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Orthogonal and nearly orthogonal designs for computer experiments

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SUMMARY

We introduce a method for constructing a rich class of designs that are suitable for use in computer experiments. The designs include Latin hypercube designs and two-level fractional factorial designs as special cases and fill the vast vacuum between these two familiar classes of designs. The basic construction method is simple, building a series of larger designs based on a given small design. If the base design is orthogonal, the resulting designs are orthogonal; likewise, if the base design is nearly orthogonal, the resulting designs are nearly orthogonal. We present two generalizations of our basic construction method. The first generalization improves the projection properties of the basic method; the second generalization gives rise to designs that have smaller correlations. Sample constructions are presented and properties of these designs are discussed.

Some key words: Fractional factorial; Hadamard matrix; J-characteristic; Kronecker product; Latin hypercube; Orthogonal array; Resolution IV design.

1. INTRODUCTION

Latin hypercube designs, which have been popular choices for computer experiments since they were introduced by McKay et al. (1979), are a very large class of designs with some desirable properties. For example, when projected on any single factor, Latin hypercubes achieve the maximum stratification; that is, if we look at the one-dimensional projections only, the equally-spaced design points cover the entire experimental region for each variable. Furthermore, a Latin hypercube does not have repeated runs, a desirable feature as they do not bring new information in computer experiments because of the deterministic nature of computer models. However, a Latin hypercube design does not necessarily compare well with respect to other useful criteria such as those related to orthogonality or space-filling. With regard to orthogonality, one natural way of finding good designs within the class of Latin hypercubes is to restrict attention to orthogonal Latin hypercubes. Ye (1998) and Steinberg & Lin (2006) provided some construction results on orthogonal Latin hypercubes. Prior to this, Owen (1994) and Tang (1998) developed computational algorithms for searching for nearly orthogonal Latin hypercubes. Butler (2001) constructed Latin hypercubes that are orthogonal with respect to models based on trigonometric functions.

The factors in a Latin hypercube design have as many levels as the run size, which makes it very difficult for a Latin hypercube to be orthogonal. In the orthogonal Latin hypercubes constructed by Ye (1998), the run size n must be of the form $n = 2^k$ and the number m of factors must satisfy $m = 2k - 2$. This means that the ratio m/n becomes very small even for moderately large k. The orthogonal Latin hypercubes constructed by Steinberg & Lin (2006) have a large ratio m/n, the price being a more severe restriction on the run size n, which now must have the form $n = 2^{2^k}$, a very large number even for k as small as 5.

Latin hypercube designs are attractive for computer experiments because they allow one to observe factors at many levels in relatively few trials. However, practical experience and interaction with researchers who use the design and analysis methodology of computer experiments in their investigations have revealed that designs with many levels are desirable, but it is not essential that the number of runs equals the number of levels at which each factor is observed, as in a Latin hypercube design. By relaxing the condition that the number of levels for each factor be identical to the run size, we construct in this paper a class of orthogonal designs for computer experiments. This very rich class of orthogonal designs includes two-level orthogonal designs and orthogonal Latin hypercubes as special cases. The construction method allows various choices for the number s of levels in the whole range $s = 2, \ldots, n$. The constructed designs have much more flexible run sizes than the designs in Ye (1998) and Steinberg & Lin (2006).

With regard to space-filling designs for computer experiments, see chap. 5 and 6 of Santner et al. (2003) for discussion and useful ideas. A full investigation is beyond the scope of the paper.

Many researchers are increasingly interested in using polynomial models for computer experiments though Gaussian-process models are still very popular. Polynomials are attractive because they allow gradual building of a suitable model by starting with simple linear terms and then gradually introducing higher-order terms. Orthogonal and nearly orthogonal designs are directly useful when polynomial models are considered. If one insists on using Gaussian-process models, orthogonality and near orthogonality can be viewed as stepping stones to space-filling designs. This is because a good space-filling design must be orthogonal or nearly so, as the design points should be uniformly scattered when projected onto two dimensions. Thus, the search for space-filling designs can be restricted to orthogonal and nearly orthogonal designs.

2. DESIGN CONSTRUCTION

2·1. *Notation, definition and background material*

Consider designs of n runs for m factors of s levels, where $s = 2, \ldots, n$. For convenience, the s levels are chosen to be centred, equally spaced and integer-valued. When s is odd, the levels are taken to be $-(s-1)/2, \ldots, -1, 0, 1, \ldots, (s-1)/2$. When s is even, the levels are chosen as $-s+1, -s+3, \ldots, -1, 1, \ldots, s-1$. For example, the levels are $-2, -1, 0, 1, 2$ for $s = 5$ and $-3, -1, 1, 3$ for $s = 4$. The levels except for level 0 in the case of odd s are assumed to be equally replicated in each design column to ensure that linear main effects are all orthogonal to the grand mean. Such a design is denoted by $\mathrm{D}(n, s^m)$ and can be represented by an $n \times m$ matrix $D = (d_{ij})$ with entries from the set of s levels as described above. Clearly, a $\mathrm{D}(n, s^m)$ becomes a Latin hypercube design when $s = n$ and a two-level fractional factorial when $s = 2$. Design D is said to be orthogonal if the inner product of any two columns of D is zero, that is, $\sum_{i=1}^{n} d_{ij_1} d_{ij_2} = 0$ for any $j_1 < j_2$. This definition of orthogonality is not to be confused with the combinatorial definition used for orthogonal arrays (Hedayat et al., 1999). We use $\mathrm{OD}(n, s^m)$ to denote an orthogonal design with m factors at s levels. We will use this shorthand for $\mathrm{D}(n, s^m)$ and $\mathrm{OD}(n, s^m)$ throughout.

For an arbitrary number of vectors $b_j = (b_{1j}, \ldots, b_{nj})^{\mathrm{T}}$, where $j = 1, \ldots, k$, their J-characteristic is defined as

$$J(b_1, \ldots, b_k) = \sum_{i=1}^{n} b_{i1} \cdots b_{ik}.$$

For a pair of columns, the J-characteristic is just the inner product of the two columns. Therefore, design $D = (d_1, \ldots, d_m)$ is orthogonal if and only if $J(d_{j_1}, d_{j_2}) = 0$ for any $j_1 < j_2$, where d_j denotes the jth column of D. Let $A = (a_{ij})_{n_1 \times m_1}$ and $B = (b_{ij})_{n_2 \times m_2}$ be two matrices. Their Kronecker product is defined as

$$A \otimes B = \begin{pmatrix} a_{11}B & a_{12}B & \cdots & a_{1m_1}B \\ a_{21}B & a_{22}B & \cdots & a_{2m_1}B \\ \vdots & \vdots & & \vdots \\ a_{n_1 1}B & a_{n_1 2}B & \cdots & a_{n_1 m_1}B \end{pmatrix}.$$

The following result from Tang (2006) is useful for later development.

