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A CONSTRUCTION METHOD FOR ORTHOGONAL LATIN HYPERCUBE DESIGNS WITH PRIME POWER LEVELS

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Abstract: Latin hypercube design (LHD) is popularly used in designing computer experiments. This paper explores how to construct LHDs with p^d ($d = 2^c$) runs and up to $(p^d-1)/(p-1)$ factors in which all main effects are orthogonal. This is accomplished by rotating groups of factors in a p^d-run regular saturated factorial design. These rotated factorial designs are easy to construct and preserve many attractive properties of standard factorial designs. The proposed method covers the one by Steinberg and Lin (2006) as a special case and is able to generate more orthogonal LHDs with attractive properties. Theoretical properties as well as the construction algorithm are discussed, with an example for illustration.

Key words and phrases: Computer experiment, factorial design, galois field, rotation.

1. Introduction

Many physical phenomena encountered in science and engineering can be modeled by a set of complicated equations. These equations often have only numerical solutions that are carried out by computer programs. These so-called computer models are used by scientists and engineers to understand complicated physical phenomena. Latin hypercube design (LHD) is popularly used in designing computer experiments. In this paper, we are particularly interested in orthogonal LHDs.

LHDs were introduced by McKay, Beckman and Conover (1979) for computer experiments. An $n \times m$ LHD for m factors in n runs is usually specified by an $n \times m$ matrix $D = (d_{ij})$, where d_{ij} is the level of factor j on the ith experimental run, and each column in D includes n uniformly spaced levels. Box and Draper (1959) showed that when the true model is a polynomial (of unknown degree), the property of equally-spaced points over the design region is desirable. Thus, equally-spaced projections are of value. However, the original construction of LHDs by mating factors randomly is susceptible to potentially high correlations between factors.

Efforts have been made to optimize LHDs. Thus Owen (1992) and Tang (1993) proposed orthogonal array-based LHDs whose r-dimensional projections are all stratified. Owen (1994) attempted to minimize pairwise correlations between input factors. Tang (1998) extended this approach by considering correlations among higher-order terms derived from the factors. Ye (1998) presented a construction method for orthogonal column LHDs in which all the input factors have zero correlation. Butler (2001) showed how to construct LHDs in which the terms of a class of trigonometric regression models are orthogonal to one another. Beattie and Lin (1998, 2004, 2005) showed that certain LHDs can be constructed by rotating the points in a p-level full factorial design. Bursztyn and Steinberg (2002) applied the rotation to groups of factors to increase the number of factors in the resulting design. Recently, Joseph and Hung (2008) proposed a multi-objective optimization approach to find good LHDs by combining correlation and distance performance measures, while Steinberg and Lin (2006) proposed a method to construct 2^d-level orthogonal LHDs by means of rotating factors in groups, this method can generate more orthogonal factor columns than those proposed by Ye (1998). However, the primary limitation of their method is the constraint that the sample size is $n = 2^d$, where d is a power of 2, $d = 2^c$. In this paper we construct orthogonal LHDs with p^d runs and up to $(p^d-1)/(p-1)$ factors that can be used in a comparatively general way.

This paper is organized as follows. Section 2 discusses some related work on rotating designs. A general approach for constructing orthogonal LHDs by rotating groups of factors in a p^d-run regular saturated factorial design is proposed in Section 3, along with a discussion of properties of the resulting designs and an illustrative example. Section 4 provides some concluding remarks.

2. Related Work on Rotation Designs

Beattie and Lin (1998, 2004, 2005) showed that a class of LHDs can be constructed by rotating the points in p-level, d-factor standard full factorial designs, where d is a power of 2.

Let D be a $p^d \times d$ full factorial design with levels $i-(p+1)/2$ for $i = 1, \ldots, p$. A $d \times d$ matrix R acts as a rotation matrix if $R'R = I_d$, where I_d is a $d \times d$ identity matrix. Then $X = DR$ is an orthogonal LHD matrix.

