

ORTHOGONAL ARRAYS WITH VARIABLE NUMBERS OF SYMBOLS¹

BY CHING-SHUI CHENG

University of California, Berkeley

Orthogonal arrays with variable numbers of symbols are shown to be universally optimal as fractional factorial designs. The orthogonality of completely regular Youden hyperrectangles (F -hyperrectangles) is defined as a generalization of the orthogonality of Latin squares, Latin hypercubes, and F -squares. A set of mutually orthogonal F -hyperrectangles is seen to be a special kind of orthogonal array with variable numbers of symbols. Theorems on the existence of complete sets of mutually orthogonal F -hyperrectangles are established which unify and generalize earlier results on Latin squares, Latin hypercubes, and F -squares

1. Introduction. The concepts of hypercubes and orthogonal arrays were first introduced by Rao (1946, 1947). They were applied in the construction of symmetrical confounded factorial designs, fractional replications, and so on. Generalization to the asymmetrical case, i.e., an orthogonal array with variable numbers of symbols, is obvious. This is discussed in some detail in Rao (1973).

The purposes of this paper are twofold. Firstly, using a tool recently developed by Kiefer, we give a precise statement and a rigorous proof of the universal optimality of an orthogonal array with variable numbers of symbols as a fractional factorial design. Such a proof seems to be not available in the literature. In proving this, we also use a recent result of Cheng (1978) concerning the computation of generalized inverses of some special kind of matrices. Secondly, we define the notion of mutually orthogonal completely regular Youden hyperrectangles which is a special kind of orthogonal array with variable numbers of symbols and is a generalization of the well-known combinatorial structures such as mutually orthogonal Latin squares, F -squares, and Latin hypercubes. Two theorems on the existence of complete sets of mutually orthogonal completely regular Youden hyperrectangles are established which generalize and unify the earlier results on the above-mentioned combinatorial structures.

We define a *rectangular array*, denoted by $(N, r, s_1 \times \cdots \times s_r)$ as an $r \times N$ matrix with entries in the i th row from a set S_i of s_i elements, $1 \leq i \leq r$. A $(N, r, s_1 \times \cdots \times s_r)$ array is said to be an *orthogonal array (with variable numbers of symbols) of strength d* if for any selection of d rows, say the α_1 th, \cdots , α_d th, the

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number of times that the column vector $(i_1, \dots, i_d)'$, $i_1 \in S_{\alpha_1}, \dots, i_d \in S_{\alpha_d}$, occurs in the $d \times N$ submatrix specified by the d selected rows is constant for all combinations $i_1 \in S_{\alpha_1}, \dots, i_d \in S_{\alpha_d}$. The constant may, however, depend on the set of selected rows. We denote such an orthogonal array by $OA(N; s_1, s_2, \dots, s_r; d)$. When $s_1 = s_2 = \dots = s_r = s$, we also write it as $OA(N, r, s, d)$ and call it a *symmetric orthogonal array*. We will restrict ourselves to orthogonal arrays of strength 2 in this paper.

2. Orthogonal arrays as universally optimal fractional factorial designs. Consider a factorial design with n factors, the i th factor being experimented with at s_i levels ($i = 1, \dots, n$). Assume that the expected value of an observation taken on the i_1 th level of the first factor, i_2 th level of the second factor, \dots , and the i_n th level of the n th factor is specified by

$$(2.1) \quad E(y_{i_1 i_2 \dots i_n}) = \alpha_{i_1}^{(1)} + \alpha_{i_2}^{(2)} + \dots + \alpha_{i_n}^{(n)},$$