Lemma 1. *We have that*

$$J(a_1 \otimes b_1, \ldots, a_k \otimes b_k) = J(a_1, \ldots, a_k)\, J(b_1, \ldots, b_k),$$

where $a_j = (a_{1j}, \ldots, a_{n_1 j})^{\mathrm{T}}$ *and* $b_j = (b_{1j}, \ldots, b_{n_2 j})^{\mathrm{T}}$ *for* $j = 1, \ldots, k$.

2·2. *Design construction and its orthogonality*

Let $A = (a_{ij})$ be an $n_1 \times m_1$ matrix with entries $a_{ij} = \pm 1$. In what follows, we always use A to denote a matrix only having entries ± 1 unless otherwise stated. Furthermore, let D_0 be a $\mathrm{D}(n_2, s^{m_2})$. Clearly, design

$$D = A \otimes D_0 \tag{1}$$

is a $\mathrm{D}(n_1 n_2, s^{m_1 m_2})$.

In the above construction it is not required that the two levels ± 1 of A be equally replicated in any column of A. As we shall see, it will be beneficial to choose A to be orthogonal. Hadamard matrices and two-level orthogonal arrays are all such orthogonal matrices. A Hadamard matrix is an orthogonal square matrix with entries ± 1. A two-level orthogonal array of strength $t \geqslant 2$, denoted by $\mathrm{OA}(n_1, 2^{m_1}, t)$, is an $n_1 \times m_1$ matrix with entries ± 1 such that, in any of its $n_1 \times t$ submatrices, each of the 2^t possible row vectors occurs the same number of times. Clearly, attaching a column of all plus ones to a two-level orthogonal array still gives an orthogonal matrix.

Proposition 1. *Let A be orthogonal. Then design $D = A \otimes D_0$ in* (1) *is orthogonal if and only if D_0 is orthogonal.*

Proposition 1 can be verified directly using Lemma 1, and its validity also follows from Proposition 2 in the next section. The construction in equation (1) and Proposition 1 are well-known results in the construction of Hadamard matrices and two-level orthogonal arrays of strength two. The use of this Kronecker product method in constructing two-level orthogonal arrays of strength three has recently been investigated by Chen & Cheng (2006) and Cheng et al. (2008). We see from Proposition 1 that the same idea allows us to construct a rich class of orthogonal designs suitable for computer experiments. The next two examples illustrate the power of this method.

Example 1. Let A be a Hadamard matrix of order k, and let D_0 be the orthogonal Latin hypercube $\mathrm{OD}(8, 8^4)$ constructed by Ye (1998). Applying the construction in (1), we obtain a series of $\mathrm{OD}(8k, 8^{4k})$s, where k is an integer such that a Hadamard matrix of order k exists.

Adding a centrepoint $(0, \ldots, 0)$ to these designs and rescaling the levels, we obtain a series of $\mathrm{OD}(8k+1, 9^{4k})$ designs.

Example 2. Steinberg & Lin (2006) constructed an orthogonal Latin hypercube of 16 runs for 12 factors. Taking this $\mathrm{OD}(16, 16^{12})$ to be D_0 in (1), we obtain a series of $\mathrm{OD}(16k, 16^{12k})$s, where k is such that a Hadamard matrix of order k exists.

2·3. *Near orthogonality*

Since there are only a handful of orthogonal Latin hypercubes available for small run sizes, choices for D_0 in (1) are quite limited. Greater flexibility is gained by allowing D_0 to be a nearly orthogonal Latin hypercube. If D_0 in (1) is nearly orthogonal, one expects that D is also nearly orthogonal. This is quantified in the present section.

For any design $C = (c_1, \ldots, c_m)$, where c_j is the jth column of C, we define $\rho_{ij}(C) = \rho(c_i, c_j)$ to be $J(c_i, c_j)/\{J(c_i, c_i)J(c_j, c_j)\}^{1/2}$. If the sum of the components in c_j for all $j = 1, \ldots, m$ is zero, as will be the case for designs in $\mathrm{D}(n, s^m)$, then $\rho_{ij}(C)$ is simply the correlation coefficient between c_i and c_j. This is the case for both D_0 and D in (1). For A in (1), the interpretation of $\rho_{ij}(A)$ is slightly different. Although it is not the correlation between the ith and jth columns, it does provide a measure of non-orthogonality of the two columns. Let $\rho_M(C) = \max_{i<j} |\rho_{ij}(C)|$ and $\rho^2(C) = \sum_{i<j} \rho_{ij}^2(C)/\{m(m-1)/2\}$.

PROPOSITION 2. *Consider design D in* (1). *Then we have that*

(i) $\rho_M(D) = \max\{\rho_M(A), \rho_M(D_0)\}$,
(ii) $\rho^2(D) = w_1\rho^2(A) + w_2\rho^2(D_0) + w_3\rho^2(A)\rho^2(D_0)$,

where $w_1 = (m_1 - 1)/(m_1m_2 - 1)$, $w_2 = (m_2 - 1)/(m_1m_2 - 1)$ *and* $w_3 = 1 - w_1 - w_2$.

Proposition 2 says that, if A and D_0 are both nearly orthogonal, then design D is nearly orthogonal as well, in terms of both measures of non-orthogonality. Lemma 1 allows Proposition 2 to be proved easily. Here we provide a sketch of the proof. Let $a_1, \ldots, a_{m_1}$ be the columns of A and let $b_1, \ldots, b_{m_2}$ be the columns of D_0. Then $a_{i_1} \otimes b_{j_1}$ and $a_{i_2} \otimes b_{j_2}$ are two columns of D. They are distinct unless $i_1 = i_2$ and $j_1 = j_2$ are both true. Lemma 1 gives $J(a_{i_1} \otimes b_{j_1}, a_{i_2} \otimes b_{j_2}) = J(a_{i_1}, a_{i_2})J(b_{j_1}, b_{j_2})$, which further implies that

$$\rho(a_{i_1} \otimes b_{j_1}, a_{i_2} \otimes b_{j_2}) = \rho(a_{i_1}, a_{i_2})\rho(b_{j_1}, b_{j_2}). \tag{2}$$

From (2), part (i) of Proposition 2 is immediate. Part (ii) follows from

$$\sum_{i_1=1}^{m_1}\sum_{i_2=1}^{m_1}\sum_{j_1=1}^{m_2}\sum_{j_2=1}^{m_2} \rho^2(a_{i_1} \otimes b_{j_1}, a_{i_2} \otimes b_{j_2}) = \sum_{i_1=1}^{m_1}\sum_{i_2=1}^{m_1} \rho^2(a_{i_1}, a_{i_2}) \times \sum_{j_1=1}^{m_2}\sum_{j_2=1}^{m_2} \rho^2(b_{j_1}, b_{j_2}).$$

If A in (1) is chosen to be orthogonal, simpler expressions are obtained.

