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Sliced space-filling designs with different levels of two-dimensional uniformity

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ABSTRACT

We consider sliced computer experiments where priori knowledge suggests that factors may have different levels of importance, and so some factors need to be paid more attention than others. A new class of sliced space-filling designs are proposed to deal with this type of sliced computer experiments, in which the whole design and each slice may have different levels of two-dimensional uniformity for different factors, besides they all achieve maximum stratification in univariate margins. They are generated by elaborately randomizing a special type of asymmetric orthogonal arrays, called asymmetric balanced sliced orthogonal arrays, which can be partitioned into several slices such that each slice is balanced and becomes an asymmetric orthogonal array after some level-collapsing. Several methods are developed to construct such asymmetric balanced sliced orthogonal arrays. Simulation study shows that the proposed designs perform well compared with other sliced designs for computer experiments.

1. Introduction

Sliced space-filling designs, proposed by Qian and Wu (2009), are intended for computer experiments with both qualitative and quantitative factors (Qian et al., 2008; Han et al., 2009), linking parameters in engineering and cross-validation. For those sliced designs constructed by Qian and Wu (2009) and Qian (2012), each slice cannot achieve the univariate and multiple-dimensional uniformity simultaneously. Recently, Xu et al. (2011) constructed Sudoku-based sliced space-filling designs in which the whole design and each slice all achieve maximum stratification in both univariate and bivariate margins. Ai et al. (2014) proposed a general approach to construct sliced space-filling designs by randomizing symmetric balanced sliced orthogonal arrays (BSOAs) so that the whole design and each slice can achieve stratification in two- or more-dimensional projections, in addition to achieving maximum stratification in univariate margins.

In this article, we consider sliced computer experiments where priori knowledge suggests that some factors are more important than others, and so need to be paid more attention. For example, in studying the heat transfer rate in a heat exchanger, the temperature of the heat source and the thermal conductivity of the material would have more influence than others. In predicting the speed of wind in an area, the local temperature and terrain may give more significant effects. Besides, interactions often arise among a group of particular factors and thus these factors deserve more attention. To deal with this issue, we are ready to propose a new class of sliced space-filling designs, in which the whole design and each slice can achieve maximum stratification in any univariate margin, but have different levels of two-dimensional uniformity

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for different factors. The proposed designs are generated by randomizing asymmetric BSOAs, which are a special class of asymmetric orthogonal arrays whose rows can be partitioned into several slices such that each slice is balanced and also becomes an asymmetric orthogonal array after some level-collapsing. Thus, the more important factors can be assigned to the columns with higher level in an asymmetric BSOA.

Compared with symmetric BSOAs of the same runs, asymmetric BSOAs can accommodate more columns with lower levels. Consequentially, the sliced space-filling designs based on asymmetric BSOAs can accommodate more factors of less importance, and hence such designs can save experimental runs if the degradation of two-dimensional uniformity for the less important factors is admissible. Furthermore, all the quantitative factors can still achieve maximum uniformity in univariate margins. So the proposed designs are expected to have high efficiency to design such sliced computer experiments.

The remainder of this article will unfold as follows. A formal definition of asymmetric BSOAs is given in Section 2. Sections 3 and 4 provide the construction of asymmetric BSOAs via the Kronecker sum and the replacement of levels, respectively. The generation of sliced space-filling designs based on asymmetric BSOAs is presented in Section 5. Some comparisons are given in Section 6 to show the performance of such designs. Section 7 concludes this article with some discussions.

2. Definition of asymmetric BSOAs

An orthogonal array (OA), denoted by $OA(n, s_1^{\gamma_1} \cdots s_k^{\gamma_k}, t)$, with n runs, $m = \sum_{i=1}^{k} \gamma_i$ factors and strength $t (m \geq t \geq 1)$, is an $n \times m$ matrix in which the first γ_1 columns have s_1 levels from a set of s_1 elements, the next γ_2 columns have s_2 levels from a set of s_2 elements, and so on, such that every $n \times t$ submatrix contains all possible level combinations as rows with the same frequency. When $s_1 = \cdots = s_k = s$, in particular, this special case is called a symmetric OA and denoted by $OA(n, s^m, t)$; otherwise, it is an asymmetric OA. An array is called *balanced* if it is an OA of strength one. Throughout, we consider only OAs of strength two and drop the strength parameter in $OA(n, s_1^{\gamma_1} \cdots s_k^{\gamma_k}, 2)$.

Let F be a set of s_1 elements and G be a set of s_2 elements with s_2 dividing s_1, denoted by $s_2 | s_1$. A level-collapsing *projection* from F to G, say δ, divides the elements of F into s_2 groups, each of size $q = s_1/s_2$, and projects any two elements of F to the same element of G if and only if they belong to the same group. The kernel matrix of δ is an $s_2 \times q$ matrix in which each row consists of the elements of F in the same group (Qian and Wu, 2009). For a matrix $\boldsymbol{A}$, let $\boldsymbol{A}'$ denote its transpose. If $\boldsymbol{A}$ takes entries from F, denote $\delta(\boldsymbol{A})$ as the array obtained from $\boldsymbol{A}$ after its entries are collapsed according to δ.