where $\alpha_{i_1}^{(1)}, \dots, \alpha_{i_n}^{(n)}$, $1 \leq i_j \leq s_j$, $1 \leq j \leq n$, are unknown constants, and all the observations are uncorrelated with common variance. A design with N observations is a selection of N combinations of the levels of the n factors. Let \mathcal{D}_N be the collection of all such designs with N observations. For a design $d \in \mathcal{D}_N$, the coefficient matrix of the normal equation for estimating $(\alpha_1^{(1)}, \dots, \alpha_{s_1}^{(1)}; \alpha_1^{(2)}, \dots, \alpha_{s_2}^{(2)}; \dots; \alpha_1^{(n)}, \dots, \alpha_{s_n}^{(n)})'$ is

$$(2.2) \quad \begin{bmatrix} \text{diag}(r_{d1}^{(1)}, \dots, r_{ds_1}^{(1)}) & & & N_{d12} & & \dots & N_{d1n} \\ & N_{d21} & & \text{diag}(r_{d1}^{(2)}, \dots, r_{ds_2}^{(2)}) & & \dots & N_{d2n} \\ & \vdots & & & \ddots & & \vdots \\ N_{dn1} & & \dots & & & \dots & \text{diag}(r_{d1}^{(n)}, \dots, r_{ds_n}^{(n)}) \end{bmatrix}$$

where $r_{dj}^{(i)}$ is the number of times that the j th level of the i th factor appears in the design, and N_{dij} is the incidence matrix between the i th and the j th factors, i.e., the (s, u) th element of N_{dij} is the number of times that the s th level of factor i and the u th level of factor j appear together in the design. Write C_{di} as the coefficient matrix of the reduced normal equation for estimating $(\alpha_1^{(i)}, \dots, \alpha_{s_i}^{(i)})'$, $i = 1, \dots, n$. For example,

$$(2.3) \quad C_{d1} = \text{diag}(r_{d1}^{(1)}, \dots, r_{ds_1}^{(1)}) - (N_{d12}, \dots, N_{d1n})E_{d1}^-(N_{d12}, \dots, N_{d1n})',$$

where E_{d1} is the matrix obtained by deleting the first s_1 rows and s_1 columns of (2.2), and E_{d1}^- is a generalized inverse of E_{d1} . C_{d2}, \dots, C_{dn} are similarly defined.

If there is an $OA(N; s_1, s_2, \dots, s_n; 2)$, then it defines a factorial design in \mathcal{D}_N for which the matrix of (2.2) is

$$(2.4) \quad \begin{bmatrix} s_1^{-1}NI_{s_1} & s_1^{-1}s_2^{-1}NJ_{s_1, s_2} & \cdots & s_1^{-1}s_n^{-1}NJ_{s_1, s_n} \\ s_1^{-1}s_2^{-1}NJ_{s_2, s_1} & s_2^{-1}NI_{s_2} & \cdots & s_2^{-1}s_n^{-1}NJ_{s_2, s_n} \\ \vdots & \vdots & \ddots & \vdots \\ s_1^{-1}s_n^{-1}NJ_{s_n, s_1} & \cdots & & s_n^{-1}NI_{s_n} \end{bmatrix}$$

where I_k is the $k \times k$ identity matrix, and J_{k_1, k_2} is the $k_1 \times k_2$ matrix consisting entirely of 1's.

We have the following optimality results:

THEOREM 2.1. *Under the model specified by (2.1), if there is an $OA(N; s_1, s_2, \dots, s_n; 2)$, then it defines a factorial design d^* with N observations which minimizes $\sum_{i=1}^n \Phi_i(C_{di})$ over \mathcal{D}_N for all functions $\Phi_i: \mathfrak{B}_{s_i, 0} \rightarrow (-\infty, +\infty)$ satisfying*

- (a) Φ_i is convex,
- (b) for any fixed $C \in \mathfrak{B}_{s_i, 0}$, $\Phi_i(bC)$ is nonincreasing in the scalar $b > 0$,
- (c) Φ_i is invariant under each simultaneous permutation of rows and columns, where $\mathfrak{B}_{s_i, 0}$ is the set of all $s_i \times s_i$ nonnegative definite matrices with zero row and column sums.