COROLLARY 1. *If A in* (1) *is orthogonal, then we have that*

(i) $\rho_M(D) = \rho_M(D_0)$,
(ii) $\rho^2(D) = w_2\rho^2(D_0)$, *where* $w_2 = (m_2 - 1)/(m_1m_2 - 1)$.

Example 3. Let D_0 be a Latin hypercube $\mathrm{D}(6, 6^2)$ given by

$$D_0^{\mathrm{T}} = \begin{pmatrix} -5 & -3 & -1 & 1 & 3 & 5 \\ 3 & -3 & 1 & -5 & 5 & -1 \end{pmatrix}.$$

The two columns of D_0 have a small correlation of $-0{\cdot}0286$. If we choose A to be a Hadamard matrix of order k, then D in (1) is a $\mathrm{D}(6k, 6^{2k})$. This design is nearly orthogonal, with $\rho_M(D) = 0{\cdot}0286$ and $\rho^2(D) = 0{\cdot}0286^2/(2k-1) = 0{\cdot}0008/(2k-1)$.

2·4. *Orthogonality of higher order*

The orthogonal Latin hypercubes constructed by Ye (1998) enjoy an orthogonality property of higher order in that, in addition to being mutually orthogonal, the linear main effects are orthogonal to the quadratic effects and the linear-by-linear two-factor interactions. Steinberg & Lin (2006) also provided a construction of Latin hypercubes with orthogonality of higher order. In this section we show that, if one of A and D_0 in (1) has this orthogonality property of higher order, then $D = A \otimes D_0$ has the same property.

For convenience of presentation, design $C = (c_1, \ldots, c_m)$ is said to be 3-orthogonal if $J(c_j) = 0$ for all j, $J(c_i, c_j) = 0$ for all $i < j$ and $J(c_i, c_j, c_k) = 0$ for all i, j, k. Clearly, a two-level design is 3-orthogonal if and only if it is an orthogonal array of strength three. A design with more than two levels is 3-orthogonal if and only if the linear main effects are orthogonal to the grand mean, linear main effects are mutually orthogonal and linear main effects are orthogonal to quadratic effects and linear-by-linear two-factor interactions.

Proposition 3. *Let both A and D_0 be orthogonal. We have that*

(i) *design D in* (1) *is* 3-*orthogonal if D_0 is* 3-*orthogonal,*
(ii) *design D in* (1) *is* 3-*orthogonal if A is an orthogonal array of strength three.*

Proposition 3 is immediate from Lemma 1. Now consider the special case in which A is a Hadamard matrix and D_0 is a two-level design. Proposition 3 concludes that $D = A \otimes D_0$ is an orthogonal array of strength three if D_0 is an orthogonal array of strength three, a result obtained earlier by Chen & Cheng (2006) and Cheng et al. (2008).

Example 4. Since the $\mathrm{OD}(8, 8^4)$ from Ye (1998) is in fact 3-orthogonal, the $\mathrm{OD}(8k, 8^{4k})$ in Example 1 is also 3-orthogonal, where k is such that a Hadamard matrix of order k exists.

Example 5. Let D_0 be the $\mathrm{OD}(16, 16^{12})$ from Steinberg & Lin (2006), and let A be a saturated orthogonal array of strength 3 with $n_1 = 2k$ runs and $m_1 = k$ factors, assuming that a Hadamard matrix of order k exists. Then D in (1) is a 3-orthogonal $\mathrm{OD}(32k, 16^{12k})$.

Remark 1. For convenience, our discussion has been restricted to designs that have the same number of levels for all factors. In fact, all the results in this section still hold true if D_0 in (1) has mixed levels, meaning that the numbers of levels may be different for different factors. Similar remarks can also be made for the results in later sections. Clearly, if D_0 has mixed levels, then D in (1) has mixed levels. Designs with mixed levels are useful if one feels the need of studying some factors in more details than others.

Remark 2. Mathematically, the results in this section are even more general than described in Remark 1. All the results rely solely on Lemma 1. There is no need to require that A have entries ± 1 and the levels of D_0 be equally spaced and integer-valued, as these requirements are never used. However, this generality appears to be only mathematically interesting. For example, if we allow A to have entries ± 1 and ± 2, the levels of D in (1) will no longer be equally-spaced even when the levels of D_0 are equally-spaced.

3. GENERALIZATIONS

3·1. *Generalization for better projection properties*

Let $A = (a_{ij})$ be an $n_1 \times m_1$ matrix with $a_{ij} = \pm 1$ as in § 2. For each $j = 1, \ldots, m_1$, let D_j be a $\mathrm{D}(n_2, s^{m_2})$. Consider the following construction:

$$D = (a_{ij} D_j) = \begin{pmatrix} a_{11}D_1 & a_{12}D_2 & \cdots & a_{1m_1}D_{m_1} \\ a_{21}D_1 & a_{22}D_2 & \cdots & a_{2m_1}D_{m_1} \\ \vdots & \vdots & & \vdots \\ a_{n_1 1}D_1 & a_{n_1 2}D_2 & \cdots & a_{n_1 m_1}D_{m_1} \end{pmatrix}. \tag{3}$$

We have the following results for design D in (3), which generalize Proposition 1 and Corollary 1.

PROPOSITION 4. *Let A be orthogonal. We have that*

(i) $\rho_M(D) = \max\{\rho_M(D_1), \ldots, \rho_M(D_{m_1})\}$,
(ii) $\rho^2(D) = w_2\{\rho^2(D_1) + \cdots + \rho^2(D_{m_1})\}/m_1$, *where* $w_2 = (m_2 - 1)/(m_1 m_2 - 1)$,
(iii) *D in (3) is orthogonal if and only if $D_1, \ldots, D_{m_1}$ are all orthogonal.*

We sketch a proof. Let a_j be the jth column of A, and let b_1, b_2 be two columns of D_j. Then we have $J(a_j \otimes b_1, a_j \otimes b_2) = n_1 J(b_1, b_2)$ according to Lemma 1. Let a_i and a_j be two distinct columns of A, let b_1 be a column of D_i and let b_2 a column of D_j. We obtain $J(a_i \otimes b_1, a_j \otimes b_2) = 0$ because A is orthogonal. Parts (i) and (ii) quickly follow from these observations. Part (iii) becomes obvious once we have part (i) or part (ii).