The rotation matrices can be defined by the following recursive scheme. Let

$$V_1 = \begin{pmatrix} p & -1 \\ 1 & p \end{pmatrix}, \tag{2.1}$$

$$V_c = \begin{pmatrix} p^{2^{c-1}} V_{c-1} & -V_{c-1} \\ V_{c-1} & p^{2^{c-1}} V_{c-1} \end{pmatrix}, \tag{2.2}$$

and then the rotation matrix can be rescaled to

$$R_c = a_c V_c, \tag{2.3}$$

with $a_c = \{\prod_{k=1}^{c}(1+p^{2^k})\}^{-1/2}$. Note that expressions (2.1)–(2.2) have slightly different representations from those of Beattie and Lin (1998, 2004, 2005).

The orthogonal LHD proposed above has many attractive properties. It possesses the orthogonality of factorial designs, i.e., the correlation of each pair of columns in the design is zero, and admits unique and equally-spaced projections to univariate dimensions while maintaining a high spatial dispersion according to minimum inter-site distance.

Bursztyn and Steinberg (2002) proposed the idea of independently rotating groups of factors in two-level designs. Let D be a 2^{m-l} factorial design and let R be a $t \times t$ rotation matrix. Suppose we can decompose the m factors in D into b sets of t factors each, with $m - bt$ factors left over. Let $D_1, \ldots, D_b$ be the design matrices obtained from projecting D onto each of the b sets of t factors. Let the rotation matrix R_b be a $bt \times bt$ block diagonal matrix with b copies of R on the diagonal. The rotation design is then $D_R = (D_1 \vdots \cdots \vdots D_b)R_b = (D_1R \vdots \cdots \vdots D_bR)$. Recently, Steinberg and Lin (2006) combined the above two ideas with the theory of Galois field to produce an orthogonal LHD matrix with n runs, where $n = 2^d$ and $d = 2^c$. The number of possible factors in their design can be as large as n.

3. General Construction Method

In this section, we propose a new class of orthogonal LHDs with p^d runs and $(p^d-1)/(p-1)$ factors, where $p \geq 3$ is a prime and d is a power of 2. Let D be a p-level, $(p^d-1)/(p-1)$-factor, p^d-run regular saturated factorial design. The levels for each factor in D are taken to be $0, \ldots, p-1$. Let $d = 2^c$ and $b = (p^d-1)/(d(p-1))$. We divide the matrix D into b groups of d factors each, $D_1, \ldots, D_b$, and rotate each group with rotation matrix R_c defined by expressions (2.1)–(2.3). An illustrative example is given below to carry out the basic idea.

Example 1.($p = 3, d = 2, b = 2$) Start with a 3^{4-2} regular factorial design D with levels 0, 1, 2:

$$\begin{pmatrix} \mathbf{1} & 0 & 0 & 0 & 1 & 1 & 1 & 2 & 2 & 2 \\ \mathbf{2} & 0 & 1 & 2 & 0 & 1 & 2 & 0 & 1 & 2 \\ \mathbf{12^2} & 0 & 2 & 1 & 1 & 0 & 2 & 2 & 1 & 0 \\ \mathbf{1^2 2^2} & 0 & 2 & 1 & 2 & 1 & 0 & 1 & 0 & 2 \end{pmatrix}'.$$

Now, columns $\mathbf{1}$ and $\mathbf{2}$ form a full factorial design, and columns $\mathbf{12^2}$ and $\mathbf{1^2 2^2}$ form another one. Centralize $(D_1 \vdots D_2) = (\mathbf{1}\ \mathbf{2} \vdots \mathbf{12^2}\ \mathbf{1^22^2})$ and rotate each D_i by R_1, where

$$R_1 = a_1 V_1 = \frac{1}{\sqrt{10}} \begin{pmatrix} 3 & -1 \\ 1 & 3 \end{pmatrix},$$

to get a 9-point rotated factorial design:

$$\frac{1}{\sqrt{10}}\begin{pmatrix} -4 & -3 & -2 & -1 & 0 & 1 & 2 & 3 & 4 \\ -2 & 1 & 4 & -3 & 0 & 3 & -4 & -1 & 2 \\ -4 & 4 & 0 & 1 & -3 & 2 & 3 & -1 & -2 \\ -2 & 2 & 0 & 3 & 1 & -4 & -1 & -3 & 4 \end{pmatrix}'.$$

This design is a 9-point orthogonal LHD and can be scaled into the proper experimental region.

