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A note on uniformity and orthogonality ☆

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Abstract

Fang et al. (Technometrics 42 (2000) 237) proposed a united approach for searching orthogonal fractional factorial designs. They conjecture an important “equivalence theorem” between the uniformity of experimental points over the domain and the design orthogonality. They showed numerically that uniformity of experimental points over the domain can imply design orthogonality and conjecture that every orthogonal design can be obtained by minimizing some measure of uniformity. This paper shows that their conjecture is only true in some special cases. © 2002 Elsevier Science B.V. All rights reserved.

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1. Introduction

Factorial experiments have become important in all kinds of investigation and have been found to be of great utility in many areas of experimentation (see, for example, Dey and Mukerjee, 1999). A complete factorial experiment may involve a large number of runs, however. This is particularly true when the number of factors and the number of levels are large. Orthogonal fractional factorial designs (orthogonal designs, or OD for short) form a major class of fractional factorial designs and have been used in various fields.

Let $\mathscr{P}=\{\boldsymbol{x}_1,\ldots,\boldsymbol{x}_n\}$ be a design of n runs and s q-level factors. A design $\mathscr{P}$ is called an orthogonal design, denoted by $L_n(q^s)$, if all the level-combinations for any two factors appear equally often. The OD is a special case of orthogonal arrays. An orthogonal array of strength r and size n with s constrains, denoted by $\mathrm{OA}(n;q^s;r)$, is

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a factorial design of n runs and s q-level factors such that all the level-combinations for any r factors appear equally often. Obviously, a $L_n(q^s)$ is an orthogonal array of strength two, OA$(n;q^s;2)$.

ODs have been obtained by Bose and Bush (1952), Raghavarao (1971), Bose et al. (1960, 1961) and Geramita and Seberry (1979), for example. Their approaches strongly depend on profound mathematics, such as Hadamard matrices, orthogonal Latin squares, coding theory and finite fields. Fang et al. (2000, FLWZ for short) proposed a way of searching for ODs based on the concept of uniform design. A uniform design is a design with experimental points uniformly scattered on the domain (Fang and Wang, 1994).

A *U-type design* $U(n;q^s)$ is an $n \times s$ matrix with entries $1,\ldots,q$ in each column such that all the entries in each column appear equally often. This is, of course, an OA of strength 1. Let $\mathscr{U}(n;q^s)$ be the set of $U(n;q^s)$'s. A U-type design $\boldsymbol{U}^* \in \mathscr{U}\ (n;q^s)$ is called a uniform design (UD) under a given measure of uniformity, denoted by $U_n(q^s)$, if it has the best uniformity over $\mathscr{U}(n;q^s)$. For given (n,q,s) and a measure of uniformity, the corresponding uniform design can be found using optimization tools. If the centered L_2-discrepancy (see Section 2) is used as the measure of uniformity, FLWZ found that for many cases the uniform design $U_n(q^s)$, especially with a small number of runs, is indeed an orthogonal design $L_n(q^s)$. They further conjectured that $U_n(q^s)$ will also be an $L_n(q^s)$ in general. If the conjecture is true, both the OD and UD can be regarded as the same type of experimental designs and we can give another justification for the UD.

This note obtains the exact conditions that their conjecture will be valid. Such an equivalence between uniformity and orthogonality provides an additional rationale for using the uniform design. Uniform design are widely used in applications. One reviewer points out that:

> Designs that are 'spread out' or 'uniform' are commonly used in the computer experiments literature. The most popular are Latin hypercube designs. The rationale for using such designs has generally been heuristic; it seems sensible to spread points evenly throughout the design space so that one can explore a variety of models. Also, if one is trying to locate maxima or minima, spreading observations throughout the design space guarantees that no unobserved points in the space are far from a point that has been observed. The connection between uniformity and orthogonality provides an additional rationale for using designs that are uniform in the sense defined in this paper. Furthermore, this connection suggests that the measures of uniformity proposed in this paper may be more sensible than others currently popular (cf. Fang and Mukerjee, 2000 and Ma et al., 2001).