What makes the construction in (3) attractive is that it offers better projection properties as compared with our basic construction method in (1). To explain this, consider the simple case in which $A = ((1, 1)^{\mathrm{T}}, (1, -1)^{\mathrm{T}})^{\mathrm{T}}$, a Hadamard matrix of order 2. Then design D given by (1) has two columns of the form

$$\begin{pmatrix} b & b \\ b & -b \end{pmatrix},$$

where b is a column of D_0. When design D is projected on to these two columns, the design points lie on the two lines $y = x$ and $y = -x$. By using two different D_1 and D_2 as in (3), we can eliminate the above pattern.

Example 6. Consider the following two $\mathrm{OD}(8, 8^4)$s.

D_1				D_2			
1	−3	7	5	−3	−1	−5	7
3	1	5	−7	−7	−5	1	−3
5	−7	−3	−1	7	5	−1	3
7	5	−1	3	3	1	5	−7
−1	3	−7	−5	5	−7	−3	−1
−3	−1	−5	7	1	−3	7	5
−5	7	3	1	−5	7	3	1
−7	−5	1	−3	−1	3	−7	−5

Design D_1 is the orthogonal Latin hypercube from Ye (1998) while D_2 is a row permutation of D_1. Let $A = ((1, 1)^{\mathrm{T}}, (1, -1)^{\mathrm{T}})^{\mathrm{T}}$. We now obtain two $\mathrm{OD}(16, 8^8)$s. The first is given by the

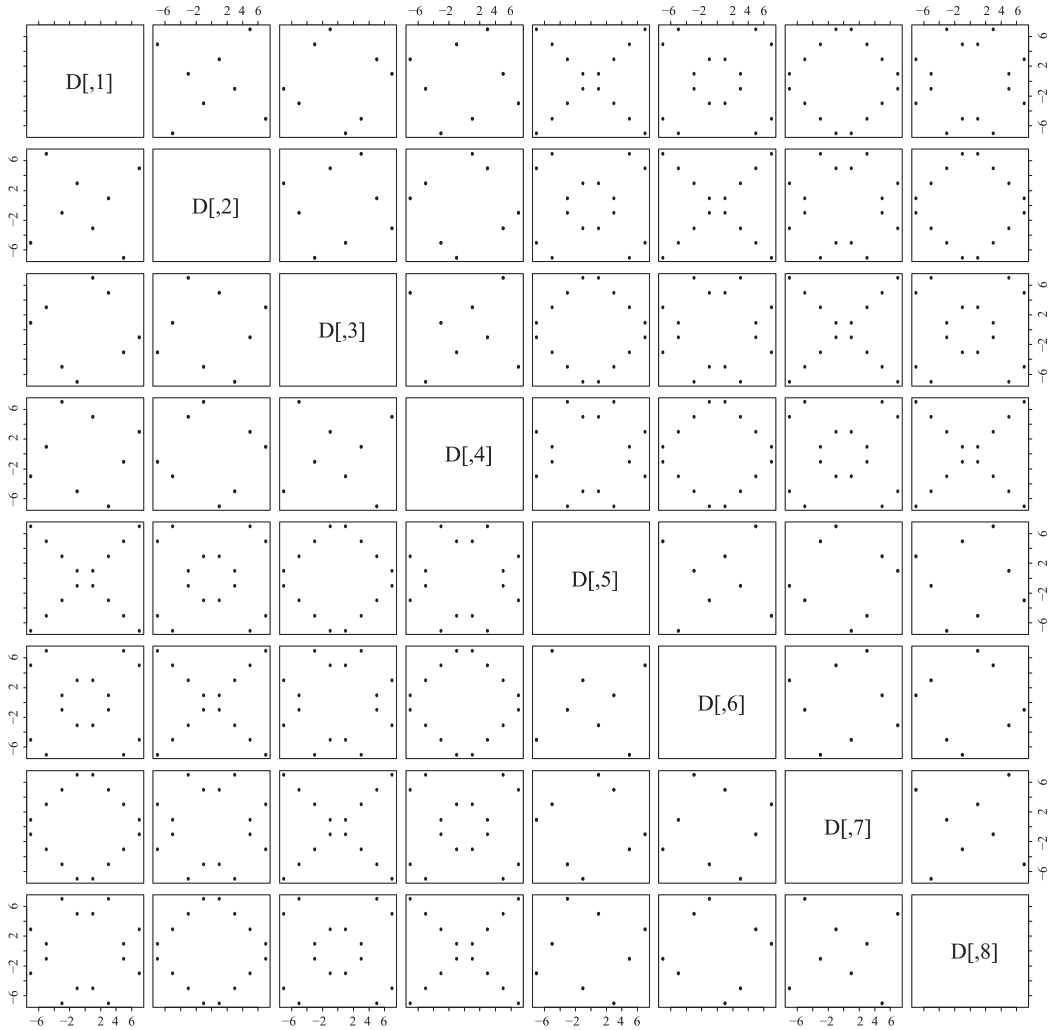

Fig. 1. The OD(16, 8^8) constructed by the basic method in (1).

basic construction in (1) by taking $D_0 = D_1$ and the second is obtained from the construction in (3) using the above D_1 and D_2. The pairwise plots of the two OD(16, 8^8)s are given in Figs. 1 and 2, respectively. In Fig. 1, four bivariate projections of the design points have the pattern that the points lie on the two diagonals of the square region. No such pattern is apparent in Fig. 2.

