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Miscellanea

Construction of orthogonal Latin hypercube designs

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SUMMARY

Latin hypercube designs have found wide application. Such designs guarantee uniform samples for the marginal distribution of each input variable. We propose a method for constructing orthogonal Latin hypercube designs in which all the linear terms are orthogonal not only to each other, but also to the quadratic terms. This construction method is convenient and flexible, and the resulting designs can accommodate many more factors than can existing ones.

Some key words: Computer experiment; Factorial design; Orthogonality; Second-order model.

1. INTRODUCTION

Many physical phenomena encountered in science and engineering are governed by a set of equations that can only be solved by a computer. Because such models are mostly deterministic, computer experiments require special designs, such as Latin hypercube designs, which possess equally spaced levels. Orthogonality is an important criterion in choosing Latin hypercube designs. Ye (1998) presented a method for constructing orthogonal Latin hypercube designs in which all the input factors have zero correlation. On the basis of Ye's procedure, Cioppa & Lucas (2007) augmented the number of factors for some cases. Beattie & Lin (2004) presented a class of orthogonal Latin hypercube designs developed from the rotation of q-level full factorial designs. Recently, Steinberg & Lin (2006) and Pang et al. (2009) proposed methods to construct orthogonal Latin hypercube designs by means of rotating factorial designs, while Bingham et al. (2009) and Lin et al. (2009) constructed many orthogonal or nearly orthogonal Latin hypercube designs.

Orthogonal Latin hypercube designs ensure independence of estimates of linear effects when a first-order model is fitted. However, a second-order model is needed when second-order effects are present. For such cases, a Latin hypercube design must satisfy the following properties: (a) each column is orthogonal to the others in the design; (b) the elementwise square of each column and the elementwise product of every two columns are orthogonal to all columns in the design. The Latin hypercube designs constructed by Ye (1998) possess these properties, but can accommodate only a few factors. In this paper, we propose a method for constructing Latin hypercube designs with properties (a) and (b) that can accommodate many more factors than existing ones.

2. THE CONSTRUCTION METHOD

2·1. *Orthogonal Latin hypercube designs with $2^{c+1}+1$ runs and 2^c factors*

We denote a Latin hypercube design with n runs, rows, and k factors, columns, by $L(n, k)$. For any integer $c \geqslant 1$, the construction algorithm for an orthogonal $L(2^{c+1}+1, 2^c)$ can be illustrated as follows.

Step 1. For $c = 1$, let

$$S_1 = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \qquad T_1 = \begin{pmatrix} 1 & 2 \\ 2 & -1 \end{pmatrix}. \tag{1}$$

Step 2. For $c > 1$, define S_c and T_c as

$$S_c = \begin{pmatrix} S_{c-1} & -S^*_{c-1} \\ S_{c-1} & S^*_{c-1} \end{pmatrix}, \quad T_c = \begin{pmatrix} T_{c-1} & -(T^*_{c-1} + 2^{c-1}S^*_{c-1}) \\ T_{c-1} + 2^{c-1}S_{c-1} & T^*_{c-1} \end{pmatrix}, \tag{2}$$

where the * operator works on any matrix with an even number of rows by multiplying the entries in the top half of the matrix by -1 and leaving those in the bottom half unchanged.

Step 3. An $L(2^{c+1}+1, 2^c)$ can be obtained as

$$L_c = \left(T_c^{\mathrm{T}},\ 0_{2^c},\ -T_c^{\mathrm{T}}\right)^{\mathrm{T}}, \tag{3}$$

where A^{T} denotes the transpose of A and 0_{2^c} denotes the $2^c \times 1$ column vector with all elements zero.

Some theoretical properties of the proposed design can be stated as the following theorem. The proof is given in the Appendix.

THEOREM 1. (i) *The T_c in* (2) *consists of rows and columns of permutations of the 2^c elements $1, \ldots, 2^c$, up to sign changes.*

(ii) *The L_c in* (3) *is a Latin hypercube design $L(2^{c+1}+1, 2^c)$ with properties* (a) *and* (b).

2·2. *Orthogonal $L(n, k)$s with $n = 2^{c+1}$ runs and $k = 2^c$ factors*

The construction method described in the previous subsection can be modified to produce $L(2^{c+1}, 2^c)$s with properties (a) and (b). The construction algorithm is as follows.

Step 1′. As equation (1) for construction of S_1 and T_1.

Step 2′. As equation (2) for construction of S_c and T_c.

Step 3′. Let $H_c = T_c - S_c/2$, $L_c = (H_c^{\mathrm{T}},\ -H_c^{\mathrm{T}})^{\mathrm{T}}$.

Then from a similar argument given in the proof of Theorem 1 in the Appendix, it can easily be shown that $H_c^{\mathrm{T}} H_c = h_c I_{2^c}$, where $h_c = 2^c(2^{2c+2} - 1)/12$. This leads to Theorem 2.

THEOREM 2. *The L_c obtained in Step 3′ is a Latin hypercube design $L(2^{c+1}, 2^c)$ with properties* (a) *and* (b).