This paper is organized as follows. Section 2 introduces the centered L_2-discrepancy criterion and derives a useful quadratic form for such a criterion. Some properties of this quadratic form are also discussed. The main results are presented in Section 3, where we show that the FLWZ conjecture is true only if $(n,q)=(q^s,2)$, $(q^s$, odd), or $(2^{s-1}, 2)$, where n is the number of runs and q is the number of levels. Some concluding remarks are given in Section 4. Throughout this paper, we use bold small letters for column vectors and bold capital letters for matrices. The m-column vector of 1's (0's) is denoted by $\mathbf{1}_m$ or $\mathbf{1}$ ($\mathbf{0}_m$ or $\mathbf{0}$). The determinant of $\boldsymbol{A}$ is denoted by $|\boldsymbol{A}|$. The Kronecker product of two matrices/vectors is denoted by $\boldsymbol{A} \otimes \boldsymbol{B}$.

2. Centered L_2-discrepancy

Let $\mathscr{P} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n\}$ be a set of n points in the s-dimensional unit cube $C^s = [0, 1)^s$. Let $F_n(\boldsymbol{x})$ be the empirical distribution of $\mathscr{P}$ and $F(\boldsymbol{x})$ be the uniform distribution on C^s. The centered L_2-discrepancy (CL_2-discrepancy for short) of $\mathscr{P}$, denoted by $CL_2(\mathscr{P})$, measures the difference between $F_n(\boldsymbol{x})$ and $F(\boldsymbol{x})$ by $||F_n(\boldsymbol{x}) - F(\boldsymbol{x})||$, where the norm is defined according to the following considerations: (1) $CL_2(\mathscr{P})$ is invariant under reordering the points and relabeling the coordinates of the points; (2) $CL_2(\mathscr{P})$ is invariant under reflections of $\mathscr{P}$ about the any plane $x_j = 0.5$; (3) it considers not only the uniformity of $\mathscr{P}$ over C^s, but also the projection uniformity of $\mathscr{P}$.

The CL_2-discrepancy is defined by

$$(CL_2(\mathscr{P}))^2 = \sum_{u \neq \emptyset} \int_{C^u} \left| \frac{N(\mathscr{P}, J_{\boldsymbol{x}_u})}{n} - \mathrm{Vol}(J_{\boldsymbol{x}_u}) \right|^2 \mathrm{d}u, \tag{2.1}$$

where u is a non-empty subset of the set of coordinate indices $S = \{1, \ldots, s\}$, $|u|$ denotes the cardinality of u, C^u is the $|u|$-dimensional unit cube involving the coordinates in u, $J_{\boldsymbol{x}}$ is a rectangle uniquely determined by $\boldsymbol{x}$, $N(\mathscr{P}, J_{\boldsymbol{x}_u})$ is the number of points of $\mathscr{P}$ falling in $J_{\boldsymbol{x}_u}$ and $\mathrm{Vol}(J_{\boldsymbol{x}_u})$ is the volume of the projection of $J_{\boldsymbol{x}}$ on C^u. The rectangle $J_{\boldsymbol{x}}$ is chosen under some geometric consideration. For given $\boldsymbol{x} = (x_1, \ldots, x_s) \in C^s$, let $\boldsymbol{a} = (a_1, \ldots, a_s)$ be the closest vertex of C^s to $\boldsymbol{x}$. $J_{\boldsymbol{x}}$ is the hyper-rectangle containing $\boldsymbol{x}$ and $\boldsymbol{a}$, i.e.,

$$J_{\boldsymbol{x}} = \{\boldsymbol{y} \in C^s \mid \min(a_j, x_j) \leqslant y_j < \max(a_j, x_j), \text{ for } 1 \leqslant j \leqslant s\}.$$