To construct orthogonal designs using the construction in (3), we need several orthogonal Latin hypercubes. Orthogonal Latin hypercubes are very difficult to find, and only a handful of them are available for small run sizes. However, this is not a problem for using the construction in (3). Given an orthogonal Latin hypercube, we can obtain a large collection of orthogonal Latin hypercubes by row-permutation, column-permutation, sign-switching columns, or a combination of these operations. To use (3), one can consider different orthogonal Latin hypercubes given by permuting the rows of this given orthogonal Latin hypercube. One could also consider column-permutation and sign-switching columns as well as row-permutation. However, it should be

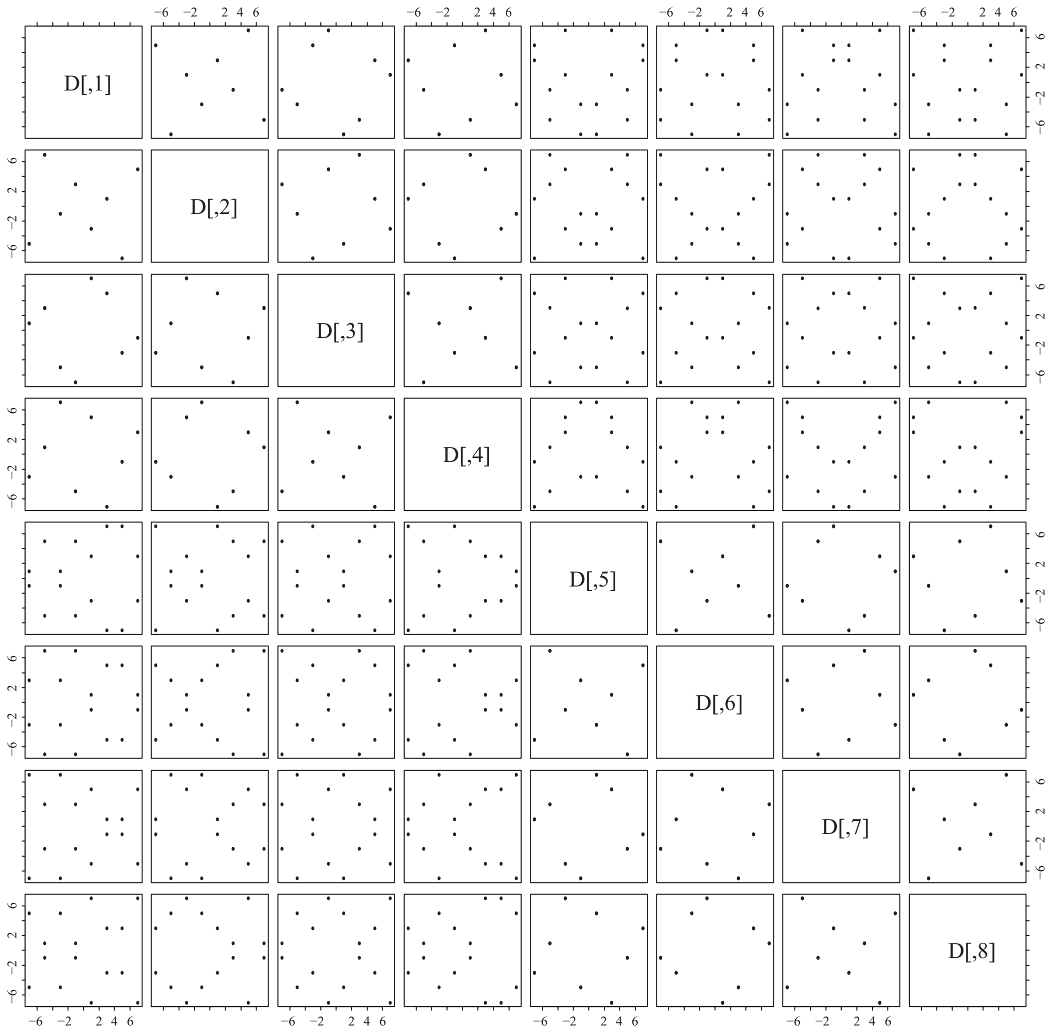

Fig. 2. The OD$(16, 8^8)$ constructed by the generalization in (3).

mentioned that column-permutation and sign-switching columns alone do not help to eliminate the diagonal pattern in the bivariate projections.

Regarding higher-order orthogonality, we can easily prove a generalization of part (ii) of Proposition 3.

PROPOSITION 5. *Let* $D_1, \ldots, D_{m_1}$ *be orthogonal. Then* D *in* (3) *is* 3-*orthogonal if* A *is an orthogonal array of strength three.*

A result analogous to part (i) of Proposition 3 is also true, which states that D in (3) is 3-orthogonal if A is orthogonal and $(D_1, \ldots, D_{m_1})$ is 3-orthogonal, but this result is hardly useful because it will give a design with far fewer columns. Simply requiring each of $D_1, \ldots, D_{m_1}$ be 3-orthogonal is not sufficient for D to be 3-orthogonal if A is only orthogonal.

3·2. *Generalization for better correlation properties*

Let $A = (a_{ij})$ be an $n_1 \times m_1$ matrix with $a_{ij} = \pm 1$ as before. For each $p = 1, \ldots, n_1$, let D_p be a $\mathrm{D}(n_2, s^{m_2})$. Now consider design D given by

$$D = (a_{ij} D_i) = \begin{pmatrix} a_{11} D_1 & a_{12} D_1 & \cdots & a_{1m_1} D_1 \\ a_{21} D_2 & a_{22} D_2 & \cdots & a_{2m_1} D_2 \\ \vdots & \vdots & & \vdots \\ a_{n_1 1} D_{n_1} & a_{n_1 2} D_{n_1} & \cdots & a_{n_1 m_1} D_{n_1} \end{pmatrix}. \tag{4}$$

For this design D in (4), we have the following results.

PROPOSITION 6. *Let A be orthogonal. Then we have that*

(i) $\rho_M(D) \leqslant \{\rho_M(D_1) + \cdots + \rho_M(D_{n_1})\}/n_1$,
(ii) $\rho^2(D) \leqslant w_2\{\rho^2(D_1) + \cdots + \rho^2(D_{n_1})\}/n_1$, *where* $w_2 = (m_2 - 1)/(m_1 m_2 - 1)$,
(iii) *D is orthogonal if $D_1, \ldots, D_{n_1}$ are all orthogonal,*
(iv) *D is 3-orthogonal if $D_1, \ldots, D_{n_1}$ are all 3-orthogonal.*

Using Lemma 1, the proofs of all the previous results in Propositions 1–5 are relatively straightforward. In contrast, Lemma 1 does not help prove Proposition 6, of which we give a full proof.