PROOF. We only have to show that d^* minimizes $\Phi_i(C_{di})$ over \mathcal{D}_N , for all $i = 1, \dots, n$. It is enough to prove the case $i = 1$.

By the same argument as in Lemma 2.2 of Cheng (1978), one can show that $N^{-1} \text{diag}(s_2I_{s_2}, s_3I_{s_3} - J_{s_3, s_3}, \dots, s_nI_{s_n} - J_{s_n, s_n})$ is a generalized inverse of $E_{d^{*1}}$. Accordingly,

$$\begin{aligned} C_{d^{*1}} &= s_1^{-1}NI_{s_1} - s_1^{-1}s_2^{-1}NJ_{s_1, s_2}(N^{-1}s_2I_{s_2})(s_1^{-1}s_2^{-1}NJ_{s_2, s_1}) \\ &\quad - \sum_{j=3}^n s_1^{-1}s_j^{-1}NJ_{s_1, s_j}[N^{-1}(s_jI_{s_j} - J_{s_j, s_j})]s_1^{-1}s_j^{-1}NJ_{s_j, s_1} \\ &= s_1^{-1}NI_{s_1} - s_1^{-2}NJ_{s_1, s_1} \end{aligned}$$

since each $s_jI_{s_j} - J_{s_j, s_j}$ has zero row sum.

So $C_{d^{*1}}$ is completely symmetric in the sense that all the diagonal elements of $C_{d^{*1}}$ are equal, and all the off-diagonal elements are also equal. Therefore, by Proposition 1 of Kiefer (1975), it suffices to show that d^* maximizes $\text{tr } C_{d1}$ over \mathcal{D}_N .

For any $d \in \mathcal{D}_N$, we have

$$E_{d1}^- > \begin{pmatrix} (\text{diag}(r_{d1}^{(2)}, \dots, r_{ds_2}^{(2)}))^- & 0 \\ 0 & 0 \end{pmatrix},$$

where $A > B$ means that $A - B$ is nonnegative definite.

Hence

$$\text{diag}(r_{d_1}^{(1)}, \dots, r_{d_{s_1}}^{(1)}) - N_{d12} [\text{diag}(r_{d_1}^{(2)}, \dots, r_{d_{s_2}}^{(2)})]^{-N'_{d12}} > C_{d1}.$$

Now,

$$\text{tr}(N_{d12} [\text{diag}(r_{d_1}^{(2)}, \dots, r_{d_{s_2}}^{(2)})]^{-N'_{d12}}) = \sum_{i=1}^{s_1} \sum_{j=1}^{s_2} [(N_{d12})_{ij}]^2 / r_{d_j}^{(2)},$$

where $[(N_{d12})_{ij}]^2 / r_{d_j}^{(2)}$ is interpreted as zero if $r_{d_j}^{(2)} = 0$.

For each $r_{d_j}^{(2)} \neq 0$, $\sum_{i=1}^{s_1} (N_{d12})_{ij} = r_{d_j}^{(2)}$. Therefore,

$$\begin{aligned} \sum_{i=1}^{s_1} [(N_{d12})_{ij}]^2 / r_{d_j}^{(2)} &\geq s_1 (s_1^{-1} r_{d_j}^{(2)})^2 / r_{d_j}^{(2)} \\ &= s_1^{-1} r_{d_j}^{(2)}. \end{aligned}$$

Hence

$$\begin{aligned} \text{tr}(C_{d1}) &\leq \sum_{j=1}^{s_1} r_{d_j}^{(1)} - \sum_{j=1}^{s_2} s_1^{-1} r_{d_j}^{(2)} \\ &= N - s_1^{-1} N \\ &= \text{tr } C_{d^*1}. \end{aligned}$$

□

Following Kiefer (1975), we say that an orthogonal array is *universally optimal*.

