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Uniform minimum moment aberration designs

Xue Yang [a,b], Gui-Jun Yang [a], Ya-Juan Su [c,*]

[a] *Tianjin University of Finance and Economics, China*
[b] *Nankai University, China*
[c] *Hebei Normal University, China*

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ABSTRACT

This paper discusses the issue of constructing uniform minimum moment aberration designs under discrepancies criteria. By considering all possible level permutations of factors, we establish a linear relationship between power moments and average discrepancy defined by a reproducing kernel for an asymmetrical or symmetrical design. We prove that minimum moment aberration designs often have low average discrepancies. Moreover, the average centered L_2-discrepancy is expressed as a linear combination of power moments for a given design. An efficient method for constructing uniform minimum moment aberration designs is proposed. Some asymmetrical uniform minimum moment aberration designs obtained by our method have low centered L_2-discrepancy and can be recommended for use in practice.

1. Introduction

Uniform designs spread their experimental points evenly throughout the design space under some discrepancy criterion (Fang and Lin, 2003; Fang et al., 2006) so that one can explore many kinds of models by using it. The commonly used discrepancies include, e.g., the centered L_2-discrepancy (CD), the wrap-around L_2-discrepancy (Hickernell, 1998) and the discrete discrepancy (Hickernell and Liu, 2002). A design is said to be uniform under some discrepancy criterion if it minimizes the discrepancy among all designs in a design space.

Constructing uniform designs is a complex and computationally intractable task, even for moderate number of runs, factors and levels (Fang et al., 2002). Many construction methods of uniform designs have been proposed, e.g., good lattice method, Latin square method and expanding orthogonal design method (Fang et al., 2006; Yang et al., 2014; Jiang and Ai, 2017). Recently, considerable studies have been done for constructing uniform designs by using the method of permutating levels of factorial designs. Tang et al. (2012) established a relationship between average CD and generalized wordlength pattern for three-level regular designs. To generalize their ideas, Tang and Xu (2013) investigated the relationship between average CD and generalized wordlength pattern for designs with arbitrary number of levels. Furthermore, Zhou and Xu (2014) obtained a unified expression between generalized wordlength pattern and any average discrepancy defined by a reproducing kernel. Generalized minimum aberration designs tend to agree with uniform designs. It is, however, often a hard task to find a generalized minimum aberration design.

Minimum moment aberration (MMA) criterion is developed for nonregular designs and supersaturated designs (Xu, 2003). It is also a good surrogate with computational advantages for the generalized minimum aberration criterion. Instead of studying the relationship between factors (i.e., columns), MMA is to sequentially minimize the power moments of the

* Corresponding author.
E-mail address: suyajuan1806@126.com (Y. Su).

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number of coincidence among runs (i.e., rows). The MMA criterion is statistically reasonable, computationally cheap, and convenient for theoretical development.

By considering all possible level permutations of factors, we establish a linear relationship between average discrepancy defined by a reproducing kernel and power moments for an asymmetrical or symmetrical design. We prove that MMA designs often have low average discrepancies. An MMA design with minimum discrepancy is called uniform MMA design. Moreover, the average centered L_2-discrepancy is expressed as a linear combination of power moments for a given design. An efficient method for constructing uniform MMA designs is proposed and some uniform MMA designs are constructed.

The remainder of this paper is organized as follows. Some notations and preliminaries are provided in Section 2. Section 3 presents a linear relationship between average discrepancy and power moments for an asymmetrical or symmetrical design. The method of constructing uniform MMA designs is also given in Section 3. Section 4 gives some concluding remarks. All proofs are deferred to Appendix A.

2. Notations and preliminaries

An $(N, s_1^{n_1}s_2^{n_2}\dots s_v^{n_v})$-design D is denoted by an array of size $N\times n$, where N and $n=\sum_{i=1}^{v}n_i$ are respectively the total number of points (rows) and factors (columns), in which the first n_1 columns have symbols from $\mathbb{Z}_{s_1}$, the next n_2 columns have symbols from $\mathbb{Z}_{s_2}$ and so on, where $\mathbb{Z}_s=\{0,1,\dots,s-1\}$. When $v=1$, the design D is denoted by (N, s^n) and is said to be symmetrical, otherwise is called asymmetrical or mixed-level. For simplicity of presentation, we only consider designs with two different levels in this paper, say $(N, s_1^{n_1}s_2^{n_2})$-design, where $n=n_1+n_2$.

For any symmetrical (N, s^n)-design $D=[x_{ik}]_{N\times n}$, let $\delta_{ij}(D)=\sum_{k=1}^{n}\delta(x_{ik},x_{jk})$ be the coincidence number of the ith and jth rows of D, where $\delta(y,z)$ is the Kronecker delta function, equals to 1 if $y=z$ and 0 otherwise. Note that $n-\delta_{ij}(D)$ is known as the Hamming distance between the ith and jth rows of D in algebraic coding theory. For an asymmetrical $(N, s_1^{n_1}s_2^{n_2})$-design D, we partition it into two symmetrical subdesigns by columns, i.e., $D=(D^{(1)} \vdots D^{(2)})$, where $D^{(r)}=(N, s_r^{n_r})$, $r=1,2$. Let $\delta_{ij}^{(r)}$ be the coincidence number of the ith and jth rows for $D^{(r)}$, and $\delta_{ij}^{*}(D)=\omega_1\delta_{ij}^{(1)}+\omega_2\delta_{ij}^{(2)}$, where $\omega_1>0$ and $\omega_2>0$ are weights, $\delta_{ij}^{*}(D)$ is called the weighted coincidence number of the ith and jth rows for D.