Proof. Let $b_j(p)$ be the jth column of design D_p. Then a column of design D in (4) has a form

$$d(i, j) = [a_{1i}\{b_j(1)\}^{\mathrm{T}}, \ldots, a_{n_1 i}\{b_j(n_1)\}^{\mathrm{T}}]^{\mathrm{T}}.$$

For two columns $d(i_1, j_1)$ and $d(i_2, j_2)$ of D, we have

$$J\{d(i_1, j_1), d(i_2, j_2)\} = \sum_{p=1}^{n_1} a_{pi_1} a_{pi_2} J\{b_{j_1}(p), b_{j_2}(p)\}. \tag{5}$$

Dividing both sides of equation (5) by

$$J\{d(i, j), d(i, j)\} = \sum_{p=1}^{n_1} a_{pi} a_{pi} J\{b_j(p), b_j(p)\} = n_1 J\{b_j(1), b_j(1)\},$$

we obtain

$$\rho\{d(i_1, j_1), d(i_2, j_2)\} = \frac{1}{n_1} \sum_{p=1}^{n_1} a_{pi_1} a_{pi_2} \rho\{b_{j_1}(p), b_{j_2}(p)\}. \tag{6}$$

If $d(i_1, j_1)$ and $d(i_2, j_2)$ are two distinct columns of D, then $(i_1 j_1) \neq (i_2, j_2)$. For the case $i_1 \neq i_2$ but $j_1 = j_2$, we have $\rho\{d(i_1, j_1), d(i_2, j_2)\} = 0$, as A is orthogonal. For the case $j_1 \neq j_2$, from (6) we obtain

$$|\rho\{d(i_1, j_1), d(i_2, j_2)\}| \leqslant \frac{1}{n_1} \sum_{p=1}^{n_1} |\rho\{b_{j_1}(p), b_{j_2}(p)\}| \leqslant \frac{1}{n_1} \sum_{p=1}^{n_1} \rho_M(D_p).$$

This gives

$$\rho_M(D) \leqslant \frac{1}{n_1} \sum_{p=1}^{n_1} \rho_M(D_p),$$

proving part (i) of Proposition 6. Part (iii) follows from part (i). Similarly to (5), for three columns $d(i_1, j_1)$, $d(i_2, j_2)$ and $d(i_3, j_3)$ of D, we have

$$J\{d(i_1, j_1), d(i_2, j_2), d(i_3, j_3)\} = \sum_{p=1}^{n_1} a_{pi_1} a_{pi_2} a_{pi_3} J\{b_{j_1}(p), b_{j_2}(p), b_{j_3}(p)\}$$

from which part (iv) is immediate. We now turn our attention to part (ii). Let $\alpha = \sum_{i_1=1}^{m_1} \sum_{i_2=1}^{m_1} \sum_{j_1=1}^{m_2} \sum_{j_2=1}^{m_2} [\rho\{d(i_1, j_1), d(i_2, j_2)\}]^2$. Then we have

$$\alpha = m_1 m_2 + (m_1 m_2)(m_1 m_2 - 1)\rho^2(D). \tag{7}$$

From (6), we further have

$$\alpha = \frac{1}{n_1} \sum_{i_1=1}^{m_1} \sum_{i_2=1}^{m_1} \sum_{j_1=1}^{m_2} \sum_{j_2=1}^{m_2} \left[\sum_{p=1}^{n_1} \frac{a_{pi_1} a_{pi_2}}{n_1^{1/2}} \rho\{b_{j_1}(p), b_{j_2}(p)\} \right]^2. \tag{8}$$

For fixed i_1 and fixed $j_1 \neq j_2$, consider

$$\beta = \sum_{i_2=1}^{m_1} \left[\sum_{p=1}^{n_1} \frac{a_{pi_1} a_{pi_2}}{n_1^{1/2}} \rho\{b_{j_1}(p), b_{j_2}(p)\} \right]^2.$$

Let

$$x = \begin{bmatrix} \rho\{b_{j_1}(1), b_{j_2}(1)\} \\ \rho\{b_{j_1}(2), b_{j_2}(2)\} \\ \vdots \\ \rho\{b_{j_1}(n_1), b_{j_2}(n_1)\} \end{bmatrix}, \qquad Q = \frac{1}{n_1^{1/2}} \begin{pmatrix} a_{1i_1}a_{11} & a_{1i_1}a_{12} & \cdots & a_{1i_1}a_{1m_1} \\ a_{2i_1}a_{21} & a_{2i_1}a_{22} & \cdots & a_{2i_1}a_{2m_1} \\ \vdots & \vdots & & \vdots \\ a_{n_1i_1}a_{n_11} & a_{n_1i_1}a_{n_12} & \cdots & a_{n_1i_1}a_{n_1m_1} \end{pmatrix}.$$

Then we have $\beta = \|Q^{\mathrm{T}}x\|^2$. As the columns of Q are orthogonal vectors of length unity, we must have

$$\beta = \|Q^{\mathrm{T}}x\|^2 \leqslant \|x\|^2 = \sum_{p=1}^{n_1} [\rho\{b_{j_1}(p), b_{j_2}(p)\}]^2. \tag{9}$$

Substituting (9) into (8), we obtain $\alpha \leqslant m_1 m_2 + m_1 n_1^{-1} \sum_{p=1}^{n_1} \sum_{j_1 \neq j_2} [\rho\{b_{j_1}(p), b_{j_2}(p)\}]^2$, which simplifies to

$$\alpha \leqslant m_1 m_2 + \frac{m_1}{n_1} m_2(m_2 - 1) \sum_{p=1}^{n_1} \rho^2(D_p). \tag{10}$$

Combining (7) and (10), we obtain part (ii). □

When orthogonal Latin hypercubes are not available, the construction method in (4) provides ample opportunities to obtain designs with correlations smaller than those from the basic construction method in (1). From the proof of Proposition 6, we see that, if $m_1 = n_1$ in which case A is a Hadamard matrix, then the equality holds in part (ii). When $m_1 < n_1$, the strict inequality holds in part (ii) unless x in (9) is in the column space of Q. Now let us look at part (i). Also from the proof, in order for the equality to be true in part (i), there must exist i_1, i_2 and $j_1 \neq j_2$ such that $\rho_M(D_p) = |\rho\{b_{j_1}(p), b_{j_2}(p)\}|$ for all p and all $a_{pi_1} a_{pi_2} \rho\{b_{j_1}(p), b_{j_2}(p)\}$ for $p = 1, \ldots, n_1$ have the same sign. In all other cases, the strict inequality in part (i) is true. An example illustrates the usefulness of this construction method.