From the proof of the above theorem, it can easily be seen that for any i with $1 < i < n$, if d is a design in \mathcal{O}_N s.t. $r_{d_j}^{(i)} = N/s_i$ for all $j = 1, 2, \dots, s_i$ (i.e., the levels of the i th factor are equally replicated), then $C_{d^*i} > C_{di}$. Hence, by a result of Ehrenfeld (1955), d^* is at least as good as d for the estimation of any contrast among the main effects of the s_i levels of factor i . Thus, if we restrict to equally replicated designs, a much stronger optimality can be proved.

3. Mutually orthogonal completely regular Youden hyperrectangles. It is well known that mutually orthogonal Latin squares and Latin hypercubes are special cases of (symmetrical) orthogonal arrays of strength 2. It is also clear that a set $\{F_1, F_2, \dots, F_n\}$ of n mutually orthogonal $N \times N$ F -squares with constant frequency vectors and s_1, s_2, \dots, s_n symbols respectively (as defined in Hedayat and Seiden (1970)) is equivalent to an $\text{OA}(N^2; N, N, s_1, s_2, \dots, s_n; 2)$. All of these can be generalized to the orthogonality of completely regular Youden hyperrectangles.

Cheng (1978) defined the notion of a completely regular Youden hyperrectangle. Given an n -dimensional hyperrectangle of size $N_1 \times N_2 \times \dots \times N_n$, we can coordinatize the $\prod_{i=1}^n N_i$ cells by the n -tuples of integers (j_1, j_2, \dots, j_n) with $1 < j_i < N_i$. An arrangement of s symbols into the $\prod_{i=1}^n N_i$ cells is called a *completely regular Youden hyperrectangle* if $s | \prod_{j \neq i} N_j$, for all $i = 1, \dots, n$, and for any fixed $i = 1, \dots, n$, each of the s symbols appears $s^{-1} (\prod_{j \neq i} N_j)$ times in each of the N_i sets $H_1^i, H_2^i, \dots, H_{N_i}^i$, where H_j^i is the set of all cells with j as the i th coordinate, $1 < j < N_i$. This apparently generalizes the notions of Latin squares, F -squares, and Latin hypercubes. For convenience, we also call a completely regular Youden hyperrectangle an *F-hyperrectangle*.

We define two F -hyperrectangles of the same size to be *orthogonal* if, when superimposed on one another, every ordered pair of symbols occurs the same number of times. It is clear that a set of m mutually orthogonal F -hyperrectangles with size $N_1 \times N_2 \times \dots \times N_n$ and s_1, s_2, \dots, s_m symbols is an $\text{OA}(\prod_{i=1}^n N_i; N_1, N_2, \dots, N_n, s_1, \dots, s_m; 2)$. Thus, a set of mutually orthogonal F -hyperrectangles is not only optimal for the elimination of multi-way heterogeneity, but also is optimal as a fractional factorial design.

Rao (1973) showed that if there is an $\text{OA}(N; s_1, \dots, s_n; 2)$, then $N - 1 \geq \sum_{i=1}^n (s_i - 1)$. Therefore, for a set of m mutually orthogonal F -hyperrectangles of size $N_1 \times \dots \times N_n$ and the same number of symbols s , we must have

$$\prod_{i=1}^n N_i - 1 \geq \sum_{i=1}^n (N_i - 1) + m(s - 1).$$

Thus

$$(3.1) \quad m \leq (\prod_{i=1}^n N_i - \sum_{i=1}^n (N_i - 1) - 1) / (s - 1).$$

This gives an upper bound for the number of mutually orthogonal F -hyperrectangles with the same number of symbols. When this upper bound is achieved, we say that a *complete set of mutually orthogonal F -hyperrectangles exists*.

We have the following results concerning the existence of a complete set of mutually orthogonal F -hyperrectangles.