The CL_2-discrepancy was proposed by Hickernell (1998) who derived an analytical expression

$$(CL_2(\mathscr{P}))^2 = \left(\frac{13}{12}\right)^s - \frac{2}{n} \sum_{k=1}^{n} \prod_{j=1}^{s} \left(1 + \frac{1}{2}|x_{kj} - 0.5| - \frac{1}{2}|x_{kj} - 0.5|^2\right)$$
$$+ \frac{1}{n^2} \sum_{k=1}^{n} \sum_{j=1}^{n} \prod_{i=1}^{s} \left[1 + \frac{1}{2}|x_{ki} - 0.5| + \frac{1}{2}|x_{ji} - 0.5| - \frac{1}{2}|x_{ki} - x_{ji}|\right]. \tag{2.2}$$

The CL_2-discrepancy can be used as a criterion for comparing factorial designs (Fang and Mukerjee, 2000) and detecting non-isomorphic factorial designs (Ma et al., 2001). This is the main reason why we choose the CL_2-discrepancy in this study, although many other measures for uniformity have been proposed (see, Hickernell, 1998).

Consider a set of lattice points $\mathscr{P}=\{\boldsymbol{x}_k,\ k=1,\ldots,n\}$ where $\boldsymbol{x}_k\in\mathscr{G}_{s,q}$ and

$$\mathscr{G}_{s,q}=\{(i_1,i_2,\ldots,i_s)|i_k=1,\ldots,q,k=1,\ldots,s\}.$$

Given n, s and q, denote $\mathscr{P}(n;q^s)$ as the set of all such $\mathscr{P}$. Obviously, $\mathscr{U}(n;q^s)\subset\mathscr{P}(n;q^s)$. A design $\mathscr{P}\in\mathscr{P}(n;q^s)$ is called a $\mathscr{P}$-uniform design (P-UD for short) if it has the smallest CL_2-value in the class $\mathscr{P}(n;q^s)$. The uniform design based on $\mathscr{U}(n;q^s)$ will be called $\mathscr{U}$-uniform design (U-UD for short). From now on, if we do not mention any specific measure of uniformity, it is under the centered L_2-discrepancy. Note that a design in $\mathscr{P}(n;q^s)$ is a factorial design of n runs and s q-level factors and is not necessary to be a U-type design and so does a $\mathscr{P}$-uniform design.

To evaluate the CL_2-value of a set $\mathscr{P}\in\mathscr{P}(n;q^s)$, we have to transform its q levels into (0,1). We will use the mapping $k\to(2k-1)/2k$, $k=1,\ldots,q$, which is common in the literature. Other transformations, such as $k\to k/(q+1)$, can be used. The CL_2-values may be different from the formula below, but the ordering will be kept.

Denote by $n(i_1,i_2,\ldots,i_s)$ the number of runs at the level-combination $(i_1,i_2,\ldots,i_s)$ in $\mathscr{P}\in\mathscr{P}(n;q^s)$. The $CL_2(\mathscr{P})$ can be expressed as

$$(CL_2(\mathscr{P}))^2=\left(\frac{13}{12}\right)^s-\frac{2}{n}\sum_{(i_1,\ldots,i_s)\in\mathscr{G}}n(i_1,\ldots,i_s)\prod_{j=1}^{s}t_{i_j}$$
$$+\frac{1}{n^2}\sum_{(i_1,\ldots,i_s)\in\mathscr{G}}\sum_{(k_1,\ldots,k_s)\in\mathscr{G}}n(i_1,\ldots,i_s)n(k_1,\ldots,k_s)\prod_{j=1}^{s}t_{i_jk_j},\tag{2.3}$$

where

$$t_i=1+\frac{1}{2}\left|\frac{2i-1-q}{2q}\right|-\frac{1}{2}\left|\frac{2i-1-q}{2q}\right|^2,\tag{2.4}$$

$$t_{ij}=1+\frac{1}{2}\left|\frac{2i-1-q}{2q}\right|+\frac{1}{2}\left|\frac{2j-1-q}{2q}\right|-\frac{1}{2}\left|\frac{i-j}{q}\right|.\tag{2.5}$$

