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Orthogonal Latin hypercube designs with special reference to four factors

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ABSTRACT

Latin hypercube designs are popular now-a-days for computer experiments. We give construction methods of orthogonal Latin hypercube designs for four factors for any number of runs for which such a design exists by combining smaller orthogonal matrices. We also propose methods for obtaining orthogonal Latin hypercube designs with larger number of factors.

1. Introduction

Computer experimentation is often performed in several scientific and engineering investigations and Latin hypercube designs introduced by McKay et al. (1979) are commonly used in such experiments. A Latin hypercube design L is an $n \times m$ matrix with each column containing n equally spaced levels $\{1, 2, \ldots, n\}$ exactly once. Here, the columns of L represent the factors and the rows represent the runs. Two kinds of models namely polynomial models and Gaussian-process models are used in computer experiments, see Bingham et al. (2009) for details. A class of Latin hypercube designs called orthogonal Latin hypercube designs are very popular for computer experiments with polynomial models. A Latin hypercube design is called orthogonal if the correlation coefficient between any two columns is zero, see Ye (1998). Henceforth, we denote an orthogonal Latin hypercube design with n runs and m factors as an OLH(n, m). As discussed in Sun et al. (2009), an OLH ensures the independence of estimates of linear effects for a first order fitted model.

There is a lot of interest in obtaining OLHs. Ye (1998) first proposed a method to construct OLH(n, m) with (a) $n = 2^{r+1}$ and $m = 2r$ (b) $n = 2^{r+1} + 1$ and $m = 2r$ for any integer $r \geq 1$. Steinberg and Lin (2006) proposed a method of construction of OLH(n, m) with $n = 2^{2^r}$ runs for any integer r. Cioppa and Lucas (2007) proposed a method to obtain OLH(n, m) for (a) $n = 2^{r+1} + 1$ and $m = \binom{r}{2} + r + 1$ (b) $n = 2^{r+1}$ and $m = \binom{r}{2} + r + 1$ by adding more factors to Ye's designs. Pang et al. (2009) constructed OLH(n, m) for $n = p^{2^r}$ and $m = (p^{2^r} - 1)/(p - 1)$ by rotating groups of factors in a p-level p^{2^r}-run regular fractional factorial designs, where p is a prime or prime power. Nguyen (2008) and Sun et al. (2009) independently constructed OLH(n, m) for (a) $n = 2^{r+1}$ runs in 2^r factors and (b) $2^{r+1} + 1$ runs in 2^r factors for any integer $r \geq 1$. Sun et al. (2010) developed a method of construction of OLH(n, m) for $n = s2^{r+1}$, $s2^{r+1} + 1$ runs and 2^r factors for all integers $s \geq 1$. Lin et al. (2009) suggested a construction method of OLH(n, m) using orthogonal designs. Lin et al. (2010) proved that no OLH (n, m) exists when $n = 4r + 2$ with r being a positive integer and provided a method for construction of OLHs and nearly OLHs. Yang and Liu (2012) provided a method to construct 2^r-order orthogonal designs which can then be utilized to construct OLH(n, m) for $n = s2^{r+1}$, $s2^{r+1} + 1$ and $m = 2^r$ where s is a positive integer. They also gave methods to obtain

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nearly OLH(n, m) for $n = 2^{r+1} + 2, 2^{r+1} + 3$ and $m = 2^r$. Georgiou and Efthimiou (2014) presented several new classes of OLHs. Dey and Sarkar (2014) presented a new result on construction of OLH(n, m) using orthogonal arrays and provided some new OLH(n, m). Parui et al. (in press) presented construction methods for OLH$(n, 3)$ for any value of n for which an OLH exists.

It may be seen from the above review that the methods of Ye (1998), Cioppa and Lucas (2007), Sun et al. (2009, 2010) and Yang and Liu (2012) fail to construct OLHs for $n \equiv s \pmod 8$, $s = 3, 4, 5, 7$ runs. Only the method of Parui et al. (in press) can construct OLHs for such number of runs, but their method is applicable for $m = 3$ factors. The purpose of this article is to give a complete solution to the existence and construction problem of OLH$(n, 4)$ for any value of n. Borrowing strength from literature, we further give methods of construction of OLHs with larger number of factors.