Beattie and Lin (2005) showed that the subdesign D_iR_c is an orthogonal LHD if D_i is a full factorial design, for all $i = 1, \ldots, b$. We next discuss how to divide the matrix D into b groups of full factorial designs, $D_1, \ldots, D_b$.

Consider $GF(p)[x] = \{a_0+a_1x+\cdots+a_{d-1}x^{d-1}, a_i \in GF(p)\}$, where $GF(p) = \{0, \ldots, (p-1)\}$. It is well known that there is a primitive polynomial f of degree d over $GF(p)$ such that the powers of x, modulo f, cycle through all $p^d - 1$ nonzero elements of $GF(p)[x]$. Each of the elements of $GF(p)[x]$ can be associated with a column of a regular $p^{bd-(b-1)d}$ factorial design in the following way. As in Example 1 above, we have $GF(3)[x] = \{a_0 + a_1x, a_0, a_1 \in GF(3)\}$ with $GF(3) = \{0, 1, 2\}$, the primitive polynomial is $f(x) = x^2 + x + 2$ and x^0, x^1, x^2, x^3, modulo $f(x)$, are 1, x, $1 + 2x$, $2 + 2x$ which correspond to columns $\mathbf{1}$, $\mathbf{2}$, $\mathbf{12}^2$, $\mathbf{1}^2\mathbf{2}^2$ of the 3^{4-2} factorial design, respectively. In general, element $a_0 + a_1x + \cdots + a_{d-1}x^{d-1}$ is associated with the generalized interaction column $\mathbf{1}^{a_0}\mathbf{2}^{a_1}\cdots \boldsymbol{d}^{a_{d-1}}$ of all factors i for which $a_{i-1} \neq 0$.

Since D has $(p^d - 1)/(p - 1) = bd$ columns, the first bd nonzero elements of $GF(p)[x]$ corresponding to the powers of x, modulo $f(x)$, are sufficient to divide D. The first d terms in the sequence, $x^0, x^1, \ldots, x^{d-1}$, correspond to the main-effect columns and clearly are a full p^d factorial design. The columns corresponding to any set of d successive terms in the sequence, $(x^{id}, x^{id+1}, \ldots, x^{id+d-1})$, for all $i = 1, \ldots, b-1$, will be a full factorial design if these terms are linearly independent. In fact, if equation $\sum_{j=0}^{d-1}\beta_j x^{id+j} = 0$ holds for a set of β_j which are not all equal to 0, then we have $\sum_{j=0}^{d-1}\beta_j x^j = 0$. This contradicts the fact that the first d columns in the ordering provide a full p^d factorial design. Thus, dividing the ordered columns into blocks of d leads to each such block D_i being a full p^d factorial design.

The above discussion ensures that the matrix D can be divided into b groups of full factorial designs and suggests how the division can be arranged. This is summarized in the following theorem.

Theorem 1. *The first bd nonzero elements of $GF(p)[x]$ corresponding to the powers of x, i.e., $x^0, x^1, \ldots, x^{bd-1}$, provide an ordering of the effect columns in* *matrix D. The sets consisting of d consecutive columns in the order are full factorial designs $D_1, \ldots, D_b$ in sequence.*

Remark 1. Note that any consecutive bd nonzero elements of $GF(p)[x]$ can be used to order the columns of matrix D, and hence the division is not unique.