3. COMPARISONS WITH EXISTING METHODS

Among the existing constructions for orthogonal Latin hypercube designs, only those proposed by Ye (1998) and Cioppa & Lucas (2007) can produce designs possessing both properties (a) and (b). For $n = 2^{c+1}$ or $2^{c+1}+1$ rows, Ye's (1998) method can construct a design with at most $k = 2c$ factors. The method of Cioppa & Lucas (2007) can generate a design with at most $k = \binom{c+1}{2} + 1$ factors, while the number of factors in the design constructed by our method is $k = 2^c$. Thus, our method allows a substantially larger number of factors than those of Ye (1998) and Cioppa & Lucas (2007), especially for large c. In fact, the number of factors k in the design constructed by our method attains its maximum value among all the corresponding Latin hypercube designs satisfying both properties (a) and (b). This conclusion is based on the following theorem, which can be straightforwardly obtained.

THEOREM 3. *If* $L(n, k) = (l_{ij})$ *is a centered Latin hypercube design with properties* (a) *and* (b), *then* $k \leqslant \lfloor n/2 \rfloor$, *where* $\lfloor x \rfloor$ *is the integer part of* x.

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APPENDIX

Proof of Theorem 1

To prove this theorem, we need the following lemma.

LEMMA 1. (i). *For any two square matrices A and B with the same even number of rows* $A^{*\mathrm{T}}B^* = A^{\mathrm{T}}B$. (ii). *For the* S_c *and* T_c *defined in* (2), *we have* $S_c^{\mathrm{T}}S_c = S_c^{*\mathrm{T}}S_c^* = 2^c I_{2^c}$, $S_c^{\mathrm{T}}T_c + T_c^{\mathrm{T}}S_c = (2^{2c} + 2^c)I_{2^c}$ *and* $S_c^{\mathrm{T}}T_c^* - T_c^{\mathrm{T}}S_c^* = 0$.

Proof of Lemma 1. Conclusion (i) as well as the first equation in (ii) are obvious. We give only the proof of the second equation $S_c^{\mathrm{T}}T_c + T_c^{\mathrm{T}}S_c = (2^{2c} + 2^c)I_{2^c}$ in (ii); the proof of the third equation in (ii) is similar.

It is easy to see that equation $S_c^{\mathrm{T}}T_c + T_c^{\mathrm{T}}S_c = (2^{2c} + 2^c)I_{2^c}$ holds for $c = 1$. Suppose it holds for a particular integer c and consider the next integer $c + 1$. From (2), Lemma 1 (i) and the first equation in Lemma 1 (ii), we get

$$S_{c+1}^{\mathrm{T}}T_{c+1} = \begin{pmatrix} 2S_c^{\mathrm{T}}T_c + 2^{2c}I_{2^c} & -2^c S_c^{\mathrm{T}}S_c^* \\ 2^c S_c^{*\mathrm{T}}S_c & 2S_c^{\mathrm{T}}T_c + 2^{2c}I_{2^c} \end{pmatrix}.$$

Then

$$S_{c+1}^{\mathrm{T}}T_{c+1} + T_{c+1}^{\mathrm{T}}S_{c+1} = \{2(2^{2c} + 2^c) + 2^{2c+1}\}I_{2^{c+1}} = (2^{2c+2} + 2^{c+1})I_{2^{c+1}},$$

and the result follows by induction. □

Proof of Theorem 1. (i) From the construction method, this assertion is obvious. (ii) First, we prove $T_c^{\mathrm{T}}T_c = t_c I_{2^c}$ by induction, where $t_c = 2^c(2^c + 1)(2^{c+1} + 1)/6$. It is easy to verify that $T_1^{\mathrm{T}}T_1 = 5I_2$. Suppose $T_c^{\mathrm{T}}T_c = t_c I_{2^c}$, then we must show $T_{c+1}^{\mathrm{T}}T_{c+1} = t_{c+1}I_{2^{c+1}}$. In fact, by the induction hypothesis and Lemma 1, we have

$$\begin{aligned} T_{c+1}^{\mathrm{T}}T_{c+1} &= \begin{pmatrix} T_c^{\mathrm{T}} & T_c^{\mathrm{T}} + 2^c S_c^{\mathrm{T}} \\ -\left(T_c^{*\mathrm{T}} + 2^c S_c^{*\mathrm{T}}\right) & T_c^{*\mathrm{T}} \end{pmatrix} \begin{pmatrix} T_c & -\left(T_c^* + 2^c S_c^*\right) \\ T_c + 2^c S_c & T_c^* \end{pmatrix} \\ &= \begin{pmatrix} \{2t_c + 2^c(2^{2c} + 2^c) + 2^{3c}\}I_{2^c} & 0 \\ 0 & \{2t_c + 2^c(2^{2c} + 2^c) + 2^{3c}\}I_{2^c} \end{pmatrix} \\ &= t_{c+1}I_{2^{c+1}}. \end{aligned}$$

The fact that $T_c^{\mathrm{T}}T_c = t_c I_{2^c}$ proves that the L_c in (3) has property (a). So now we need only prove that L_c has property (b). For any three columns of L_c, no matter whether they are distinct or not, they can be expressed as $l_i = (t_i^{\mathrm{T}}, 0, -t_i^{\mathrm{T}})^{\mathrm{T}}$ with t_i being the corresponding column in T_c for $i = 1, 2, 3$. We then have

$$(l_1 \odot l_2 \odot l_3)^{\mathrm{T}}1_{2^{c+1}+1} = (t_1 \odot t_2 \odot t_3)^{\mathrm{T}}1_{2^c} - (t_1 \odot t_2 \odot t_3)^{\mathrm{T}}1_{2^c} = 0,$$

where $a \odot b$ represents the elementwise product of a and b, and 1_h denotes the $h \times 1$ column vector with all elements unity. Thus, property (b) of L_c follows immediately, and we complete the proof. □

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