2. Methods of construction

We shall represent the levels of each factor, denoted as $\mathfrak{L}$, in its centered form. To be specific, $\mathfrak{L} = \{-(n-1)/2, -(n-3)/2, \ldots, -(n-2i+1)/2, \ldots, (n-3)/2, (n-1)/2\}$.

Now, we present a result due to Lin et al. (2010).

Lemma 1. *There exists no* OLH(n, m) *if* $n \equiv 2 \pmod 4$.

Next, we note the following trivial result.

Lemma 2. *There exists no* OLH$(n, 4)$ *for* $n < 8$ *runs.*

It is known that no OLH exists for $n < 4$ and $n = 6$ is covered by Lemma 1. The non-existence of OLH$(n, 4)$ for $n = 4, 5$ and 7 can be easily verified by an exhaustive search in computer. Thus, to have an OLH$(n, 4)$, we need $n \geq 8$ runs.

We shall call an $n \times m$ matrix $\mathbf{A} = (\mathbf{a}_1, \ldots, \mathbf{a}_m)$ as orthogonal if $\mathbf{a}_i'\mathbf{a}_j = 0$ for any $i \neq j = 1, 2, \ldots, m$. We denote an orthogonal matrix as OM(n, m). Clearly, an OM(n, m) is an OLH(n, m) if each of the columns of the OM(n, m) is a permutation of the levels in $\mathfrak{L}$. Now, we present a result for constructing an OM$(n, 4)$ with $n \equiv 0 \pmod 8$.

Lemma 3. *Let* $\pm a_i, \pm b_i, \pm c_i, \pm d_i, i = 1, 2, \ldots, r$ *be any* $8r$ *real numbers such that none of them is* 0. *Consider the matrix* $\mathbf{D} = (\mathbf{D}_1', \mathbf{D}_2', \ldots, \mathbf{D}_r')'$ *with*

$$\mathbf{D}_i = \begin{pmatrix} \mathbf{H}_i \\ -\mathbf{H}_i \end{pmatrix} \quad \textit{with } \mathbf{H}_i = \begin{pmatrix} a_i & b_i & c_i & d_i \\ b_i & -a_i & d_i & -c_i \\ c_i & -d_i & -a_i & b_i \\ d_i & c_i & -b_i & -a_i \end{pmatrix}. \tag{1}$$

Then, the $\mathbf{D}$ *is an* OM$(8r, 4)$ *and each column of the matrix* $\mathbf{D}$ *contains each of the numbers* $\pm a_i, \pm b_i, \pm c_i, \pm d_i, i = 1, 2, \ldots, r$ *exactly once.*

Lemma 3 is a strong result to obtain an OM$(8r, 4)$ and will be useful to construct OLH$(n, 4)$. We give below an example of obtaining an OM$(8, 4)$.

Example 1. Let $r = 1$. Let $a_1 = -7/2, b_1 = -5/2, c_1 = -3/2, d_1 = -1/2$. Then, the matrix

$$\mathbf{D} = \frac{1}{2}\begin{pmatrix} -7 & -5 & -3 & -1 \\ -5 & 7 & -1 & 3 \\ -3 & 1 & 7 & -5 \\ -1 & -3 & 5 & 7 \\ 7 & 5 & 3 & 1 \\ 5 & -7 & 1 & -3 \\ 3 & -1 & -7 & 5 \\ 1 & 3 & -5 & -7 \end{pmatrix}$$

is an OM$(8, 4)$.

Note that methods given in Sun et al. (2010) and Yang and Liu (2012) can be used to construct orthogonal matrices with $8r$ runs. However, Lemma 3 is more general due to flexibility in the choice of $a_i, b_i, c_i, d_i, i = 1, 2, \ldots, r$. In Lemma 3, if we choose the entries in such a way that $\{\pm a_i, \pm b_i, \pm c_i, \pm d_i, i = 1, 2, \ldots, r\} = \mathfrak{L}$, then the resulting OM becomes an OLH$(8r, 4)$.

Corollary 1. *Let* $\mathbf{D}$ *be* OM$(8r, 4)$ *as in* Lemma 3. *If each of the columns of the matrix* $\mathbf{D}$ *contains each of the elements of* $\mathfrak{L}$ *exactly once, then* $\mathbf{D}$ *is an* OLH$(8r, 4)$.

We present below another result due to Lin et al. (2010) which will be used to construct OLHs by combining two orthogonal matrices.