Example 7. Consider the four D$(6, 6^3)$s given below.

$$
\begin{array}{rrr}
\multicolumn{3}{c}{D_1} \\
-5 & 3 & -5 \\
-3 & -3 & 3 \\
-1 & 1 & 5 \\
1 & -5 & -3 \\
3 & 5 & 1 \\
5 & -1 & -1
\end{array}
\qquad
\begin{array}{rrr}
\multicolumn{3}{c}{D_2} \\
3 & -5 & -5 \\
-3 & 3 & -3 \\
1 & 5 & -1 \\
-5 & -3 & 1 \\
5 & 1 & 3 \\
-1 & -1 & 5
\end{array}
\qquad
\begin{array}{rrr}
\multicolumn{3}{c}{D_3} \\
-5 & -5 & 3 \\
3 & -3 & -3 \\
5 & -1 & 1 \\
-3 & 1 & -5 \\
1 & 3 & 5 \\
-1 & 5 & -1
\end{array}
\qquad
\begin{array}{rrr}
\multicolumn{3}{c}{D_4} \\
5 & 3 & -5 \\
3 & -3 & 3 \\
1 & 1 & 5 \\
-1 & -5 & -3 \\
-3 & 5 & 1 \\
-5 & -1 & -1
\end{array}
$$

Designs D_2 and D_3 are column permutations of design D_1. Design D_4 is obtained from D_1 by sign-switching the first column. The four designs have the same $\rho_M = 0{\cdot}086$ and $\rho^2 = 0{\cdot}003$. Let

$$A = \begin{pmatrix} 1 & -1 & -1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \\ 1 & 1 & 1 \end{pmatrix}.$$

Consider the two D$(24, 6^9)$s, D^* and D^{**}, where D^* is given by the construction in (4) and D^{**} is obtained from the construction in (1) by taking $D_0 = D_1$. For design D^*, we have $\rho_M(D^*) = 0{\cdot}057$ and $\rho^2(D^*) = 0{\cdot}00054$. For design D^{**}, we have $\rho_M(D^{**}) = 0{\cdot}086$ and $\rho^2(D^{**}) = 0{\cdot}00075$. Design D^* improves upon design D^{**} in terms of both measures of non-orthogonality.

In applying the construction in (4), we need several Latin hypercubes. Given a Latin hypercube, we can obtain a large collection of Latin hypercubes by row-permutation, column-permutation, sign-switching columns or a combination of these operations. To use (4), one can consider different Latin hypercubes given by a combination of permutation and sign-switching the columns of a given Latin hypercube, as illustrated in Example 7. Row-permutation does not help here as permuting the rows of one or more D_ps in (4) gives essentially the same design.

The construction in (4) can also be used to obtain designs with better projection properties. Although it cannot eliminate the diagonal pattern, it can improve other two-dimensional projections. Example 7 provides an illustration. Some two-dimensional projections of design D^{**} given in (1) have only six distinct points while all two-dimensional projections of design D^* given in (4) have at least twelve distinct points.

4. Repeated runs

Repeated trials in computer experiments are often viewed as undesirable. This is because the computer simulator is often deterministic, and, therefore, running the code at the same input setting gives the same output. However, if one considers how the design is likely to be used, the implications are not so severe.

If the goal of the computer experiment is numerical integration (Owen, 1997), the design points represent strata from which the settings of the factors are randomly selected, rather than points where trials are performed. Therefore, a design with repeated trials has two or more points from the same strata and the probability of a repeated run is zero. On the other hand, if the goal is response surface estimation, the data analysis is likely to be carried out using a Gaussian spatial process (Sacks et al., 1989). Again, if one views the design points as strata, instead of the collection of points where trials are to be performed, then repeated runs are avoided and one obtains good space-filling properties from the design as well as some localized information where there are repeated trials. This can be important for fitting the spatial model and, in particular, estimating the correlation parameters (Handcock, 1991). Having some trials from the same strata can help detect high-frequency changes in the response surface.

Nevertheless, some experimenters would prefer to use the available resources to fill the design region, and avoid repeated runs. This section provides an investigation of this issue. We obtain some results about when repeated runs can occur and how they can be eliminated, if desired. We first present a lemma that will be useful for constructing designs without repeated runs. A design $C = (c_{ij})_{n\times m}$ is said to have mirror-image runs if there exist $k \neq l$ such that $(c_{k1}, \ldots, c_{km}) = -(c_{l1}, \ldots, c_{lm})$.

LEMMA 2. (i) *If $A = (a_{ij})_{n\times m}$ is orthogonal such that $m \geqslant n/2 + 1$, then A has no repeated run nor mirror-image runs.*

(ii) *If A is an* OA$(n, 2^m, 3)$ *with $m \geqslant n/4 + 2$, then A has no repeated run.*

Proof. (i) From the well-known fact that $\mathrm{tr}(AA^{\mathrm{T}}AA^{\mathrm{T}}) = \mathrm{tr}(A^{\mathrm{T}}AA^{\mathrm{T}}A)$, we obtain

$$2 \sum_{1\leqslant i<j\leqslant n} r_{ij}^2 + nm^2 = mn^2, \tag{11}$$

where r_{ij} denotes the inner product of runs i and j. Suppose that A has repeated runs. Without loss of generality, let the first two runs be identical, that is, $(a_{11}, \ldots, a_{1m}) = (a_{21}, \ldots, a_{2m})$. We can also assume that both equal $(1, \ldots, 1)$, for otherwise we use $(a_{1j}a_{ij})_{n\times m}$, also an orthogonal matrix. Now consider the matrix A' obtained from A by deleting the first two runs. Since the columns of A are orthogonal, the inner product of any two columns of A' must be -2. For A', we obtain

$$2 \sum_{3\leqslant i<j\leqslant n} r_{ij}^2 + (n-2)m^2 = m(n-2)^2 + (-2)^2 m(m-1). \tag{12}$$

Since $\sum_{1\leqslant i<j\leqslant n} r_{ij}^2 - \sum_{3\leqslant i<j\leqslant n} r_{ij}^2 \geqslant r_{12}^2 = m^2$, from (11) and (12) we have

$$mn^2 - nm^2 + (n-2)m^2 - m(n-2)^2 - 4m(m-1) \geqslant 2m^2,$$

which simplifies to $m \leqslant n/2$, contradicting that $m \geqslant n/2 + 1$. If A has mirror-image runs, the above argument also goes through. The matrix A' obtained by deleting the first two runs still has the property that the inner product of any two columns is equal to -2 with the only difference being that the first two runs are now supposed to be $(1, \ldots, 1)$ and $(-1, \ldots, -1)$.