Let $D^* = (D_1 \vdots \cdots \vdots D_b)$ and

$$R_b = \begin{pmatrix} R_c & & \\ & \ddots & \\ & & R_c \end{pmatrix}, \tag{3.1}$$

with b copies of R_c on the diagonal. Centralizing the levels in each column of D^* so that all level values spread as $i - (p+1)/2$ for $i = 1, \ldots, p$, denoting the resulting design by D^*_c and rotating it by R_b, the design matrix $D^*_c R_b$ can thus be obtained.

Lemma 1. (Beattie and Lin (2005)) *Let X be an orthogonal design matrix of n rows and d columns in which the sums of squares for columns are equal, and let R be a $d \times d$ rotation matrix satisfying $R' R = I_d$, where I_d is an identity matrix. Then the design XR is orthogonal.*

Lemma 2. *The matrix V_c in (2.2) is a rotation of the d-factor ($d = 2^c$), p-level standard full factorial design which yields unique and equally-spaced projections to each dimension.*

Lemma 2 can be proved in similar fashion to the proof of Theorem 3 in Beattie and Lin (2005), even though the matrix V_c in (2.2) has a different form. It can be easily seen that the matrix D^*_c obtained above is an orthogonal design matrix as the X in Lemma 1. Then based on Lemmas 1 and 2, the following theorem can be established.

Theorem 2. *The design $D^*_c R_b$ is an orthogonal LHD with unique and equally-spaced projections to univariate dimensions, and has uncorrelated regression estimates of main effects.*

We next present a construction algorithm for orthogonal LHDs.

Step 1. Give a design matrix D with p^d runs and $(p^d - 1)/(p-1)$ p-level factors, where $p \geq 3$ is a prime, d is a power of 2, and the p levels are $0, \ldots, p-1$. Let $b = (p^d - 1)/(d(p-1))$.

Step 2. Find a primitive polynomial $f(x)$ corresponding to the Galois field $GF(p)[x]$; obtain an ordering of the bd effect columns in D by associating them with the first bd nonzero elements of $GF(p)[x]$ corresponding

Table 1. Orthogonal LHDs obtainable from the proposed method ($n < 1,000$ and $p \geq 3$).

p	d	n	m
3	2	9	4
3	4	81	40
5	2	25	6
5	4	625	156
7	2	49	8
11	2	121	12
13	2	169	14
17	2	289	18
19	2	361	20
23	2	529	24
29	2	841	30
31	2	961	32

to the powers of x modulo $f(x)$; divide the ordered bd columns in D into b blocks, $D_1, \ldots, D_b$, to form the matrix $D^* = (D_1 \vdots \cdots \vdots D_b)$.

Step 3. Obtain D_c^* by centralizing the levels of D^* and R_b using (2.1)–(3.1) to get $D_c^* R_b$ as an orthogonal LHD.

Step 4. Scale the orthogonal LHD $D_c^* R_b$ to fit the desired experimental region.

Remark 2. Obviously, the method of Steinberg and Lin (2006) is the special case of our construction method at $p = 2$. In this case, however, the number of subgroups, b, should be $\lfloor (p^d - 1)/(d(p-1)) \rfloor$, where $\lfloor x \rfloor$ is the integer part of x.

Table 1 lists all possible orthogonal LHDs that can be constructed by our method for $n < 1,000$ and $p \geq 3$. These *orthogonal* LHDs are apparently new except for the case of $n = 9$, which can be obtained by Ye's (1998) method.

4. Concluding Remarks

In this paper, we propose a general construction method for orthogonal LHDs. The construction method here includes the one proposed by Steinberg and Lin (2006) as a special case, and leads to a much larger class of orthogonal LHDs than was previously known. The resulting LHDs have many attractive properties, for example, zero correlation between pairwise factors, unique and equally-spaced projections to univariate dimensions, and uncorrelated regression estimates of main effects. The primary limitation to our method is the sample size constraint; it requires the sample size to be $n = p^d$, where p is a prime and d is a power of 2.

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