ldots,s-1$ and a_1 is (k+1)-trend free over U^* .

LEMMA 2. Suppose that factor a_1 is at nonzero level e in between block generator g_{h+m} , so s^{m-1} blocks have been generated so far, $m \in \{1, \ldots, r\}$. Recall that we assume that each level of a factor appears equally often in every block. Suppose that a_1 is at level t in run position i_0 of an already existing block, B_j , for some $j=1,...,s^{m-1}$. When generator g_{h+m} is used with the generalized foldover scheme (4.2), factor a_1 will be at level t+qe, q=1,...,s-1 in position i_0 in some s-1 new blocks $B_{j_1},\ldots,B_{j_{s-1}}$. Again, as q ranges over the set 0,...,s-1, so too does t+qe. Hence, the time count with respect to the trend component of degree l contributed by this starting run position i_0 in block B_j for the i^{th} main effects component is

$$\sum_{q=0}^{s-1} P_{IR}(i_0) P_{is}(t+qe) = P_{IR}(i_0) \sum_{q=0}^{s-1} P_{is}(t+qe) = 0$$

by Definitions 2 and 3. So each starting level of factor a_1 in any starting position in an already existing block contributes zero to the time count with respect to any trend component in the model. So factor a_1 is orthogonal to any trend component in the model.

THEOREM 3. By Theorem 2, if the run order is constructed by applying the generalized foldover scheme (4.2) to the sequence of generators $\{g_1, \ldots, g_{n-p}\}$, factor a_i is k-trend free over G if a non-zero level of this factor appears in at least (k+1) of the generators. From this and Lemma 2, Theorem 3 follows.

LEMMA 3. By (4.3), d_i is the number of factor level changes between the i^{th} generator g_i and the last run of the first s^{i-1} runs. Hence, by the definition of the generalized foldover scheme (4.2), d_i is the number of factor level changes between each adjacent pair of groups of s^{i-1} runs within each group of s^i runs. There are s^{n-p-i} groups of s^i runs, and s groups of s^{i-1} runs within each such group of s^i runs. Thus, the number of factor level changes between groups of size s^{i-1} within groups of size s^i is $s^{n-p-i}(s-1)d_i$. Summing over $i=1,\ldots,n-p$ gives the result (4.5).

THEOREM 4. Set $R_0=0$, $R_i=r_1+\cdots+r_i$, $i=1,\ldots,n-p$. By (4.3), generator \mathbf{g}_{ij} of (4.6) is \mathbf{z}_{ij} multiplied by the last run in the first $\mathbf{s}^{R_{i-1}+j-1}$ runs. So the number of level changes between these two runs is $d(\mathbf{1},\mathbf{z}_{ij})=c_i$ by the definition of the runs $\{\mathbf{z}_{ij}\}$. Hence, at each stage $i=1,\ldots,n-p$, the number of level changes between each group of \mathbf{s}^{i-1} runs within each group of \mathbf{s}^i runs is the minimum possible. Therefore, the resulting run order has minimum cost. The $\{d_{i_1},i_1=1,\ldots,n-p\}$ of (4.4) are given by :

$$d_{i_1} = c_i, \quad i_1 = \sum_{j=1}^{i-1} r_j + 1, \dots, \sum_{j=1}^{i} r_j ; \quad i = 1, \dots, t + t'$$
(A.4)

Note that $s^{R_i} = N_0/N_i$. The minimum cost of this run order is, from (4.5) and (A.4):

$$\begin{split} \sum_{i=1}^{n-p} (s-1) \, s^{n-p-i} d_i &= \sum_{i=1}^{t+t'} \sum_{i_1=R_{i-1}+1}^{R_i} c_i \, (s-1) \, s^{n-p-i_1} \\ &= \sum_{i=1}^{t+t'} (s-1) \, c_i \, \left\{ s^{n-p-R_i} \, (1-s^{r_i}) / (1-s) \right\} \\ &= \sum_{i=1}^{t+t'} c_i \, N_0 N_i / N_0 \, (s^{r_i}-1) \\ &= \sum_{i=1}^{t+t'} c_i \, (N_i m_i - N_i) \\ &= \sum_{i=1}^{t+t'} c_i \, (N_{i-1} - N_i) \end{split}$$

which gives (4.8).

THEOREM 5. Follows directly from Theorem 3 and Theorem 4 for the stated choice of minimum cost generator sequence.

THEOREM 6. Let \mathbf{x}_1 and \mathbf{x}_2 be the columns of the design matrix corresponding to the main effect of any two factors a_1 and a_2 . All entries in \mathbf{x}_1 and \mathbf{x}_2 are either +1 or -1. Then the two factor interaction column \mathbf{x} has \mathbf{i}^{th} entry $\mathbf{x}_{i1} \times \mathbf{x}_{i2}$. We assume that the interaction is estimable when no time trend is present.

Without loss of generality, both factors are at the same level in g_1 , ..., g_{k-1} ; a_1 is high, a_2 low in g_k ; both are at the same level in g_{k+1} , ..., g_{m-1} and a_1 is high, a_2 low in g_m , m > k. Then the interaction column x contains +1 in the first 2^{k-1} rows and -1 in the next 2^{k-1} rows giving a time count of $2^{2(k-1)}$ over the first 2^k runs. Note that since the trend is linear, we have shifted the values of the trend polynomial to $1, \ldots, R$ rather than $P_{1R}(i)$, $i=0,\ldots,R-1$. This results in a linear rescaling of the time count but does not affect the result stated here. This same time count is contributed by each of the first 2^{m-k-1} groups of 2^k runs. So the time count after 2^{m-1} runs is 2^{m+k-3} . When g_m is used, the entries in the interaction column are all multiplied by -1 and the second group of 2^{m-1} runs contributes a time count of exactly -2^{m+k-3} and hence the time count for the interaction effect becomes zero after 2^m runs. This time count remains zero in all future foldovers by Theorem 2. So interaction column x is orthogonal to a linear trend. By the assumptions of the Theorem, this is true for all two factor interactions.

COROLLARY 1. The n runs in (5.2) are independent so generate the complete factorial design. Referring to (4.5), the runs (5.2) have cost $d_i = 1$ if $i \neq n-3, n-2$, and $d_{n-3} = d_{n-2} = 2$. By (4.5), the cost of the run order is $\sum_{i=1}^{n} (1 \times 2^{n-i}) + 2^3 + 2^2$ which gives $2^n + 11$ as required.

The generator sequence $\{g_1, \ldots, g_n\}$ found from runs (5.2) by (4.6) is

$$a_n, \ a_n a_{n-1} \ , \dots \ , \ a_6 a_5, \ a_1 a_2 a_5, \ a_2 a_3, \ a_1 a_3 a_4, \ a_2 a_4$$

namely the i^{th} generator is the product of runs \mathbf{z}_i and \mathbf{z}_{i-1} , as stated in Section 5. Inspecting this sequence shows that, for any two factors, two generators in which only one factor name appears may be found. The conditions of Theorem 6 are met so all two factor interactions are linear trend free.

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