For a positive integer t, we define the tth power moment of an asymmetrical design D to be

$$K_t^{*}(D)=[N(N-1)/2]^{-1}\sum_{1\le i<j\le N}[\delta_{ij}^{*}(D)]^t. \tag{1}$$

The MMA criterion is to sequentially minimize the power moments $K_t^{*}(D)$, $t=1,2,\dots,n$. For two $(N, s_1^{n_1}s_2^{n_2})$-designs D_1 and D_2, D_1 is said to have less moment aberration than D_2 if there exists a t, such that $K_t^{*}(D_1)<K_t^{*}(D_2)$ and $K_i^{*}(D_1)=K_i^{*}(D_2)$ for $i=1,2,\dots,t-1$. D_1 is said to have MMA if there is no other design with less moment aberration than D_1. For $s_1=s_2=s$, Eq. (1) can be expressed as $K_t(D)=[N(N-1)/2]^{-1}\sum_{1\le i<j\le N}[\delta_{ij}(D)]^t$.

Let $\mathcal{X}$ be an experimental domain. A reproducing kernel $\mathcal{K}(\boldsymbol{x},\boldsymbol{y})$ defined on $\mathcal{X}^2=\mathcal{X}\times\mathcal{X}$ satisfies two properties: (i) $\mathcal{K}(\boldsymbol{x},\boldsymbol{y})=\mathcal{K}(\boldsymbol{y},\boldsymbol{x})$ for all $\boldsymbol{x},\boldsymbol{y}\in\mathcal{X}$, and (ii) $\sum_{i,j=1}^{N}c_i\mathcal{K}(\boldsymbol{x}_i,\boldsymbol{y}_j)c_j\ge 0$ for all $\boldsymbol{x}_i,\boldsymbol{y}_j\in\mathcal{X}$ and $c_i,c_j\in\mathbb{R}$. For an N-point design $D=\{\boldsymbol{x}_1,\dots,\boldsymbol{x}_N\}$ over $\mathcal{X}$, the L_2-type discrepancy for a given $\mathcal{K}(\boldsymbol{x},\boldsymbol{y})$ is defined as (see Hickernell, 1998)

$$\mathrm{Disc}(D,\mathcal{K})=\int_{\mathcal{X}^2}\mathcal{K}(\boldsymbol{x},\boldsymbol{y})dF_u(\boldsymbol{x})dF_u(\boldsymbol{y})-\frac{2}{N}\sum_{i=1}^{N}\int_{\mathcal{X}}\mathcal{K}(\boldsymbol{x}_i,\boldsymbol{y})dF_u(\boldsymbol{y})+\frac{1}{N^2}\sum_{i,j=1}^{N}\mathcal{K}(\boldsymbol{x}_i,\boldsymbol{x}_j), \tag{2}$$

where $F_u(\cdot)$ is the uniform distribution in the experimental domain $\mathcal{X}$. Different kernel functions $\mathcal{K}(\cdot,\cdot)$ induce different discrepancies. Commonly used reproducing kernels for discrepancies in the literature are defined on $\mathcal{X}=[0,1]^n$ and have a multiplicative form $\mathcal{K}(\boldsymbol{x},\boldsymbol{y})=\prod_{k=1}^{n}f(x_k,y_k)$, where $f(\cdot,\cdot)$ satisfies

$$f(x,y)\ge 0 \quad \text{and} \quad f(x,x)+f(y,y)>f(x,y)+f(y,x), \tag{3}$$

for any $x\ne y$, $x,y\in[0,1]$. Then the corresponding discrepancy in Eq. (2) can be expressed by

$$\mathrm{Disc}(D,\mathcal{K})=\mathcal{K}_1-\frac{2}{N}\sum_{i=1}^{N}\prod_{k=1}^{n}f_1(x_{ik})+\frac{1}{N^2}\sum_{i,j=1}^{N}\prod_{k=1}^{n}f(x_{ik},x_{jk}), \tag{4}$$

where $f_1(x)=\int_0^1 f(x,y)dy$ and $\mathcal{K}_1=\int_{\mathcal{X}^2}\mathcal{K}(\boldsymbol{x},\boldsymbol{y})dF_u(\boldsymbol{x})dF_u(\boldsymbol{y})$ which is a constant.

For multilevel designs, different level permutations may lead to different geometrical structures and statistical properties. And one may improve design properties by permuting levels of some factors. For an $(N, s_1^{n_1}s_2^{n_2})$-design D, let G_{s_k} be the s_kth permutation group, $k=1,2$, and $P_D(\pi_1,\pi_2,\dots,\pi_n)$ be a design obtained by permuting levels in the lth column of D by π_l, where $\pi_l\in G_{s_1}$, for $l=1,\dots,n_1$ and $\pi_l\in G_{s_2}$, for $l=n_1+1,\dots,n$. The set of all designs obtained via level permutations of D is denoted by $\mathcal{P}(D)$.

Note that there are total $(s_1!)^{n_1}(s_2!)^{n_2}$ designs in the set $\mathcal{P}(D)$. All designs in $\mathcal{P}(D)$ are combinatorially isomorphic to each other and share the same power moments, but may have different $\mathrm{Disc}(D,\mathcal{K})$ values. We can compute $\mathrm{Disc}(D,\mathcal{K})$ value for

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