(ii) Let A be an OA$(n, 2^m, 3)$ with $m \geqslant n/4 + 2$. Suppose that the first two runs are identical and that both equal $(1, \ldots, 1)$. Taking the half fraction of A by selecting the rows with their entries in the first column equal to 1 and then deleting the first column, we obtain an OA$(n/2, m-1, 2)$ with repeated runs. From Lemma 2(i), we must have $(m-1) \leqslant n/4$, a contradiction. □

Lemma 3 of Butler (2003) is closely related to our Lemma 2(i). Lemma 2(i) does not follow from his result but his proof can be modified to prove our Lemma 2(i). We choose to present this alternative proof as it appears to us more intuitive.

We now look at the three constructions as given in (1), (3) and (4). In the following discussion, we assume that $n_1, n_2 \geqslant 2$. Results for the trivial cases $n_1 = 1$ or $n_2 = 1$ are obvious. The following result provides a complete characterization of repeated runs for the construction in (1).

LEMMA 3. *Consider the construction in* (1). *Then design D has repeated runs if and only if at least one of the following conditions is satisfied:* (i) *D_0 contains the centrepoint* $(0, \ldots, 0)$*,* (ii) *D_0 has repeated runs,* (iii) *A has repeated runs and* (iv) *both A and D_0 have mirror-image runs.*

Proof. It is straightforward to verify that, if one of the four conditions holds, design D has repeated runs. It remains to be shown that, if design D has repeated runs and none of the conditions (i), (ii) and (iii) holds, it is necessary that both A and D_0 have mirror-image runs. Let $A = (a_{ij})$ and $D_0 = (b_{pq})$. Since D has repeated runs, there exist i_1, i_2, p_1 and p_2, where $(i_1, p_1) \neq (i_2, p_2)$, such that

$$a_{i_1 j}(b_{p_1 1}, \ldots, b_{p_1 m_2}) = a_{i_2 j}(b_{p_2 1}, \ldots, b_{p_2 m_2})$$

for all $j = 1, \ldots, m_1$. Since none of the conditions (i), (ii) and (iii) is true, we must have $a_{i_1 j} = -a_{i_2 j}$ for all $j = 1, \ldots, m_1$ and $(b_{p_1 1}, \ldots, b_{p_1 m_2}) = -(b_{p_2 1}, \ldots, b_{p_2 m_2})$, showing that both A and D_0 have mirror-image runs. □

The following result is now immediate.

PROPOSITION 7. *Consider design D given by the construction in* (1). *Suppose that D_0 has no centrepoint nor repeated run. We have that*

(i) *if A is orthogonal with $m_1 \geqslant n_1/2 + 1$, then D has no repeated run, and*
(ii) *if A is an* $\text{OA}(n_1, 2^{m_1}, 3)$ *with $m_1 \geqslant n_1/4 + 2$, then D has no repeated run, provided that D_0 has no mirror-image run.*

If D_0 is a Latin hypercube with even run size, then it has no centrepoint nor a repeated run. According to Proposition 7, $D = A \otimes D_0$ has no repeated run for any A that is orthogonal with $m_1 \geqslant n_1/2 + 1$. The orthogonal Latin hypercube $\text{OD}(16, 16^{12})$ from Steinberg & Lin (2006) has no mirror-image run. If it is used as D_0, for $D = A \otimes D_0$ to have no repeated run one can also choose A to be an $\text{OA}(n_1, 2^{m_1}, 3)$ with $m_1 \geqslant n_1/4 + 2$, which results in a 3-orthogonal design. The orthogonal Latin hypercubes in Ye (1998) and some of the designs in Steinberg & Lin (2006) have mirror-image runs. If we use one of these orthogonal Latin hypercubes as D_0, design D is still without repeated runs as long as A is orthogonal with $m_1 \geqslant n_1/2 + 1$. In this case, choosing A to be an orthogonal array of strength three may result in repeated runs in D. However, there is no loss in our ability to construct 3-orthogonal designs, as these designs with mirror-image runs are already 3-orthogonal, implying that $D = A \otimes D_0$ is also 3-orthogonal as long as A is orthogonal.

Next we consider repeated runs for the two generalizations of our basic construction. For each generalization, a complete characterization of repeated runs similar to that in Lemma 3 can be obtained but is less attractive as the corresponding results become more complicated. In the interest of space, we choose to present directly the counterparts of Proposition 7 for the two generalizations, sacrificing mathematical generality for user-friendliness.

PROPOSITION 8. *Consider design D given by the construction in* (3). *For each $j = 1, \ldots, m_1$, let D_j have no centrepoint nor a repeated run. We have that*

(i) *if A is orthogonal with $m_1 \geqslant n_1/2 + 1$, then D has no repeated run; and*
(ii) *if A is an* $\text{OA}(n_1, 2^{m_1}, 3)$ *with $m_1 \geqslant n_1/4 + 2$, then D has no repeated run, provided that at least one D_j has no mirror-image run.*

PROPOSITION 9. *Consider the construction in* (4). *Suppose that none of the D_ps has repeated runs and at most one of the D_ps has a centrepoint. We have that*

(i) *if A is orthogonal with $m_1 \geqslant n_1/2 + 1$, then D has no repeated run; and*
(ii) *if A is an* OA$(n_1, 2^{m_1}, 3)$ *with $m_1 \geqslant n_1/4 + 2$, then D has no repeated run, provided that there do not exist D_{p_1} and D_{p_2} with $p_1 \neq p_2$ such that D_{p_1} has a run that is the mirror-image of a run in D_{p_2}.*

5. DISCUSSION

The construction methods in this paper use small two-level orthogonal or nearly orthogonal arrays together with small orthogonal or nearly orthogonal Latin hypercube designs to construct a large class of bigger designs that retain the orthogonality properties of the small designs and many of their other desirable properties. This allows one to exploit existing tables of small designs, and methods and algorithms for the construction of small designs. Examples for Latin hypercube designs already mentioned include construction methods for orthogonal Latin hypercubes in Ye (1998) and Steinberg & Lin (2006), and algorithms for obtaining nearly orthogonal Latin hypercubes in Owen (1994) and Tang (1998). There is also a rich literature on minimal and efficient nearly orthogonal two-level designs. Margolin (1969) points out the connection between such designs and non-orthogonal, chemical-balance, weighing designs; see Hotelling (1944), Kishen (1945), Mood (1946), Raghavarao (1959) and Yang (1966, 1968), for example.

Even without these specific methods and algorithms, because only small designs are needed, one can quite easily obtain very good nearly orthogonal two-level designs and Latin hypercubes via more general robust optimization routines, such as simulated annealing and genetic algorithms, merely by using ρ^2 or ρ_M^2 as an objective function.

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