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Construction of second-order orthogonal sliced Latin hypercube designs

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ABSTRACT

Sliced Latin hypercube designs are useful for computer experiments with qualitative and quantitative factors, model calibration, cross validation, multi-level function estimation, stochastic optimization and data pooling. Orthogonality and second-order orthogonality are crucial in identifying important inputs. Besides orthogonality, good space-filling properties are also necessary for Latin hypercube designs. In this paper, a construction method for second-order orthogonal sliced Latin hypercube designs is proposed. The constructed designs are further optimized to achieve better space-filling properties. Furthermore, the method is extended to construct nearly orthogonal sliced Latin hypercube designs. The numbers of slices and columns as well as the levels of the resulting designs are more flexible than those obtained by existing methods.

1. Introduction

Sliced Latin hypercube designs (SLHDs), first proposed by Qian [14], are able to fulfill various kinds of modeling circumstances such as computer experiments with qualitative and quantitative factors, model calibration, cross validation, multi-level function estimation, stochastic optimization and data pooling. The feature of an SLHD is that the whole design is so well organized that it can be divided into several slices which are still Latin hypercube designs (LHDs)(Mckay et al. [12]) when the levels of each slice are collapsed properly. Since the whole design and each slice are LHDs, they have

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the attractive marginal property that the maximum uniformity in any one-dimensional projection is achieved. Besides uniformity, orthogonality is another character favored by the experimenters since it can eliminate the disturbance of other inputs on the estimation of one input, making it easy to identify the most important inputs. When a second-order effect is potentially present in the model, we would like the estimations of the main effects not to be affected by this second-order effect. Thus a second-order orthogonal design is preferred. Literatures concerning the construction of orthogonal and nearly orthogonal LHDs are rather plenty, including Ye [22], Steinberg and Lin [15], Lin et al. [11], Bingham et al. [2], Pang et al. [13], Georgiou [3], Sun et al. [16,17], Lin et al. [10], Sun et al. [18], Georgiou and Stylianou [5], Yang and Liu [19], Ai et al. [1], Georgiou and Efthimiou [4], among others. As for SLHDs, the idea of making them possess the orthogonality or projection uniformity has come to researchers' attention. Yin et al. [23] and Yang et al. [20] constructed SLHDs via both symmetric and asymmetric (resolvable) orthogonal arrays so that the resulting designs possess an attractive low-dimensional uniformity. Yang et al. [21] constructed a series of orthogonal SLHDs and Huang et al. [8] provided another method for constructing orthogonal and nearly orthogonal SLHDs.

In this paper, we propose a new construction method for second-order orthogonal SLHDs. The proposed designs and their slices not only have zero correlations among the columns, but also possess a foldover structure and the second-order orthogonality, which is not guaranteed in Huang et al. [8]. The number of slices of the proposed designs could be any positive integer, and the levels are far more flexible than those constructed by the two existing methods on orthogonal SLHDs (i.e., Yang et al. [21]; Huang et al. [8]). And for a given number of runs of each slice, the maximum number of columns is attained by the resulting second-order orthogonal SLHDs. Apart from the orthogonality, we further suggest a strategy to optimize the designs to possess better space-filling properties.

The remainder of this paper is organized as follows. Section 2 provides some useful definitions and notation. Section 3 proposes the construction method for second-order orthogonal SLHDs including the space-filling property improving strategy. In Section 4, the construction method is extended to construct nearly orthogonal SLHDs. Section 5 contains some concluding remarks.

2. Definitions and notation

An $N \times p$ matrix is called a Latin hypercube design (LHD) consisting of N runs and p factors, when each of its columns is a uniform permutation of N equally spaced levels. Such a design is denoted by LHD(N, p) and, in this paper, we take the levels to be $-(N-1)/2, -(N-3)/2, \ldots, (N-1)/2$. If an LHD$(N, p)$ with $N = mt$ can be divided into t slices and each slice forms a smaller LHD(m, p) with levels $-(m-1)/2, -(m-3)/2, \ldots, (m-1)/2$ when collapsed according to $\lceil (i + (N+1)/2)/t \rceil - (m+1)/2$ for level i, where $\lceil a \rceil$ means the smallest integer greater than or equal to a, then this is called a sliced LHD (SLHD), denoted by SLHD(m, t, p). An LHD is said to be orthogonal if the correlation between any two distinct columns is zero. If an SLHD as a whole design is orthogonal as well as each slice of it, it is called an orthogonal SLHD.

A p-factor q-degree polynomial full model is of the following form

$$Y = \mu + \sum_{1 \le i \le p} \beta_i x_i + \sum_{1 \le i_1 \le i_2 \le p} \beta_{i_1 i_2} x_{i_1} x_{i_2} + \cdots + \sum_{1 \le i_1 \le \cdots \le i_q \le p} \beta_{i_1 \ldots i_q} x_{i_1} \cdots x_{i_q} + \varepsilon,$$

where β_i is the linear effect of x_i, $\beta_{i_1 \ldots i_l}$ is the l-order interaction of $x_{i_1}, \ldots, x_{i_l}$, specially β_{ii} represents the quadratic effect of factor x_i and $\beta_{i_1 i_2}$ represents the bilinear interaction of factors x_{i_1} and x_{i_2} for $i_1 \neq i_2$. In regression analysis, it is desirable that the variables in the model are orthogonal to each other, in which case the estimates of the regression coefficients are uncorrelated. When it comes to fitting a q-degree polynomial regression model, orthogonal LHDs can guarantee the estimates of linear effects uncorrelated to each other. While sometimes second-order effects may be present, we seek designs with the following properties:

(a) each column is orthogonal to the others in the design;
(b) the sum of the elementwise product of any three columns is zero.

We call a design satisfying these two properties a second-order orthogonal design. It is well known that if a design D has the foldover structure $D = \left(D_0', -D_0'\right)'$, where D' is the transpose of D, it naturally