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Construction of sliced (nearly) orthogonal Latin hypercube designs

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ABSTRACT

Sliced Latin hypercube designs are very useful for running a computer model in batches, ensembles of multiple computer models, computer experiments with qualitative and quantitative factors, cross-validation and data pooling. However, the presence of highly correlated columns makes the data analysis intractable. In this paper, a construction method for sliced (nearly) orthogonal Latin hypercube designs is developed. The resulting designs have flexible sizes and most are new. With the orthogonality or near orthogonality being guaranteed, the space-filling property of the resulting designs is also improved. Examples are provided for illustrating the proposed method.

1. Introduction

Sliced Latin hypercube designs (SLHDs), first proposed by Qian [14], are motivated by several new problems recently arising in computer experiments such as running a computer model in batches with each batch of input values being one slice of the design, running multiple computer models based on similar mathematics [22] where each model uses one slice of the design, and computer experiments with both qualitative and quantitative factors [16,8,15,27]. A common feature of these applications is that the used design needs to be divided into batches. In view of this, it is natural to require that each batch has some good properties, as well as the whole design. An SLHD meets these requirements. Such a design is a special Latin hypercube design (LHD) that can be partitioned into slices each of which constitutes a smaller LHD. An LHD [12] has the appealing marginal property in the sense that it achieves maximum uniformity in any one-dimensional projection. Therefore, viewing the slices of an SLHD as the batches, each batch has the appealing marginal property. Furthermore,

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when collapsing over all the batches, the whole design also possesses the appealing marginal property. Beyond the above applications, SLHDs are also useful for validating a computer model [2], data pooling and stochastic optimization [14,23]. However, the original construction of Qian [14] cannot guarantee the low correlations among the columns of each slice of the design, and the columns of the whole design. Consequently, when applying SLHDs to the applications mentioned above, the presence of potentially highly correlated input factors may complicate the subsequent data analysis. For example, polynomial models are commonly used for computer experiments when the goal is screening. Designs with poor orthogonality will make it difficult to identify the most important input factors. In particular, orthogonality is directly useful when the first-order polynomial models are considered, and exact or near orthogonality can be viewed as stepping stones to space-filling designs. The rationales for using designs with exact or near orthogonality can be found in Ye [26], Steinberg and Lin [18], and Bingham et al. [3] among others.

In view of the fact that SLHDs with good orthogonality are often required, Yang et al. [23] proposed a class of sliced orthogonal LHDs (SOLHDs). Such designs preserve zero correlations among the columns and can be divided into slices of smaller orthogonal LHDs. For some parameters, however, the SOLHDs are non-existent or difficult to be constructed. In such cases, sliced nearly orthogonal LHDs (SNOLHDs), as alternatives to SOLHDs, are necessary.

In this paper, a new construction method for SOLHDs and SNOLHDs is introduced. Any design derived from the proposed method preserves zero or low correlations among the columns and can be divided into slices of smaller orthogonal or nearly orthogonal LHDs. The resulting SOLHDs can have different parameters from those constructed in Yang et al. [23]; and the resulting SNOLHDs are very flexible in design parameters.

The remainder of this paper is organized as follows. Section 2 presents some useful definitions and notation. Section 3 provides the construction method for SOLHDs and SNOLHDs. A strategy for improving the space-filling property of the constructed SOLHDs and SNOLHDs is given in Section 4. Section 5 contains some further discussion and concluding remarks. All proofs are deferred to the Appendix.

2. Definitions and notation

A Latin hypercube design (LHD) with N runs and p factors, denoted by LHD(N, p), is an $N \times p$ matrix in which each column is a permutation of N equally-spaced levels, taken to be $\{-(N-1)/2, -(N-3)/2, \ldots, (N-3)/2, (N-1)/2\}$ in this paper. For integers m and s, a sliced LHD (SLHD) with $N = ms$ runs, p factors and s slices, denoted by SLHD(m, s, p), is an LHD(N, p) that can be divided into s $m \times p$ subarrays each of which becomes an LHD(m, p) after the N levels are collapsed to m equally-spaced levels. Take the following design

$$D = \left(D_{(1)}^T, D_{(2)}^T\right)^T = \left(\begin{array}{cccc|cccc} 1.5 & 3.5 & -0.5 & -2.5 & 0.5 & 2.5 & -1.5 & -3.5 \\ 2.5 & -1.5 & -3.5 & 0.5 & 3.5 & -0.5 & -2.5 & 1.5 \end{array}\right)^T \tag{1}$$

as an example. The whole design D is an LHD(8,2), and the two subarrays $D_{(1)}$ and $D_{(2)}$ become two LHD(4,2)'s after the levels are collapsed according to

$$\{-3.5, -2.5\} \to -1.5,\ \{-1.5, -0.5\} \to -0.5,\ \{0.5, 1.5\} \to 0.5,\ \{2.5, 3.5\} \to 1.5.$$

Therefore, D is an SLHD(4,2,2).

The correlation between two vectors $u = (u_1, \ldots, u_n)^T$ and $v = (v_1, \ldots, v_n)^T$ is defined as

$$\rho(u, v) = \frac{\sum_{i=1}^{n}(u_i - \overline{u})(v_i - \overline{v})}{\sqrt{\sum_{i=1}^{n}(u_i - \overline{u})^2 \sum_{i=1}^{n}(v_i - \overline{v})^2}}, \tag{2}$$

where $\overline{u} = \sum_{i=1}^{n} u_i/n$ and $\overline{v} = \sum_{i=1}^{n} v_i/n$. Two vectors u and v are called orthogonal if $\rho(u, v) = 0$.