THEOREM 3.1. *If s is a prime power, and each N_i is a power of s , $i = 1, \dots, n$, then there exists a complete set of mutually orthogonal F -hyperrectangles of size $N_1 \times N_2 \times \dots \times N_n$ and s symbols.*

PROOF. By assumption, $N_i = s^{t_i}$ for some integer t_i . Write $u = \sum_{i=1}^n t_i$. Let $\text{EG}(u; s)$ be the u -dimensional Euclidean geometry based on the Galois field with s elements. One can choose u independent pencils of $(u - 1)$ -flats in $\text{EG}(u; s)$ and divide them into n groups B_1, B_2, \dots, B_n such that for each i , $1 \leq i \leq n$, B_i contains t_i pencils. If we take an arbitrary $(u - 1)$ -flat from each pencil in B_i , then these t_i $(u - 1)$ -flats intersect in a $(u - t_i)$ -flat. Altogether, there are $N_i = s^{t_i}$ such $(u - t_i)$ -flats. Denote these $(u - t_i)$ -flats by $F_1^{(i)}, \dots, F_{N_i}^{(i)}$. If we take an arbitrary $(u - t_i)$ -flat from $F_1^{(i)}, \dots, F_{N_i}^{(i)}$, $i = 1, \dots, n$, then the intersection of the n chosen flats with dimensions $(u - t_1), \dots, (u - t_n)$, respectively, is a point. So we can use the set $\cup_{i=1}^n \{F_1^{(i)}, \dots, F_{N_i}^{(i)}\}$ to set up a coordinate system for $\text{EG}(u; s)$. A point has coordinate (i_1, \dots, i_n) if it is the intersection of $F_{i_1}^{(1)}, F_{i_2}^{(2)}, \dots$, and $F_{i_n}^{(n)}$.

Now, there are $(s^u - 1)/(s - 1) - \sum_{i=1}^n (s^{t_i} - 1)/(s - 1) = (\prod_{i=1}^n N_i - \sum_{i=1}^n (N_i - 1) - 1)/(s - 1)$ pencils of $(u - 1)$ -flats which are linearly dependent on none of the B_i 's. For each of these pencils, we can label the s $(u - 1)$ -flats in it by $1, 2, \dots, s$, and define an F -hyperrectangle of size $N_1 \times \dots \times N_n$ and s symbols in the following way: for each cell (i_1, i_2, \dots, i_n) , $1 \leq i_j \leq N_j$, if the point of $\text{EG}(u; s)$ with coordinates (i_1, i_2, \dots, i_n) is in the j th flat of the pencil, then we assign symbol j to the cell (i_1, \dots, i_n) .

This clearly defines an F -hyperrectangle, and the $(\prod_{i=1}^n N_i - \sum_{i=1}^n (N_i - 1) - 1)/(s - 1)$ F -hyperrectangles obtained are mutually orthogonal. \square

REMARK. In the above theorem,

(a) if $n = 2$ and $s = N_1 = N_2$, then it reduces to the classical result on the existence of a complete set of mutually orthogonal Latin squares with a prime power as the size;

(b) if $n > 2$, and $s = N_1 = \dots = N_n$, then it reduces to Kishen's (1949) result on orthogonal Latin hypercubes;

(c) if $n = 2$ and $N_1 = N_2$, then it reduces to the result of Hedayat, Raghavarao and Seiden (1975) on orthogonal F -squares.

THEOREM 3.2. *If there exist orthogonal arrays $OA(N_i, n_i, s, 2)$ for $i = 1, \dots, k$, then there exist m mutually orthogonal F -hyperrectangles of size $N_1 \times N_2 \times \dots \times N_k$ and s symbols, where $m = \prod_{i=1}^k (n_i + 1) - 1 - \sum_{i=1}^k n_i$.*