The definition of asymmetric BSOAs is given as follows. Let $\boldsymbol{H}$ be an $OA(n_1, s_{11}^{\gamma_1} \cdots s_{k1}^{\gamma_k})$. Suppose the n_1 rows of $\boldsymbol{H}$ can be partitioned into v subarrays each with n_2 rows, denoted by $\boldsymbol{H}_i$, $i = 1, \ldots, v$, and each $\boldsymbol{H}_i$ becomes an $OA(n_2, s_{12}^{\gamma_1} \cdots s_{k2}^{\gamma_k})$ after the s_{j1} levels of the s_{j1}-level factors are collapsed to s_{j2} levels according to some level-collapsing projection δ_j, for $j = 1, \ldots, k$. Then $\boldsymbol{H}$, or more precisely $(\boldsymbol{H}_1', \ldots, \boldsymbol{H}_v')'$, is called a sliced orthogonal array (SOA). For an SOA $\boldsymbol{H}$ in which each slice $\boldsymbol{H}_i$ is balanced, it is called a balanced SOA (BSOA). Provided that the s_{j1}'s are not all the same, it is an asymmetric BSOA.

3. Construction of asymmetric BSOAs via Kronecker sum

Similar to the construction of nested OAs with mixed levels in Qian et al. (2009), we propose three methods of constructing asymmetric BSOAs via the Kronecker sum. Throughout this section, we consider only the level-collapsing projection δ from an abelian group F to another abelian group G that has the additivity property, i.e., $\delta(f_1 + f_2) = \delta(f_1) + \delta(f_2)$ for any $f_1, f_2 \in F$.

The Kronecker sum of an $n \times m$ matrix $\boldsymbol{A} = (a_{ij})$ and a $u \times v$ matrix $\boldsymbol{B} = (b_{lk})$ based on the same abelian group with the addition operation '+', is defined to be the $nu \times mv$ matrix $\boldsymbol{A} \oplus \boldsymbol{B} = (a_{ij} + \boldsymbol{B})$, where $a_{ij} + \boldsymbol{B}$ denotes the $u \times v$ matrix with entries $a_{ij} + b_{lk}$, $1 \leq l \leq u$ and $1 \leq k \leq v$. Let $D(r, c, g)$ denote a difference matrix (DM), which is an $r \times c$ array based on an abelian group $\mathcal{A}$ of g elements such that every element of $\mathcal{A}$ appears equally often in the vector difference between any two columns of the array. Here we present an obvious conclusion for constructing asymmetric OAs in the following lemma for convenience of later use (Wang and Wu, 1991).

Lemma 1. *Suppose* $\boldsymbol{A} = (\boldsymbol{A}_1, \ldots, \boldsymbol{A}_k)$ *is an* $OA(n, s_1^{\gamma_1} \cdots s_k^{\gamma_k})$, *where* $\boldsymbol{A}_j$ *is the subarray corresponding to the* s_j*-level factors with levels from an abelian group* $\mathcal{A}_j$. *Let* $\boldsymbol{B}_j$ *be a* $D(r, c_j, s_j)$ *based on* $\mathcal{A}_j$, *for* $j = 1, \ldots, k$. *Then* $\boldsymbol{H} = (\boldsymbol{A}_1 \oplus \boldsymbol{B}_1, \ldots, \boldsymbol{A}_k \oplus \boldsymbol{B}_k)$ *is an* $OA(nr, s_1^{\gamma_1 c_1} \cdots s_k^{\gamma_k c_k})$.

3.1. Using sliced orthogonal arrays and difference matrices

This construction makes use of SOAs and difference matrices. For $j = 1, \ldots, k$, let $s_{j1} \geq s_{j2} > 1$ with $s_{j2} | s_{j1}$, F_j be an abelian group of s_{j1} elements, G_j be an abelian group of s_{j2} elements, and δ_j be a level-collapsing projection from F_j to G_j, where the s_{j1}'s are assumed to be all distinct. Suppose $\boldsymbol{A} = (\boldsymbol{A}_1, \ldots, \boldsymbol{A}_k)$ is an SOA with v slices, where $\boldsymbol{A}$ is an $OA(n_1, s_{11}^{\gamma_1} \cdots s_{k1}^{\gamma_k})$, $\boldsymbol{A}_j = (\boldsymbol{A}_{j1}', \ldots, \boldsymbol{A}_{jv}')'$ is the subarray of $\boldsymbol{A}$ corresponding to the s_{j1}-level factors with levels from F_j, and each slice $(\boldsymbol{A}_{1i}, \ldots, \boldsymbol{A}_{ki})$ becomes an $OA(n_2, s_{12}^{\gamma_1} \cdots s_{k2}^{\gamma_k})$ after the levels of the s_{j1}-level factors are collapsed according to δ_j, for $j = 1, \ldots, k$ and $i = 1, \ldots, v$.