Let $\boldsymbol{y}(\mathscr{P})$ (or $\boldsymbol{y}$ for short) be a q^s-vector with elements $n(i_1,\ldots,i_s)$ arranged lexicographically. For example, when $q=2$ and $s=3$, the order is $n(1,1,1)$, $n(1,1,2)$, $n(1,2,1)$, $n(1,2,2)$, $n(2,1,1)$, $n(2,1,2)$, $n(2,2,1)$, and $n(2,2,2)$. Let $\boldsymbol{b}_0=(t_1,\ldots,t_q)'$, $\boldsymbol{A}_0=(t_{ij},i,j=1,\ldots,q)$, $\boldsymbol{b}_s=\otimes^s\boldsymbol{b}_0$ and $\boldsymbol{A}_s=\otimes^s\boldsymbol{A}_0$, where $\otimes$ is the Kronecker product. Now we can express $CL_2(\mathscr{P})$ as a quadratic form of $\boldsymbol{y}$ from (2.3).

Lemma 1.

$$[CL_2(\mathscr{P})]^2=\left(\frac{13}{12}\right)^s-\frac{2}{n}\boldsymbol{b}_s'\boldsymbol{y}+\frac{1}{n^2}\boldsymbol{y}'\boldsymbol{A}_s\boldsymbol{y}.\tag{2.6}$$

3. Connections between uniformity and orthogonality

A design is called a *complete design* if all level-combinations of the factors appear equally often. Any complete design is an OD and the corresponding vector of integers

$\boldsymbol{y}(\mathscr{P})$ is a multiple of $\mathbf{1}$. For any factorial design $\mathscr{P} \in \mathscr{P}(n; q^s)$, $\boldsymbol{y}(\mathscr{P})/n$ can be regarded as a probability measure over q^s level-combinations. Therefore, we can extend $\boldsymbol{y}(\mathscr{P})$ to be a measure on q^s level-combinations, i.e. $\boldsymbol{y}(\mathscr{P})$ is a q^s-real vector with constraint $\boldsymbol{y}'\mathbf{1} = n$.

Theorem 1. *Let $\mathscr{P} \in \mathscr{P}(n; q^s)$ be a set of n lattice points. Then,*

(1) *when $q = 2$ or q is odd, $\mathscr{P}$ minimizes $CL_2(\mathscr{P})$ over $\mathscr{P}(n, q^s)$ if and only if $\boldsymbol{y}(\mathscr{P}) = (n/q^s)\mathbf{1}$;*

(2) *when q is even (but not 2), $\mathscr{P}$ minimizes $CL_2(\mathscr{P})$ over $\mathscr{P}(n, q^s)$ if and only if*

$$\boldsymbol{y}(\mathscr{P}) = \frac{n}{q^s} \otimes^s \begin{pmatrix} \mathbf{1}_{q/2-1} \\ 1 - \frac{1}{4(4q+1)} \\ 1 - \frac{1}{4(4q+1)} \\ \mathbf{1}_{q/2-1} \end{pmatrix} + n\frac{1 - (1 - 1/(2q(4q+1)))^s}{2^s} \otimes^s \begin{pmatrix} \mathbf{0}_{q/2-1} \\ 1 \\ 1 \\ \mathbf{0}_{q/2-1} \end{pmatrix}$$

(3) *when q is even (but not 2) and $\mathscr{P} \in \mathscr{U}(n; q^s)$, $\mathscr{P}$ minimizes $CL_2(\mathscr{P})$ over $\mathscr{P}(n, q^s)$ if and only if*

$$\boldsymbol{y} = nA_s^{-1}\boldsymbol{b}_s - n\left[\frac{\mathbf{1}'A_s^{-1}\boldsymbol{b}_s}{\mathbf{1}'A_s^{-1}\mathbf{1}}\left(1 - \frac{s(8q^2+2q)}{8q^2+2q-1}\right) + \frac{s-1}{\mathbf{1}'A_s^{-1}\mathbf{1}}\right]A_s^{-1}\mathbf{1}$$
$$- \frac{n}{q}\frac{(\mathbf{1}'A_0^{-1}\boldsymbol{b}_0)^{s-1} - 1}{(\mathbf{1}'A_0^{-1}\mathbf{1})^{s-1}}\sum_{i=1}^{s}(A_0^{-1}\mathbf{1})^{i-1} \otimes \mathbf{1} \otimes (A_0^{-1}\mathbf{1})^{i-1}.$$

Especially, for $s = 1, 2$ we have $\boldsymbol{y}(\mathscr{P}) = n/q^s\mathbf{1}$.