PROOF. Denote the s symbols by $0, 1, 2, \dots, s - 1$, i.e., the integers modulo s . To each $OA(N_i, n_i, s, 2)$, add a row consisting entirely of zeros. Designate the augmented array by D_i . Let D be the Kronecker product of D_1, D_2, \dots , and D_k . Then D is an $\prod_{i=1}^k (n_i + 1) \times \prod_{i=1}^k N_i$ array. Each entry of D is a k -tuple of integers modulo s . These $\prod_{i=1}^k (n_i + 1)$ entries can be coordinatized in the following way. Label the rows of D by the k -tuples of integers (i_1, \dots, i_k) , $1 \leq i_l \leq n_l + 1$, and the columns by the k -tuples of integers (j_1, \dots, j_k) , $1 \leq j_l \leq N_l$. Then for each h with $1 \leq h \leq k$, the h th coordinate of the entry in the (i_1, \dots, i_k) th row and the (j_1, \dots, j_k) th column of D is the element appearing in the i_h th row and the j_h th column of D_h . The (i_1, \dots, i_k) th row of D is said to be obtained from the i_1 th row of D_1, i_2 th row of D_2, \dots , and i_k th row of D_k . Now delete those rows of D which are obtained from at least $k - 1$ augmented rows (rows consisting entirely of zeros). Altogether, there are $m = \prod_{i=1}^k (n_i + 1) - 1 - \sum_{i=1}^k n_i$ remaining rows. Replacing each entry (a k -tuple) of the remaining array by the sum of its coordinates modulo s , we get a new array \bar{D} of the integers $0, 1, 2, \dots, s - 1$. Keeping the coordinates of the $\prod_{i=1}^k N_i$ columns of \bar{D} as the coordinates of a hyperrectangle of size $N_1 \times N_2 \times \dots \times N_k$, each of these m rows defines a hyperrectangle of size $N_1 \times N_2 \times \dots \times N_k$ and s symbols. It can easily be seen that these m hyperrectangles are F -hyperrectangles and are mutually orthogonal. \square

When $s = 2$, the upper bound for the number of mutually orthogonal F -hyperrectangles of size $N_1 \times N_2 \times \dots \times N_k$ is $\prod_{i=1}^k N_i - (\sum_{i=1}^k N_i - 1) - 1$. If there exist Hadamard matrices of orders N_1, N_2, \dots, N_k , then there exist k orthogonal arrays $OA(N_i, N_i - 1, 2, 2)$, $i = 1, \dots, k$, and hence by Theorem 3.2, there exist $\prod_{i=1}^k N_i - 1 - \sum_{i=1}^k (N_i - 1)$ mutually orthogonal F -hyperrectangles of size $N_1 \times N_2 \times \dots \times N_k$ and 2 symbols. This achieves the upper bound. That is, we have

COROLLARY 3.2.1. *If there exist Hadamard matrices of order N_1, N_2, \dots, N_k , where N_1, N_2, \dots , and N_k are multiples of 4, then there is a complete set of mutually orthogonal F -hyperrectangles of size $N_1 \times N_2 \times \dots \times N_k$ and 2 symbols.*

REMARK. In the above corollary, if $n = 2$, and $N_1 = N_2$, then it reduces to the result of Federer (1977) on orthogonal F -squares.

REMARK. An easy method to construct an orthogonal array with variable numbers of symbols is to identify different symbols in some rows of a symmetric orthogonal array. But not all orthogonal arrays with variable numbers of symbols can be obtained in this way. For example, by Corollary 3.2.1, there is an OA(8; 4, 2, 2, 2, 2; 2). This can not be obtained by identifying different symbols in a symmetric orthogonal array since such a symmetric orthogonal array must have at least four symbols and hence the size N must be at least 16. One more example. Corollary 3.2.1. implies the existence of an

$$OA\left(16; 4, 4, \underbrace{2, \dots, 2}_9; 2\right)$$

accommodating 11 factors. Again it can not be obtained by identifying different symbols in a symmetric orthogonal array since such a symmetric OA must have 4 symbols and hence can only accommodate at most 5 factors.

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DEPARTMENT OF STATISTICS
 UNIVERSITY OF CALIFORNIA
 BERKELEY, CALIFORNIA 94720