The following properties are useful in the proof of Theorem 1.

Lemma 2.

(1) $$|A_0| = \begin{cases} \left(\frac{1}{q}\right)^{q-1}, & q \text{ is odd} \\ \left(\frac{1}{q}\right)^{q-1}\left(1 + \frac{1}{4q}\right), & q \text{ is even.} \end{cases}$$

(2) $$\boldsymbol{b}_0'\mathbf{1} = \begin{cases} \frac{13}{12}q - \frac{1}{12q}, & q \text{ is odd}, \\ \frac{13}{12}q + \frac{1}{24q}, & q \text{ is even.} \end{cases}$$

(3) $$A_0\mathbf{1} - q\boldsymbol{b}_0 = \begin{cases} \mathbf{0}, & q \text{ is odd}, \\ \frac{1}{8q}\mathbf{1}, & q \text{ is even.} \end{cases}$$

(4) *A_0^{-1} is a tridiagonal symmetric matrix. When q is odd, its diagonal elements are $(q, 2q\mathbf{1}_{(q-3)/2}, 2q+1, 2q\mathbf{1}_{(q-3)/2}, q)'$ and its all second diagonal elements are $-q$. When q is even, the diagonal elements are $(q, 2q\mathbf{1}_{(q-4)/2}, 2q + q/(2q+1),$*

$2q + q/(2q+1), 2q\mathbf{1}_{(q-4)/2}, q)'$ *and the second diagonal elements are* $(-q\mathbf{1}_{(q-2)/2}, -q + q/(2q+1), -q\mathbf{1}_{(q-2)/2})'$.

(5) $$A_0^{-1}\mathbf{1} = \begin{cases} (\mathbf{0}', 1, \mathbf{0}')', & q \text{ is odd}, \\ \frac{2q}{4q+1}(\mathbf{0}', 1, 1, \mathbf{0}')', & q \text{ is even}. \end{cases}$$

(6) $$\mathbf{1}'A_0^{-1}\mathbf{1} = \begin{cases} 1, & q \text{ is odd}, \\ \frac{4q}{4q+1}, & q \text{ is even}. \end{cases}$$

(7) $$A_0^{-1}\mathbf{b}_0 = \begin{cases} \frac{1}{q}\mathbf{1}, & q \text{ is odd}, \\ \frac{1}{q}\mathbf{1} - \frac{1}{8q^2}A_0^{-1}\mathbf{1}, & q \text{ is even}. \end{cases}$$

Proof of Theorem 1. From Lemma 1 and the Lagrange multiplier method, let

$$L(\mathbf{y}, \lambda) = \left(\frac{13}{12}\right)^s - \frac{2}{n}\mathbf{b}_s'\mathbf{y} + \frac{1}{n^2}\mathbf{y}'A_s\mathbf{y} + \lambda(\mathbf{y}'\mathbf{1} - n).$$

The following system of equations

$$\frac{\partial L}{\partial \lambda} = \mathbf{y}'\mathbf{1} - n = 0,$$

$$\frac{\partial L}{\partial \mathbf{y}} = -\frac{2}{n}\mathbf{b}_s + \frac{2}{n^2}A_s\mathbf{y} + \lambda\mathbf{1} = \mathbf{0},$$

give

$$\lambda = \frac{2(\mathbf{1}'A_s^{-1}\mathbf{b}_s - 1)}{n\mathbf{1}'A_s^{-1}\mathbf{1}}$$

and

$$\mathbf{y} = nA_s^{-1}\mathbf{b}_s - n\frac{\mathbf{1}'A_s^{-1}\mathbf{b}_s - 1}{\mathbf{1}'A_s^{-1}\mathbf{1}}A_s^{-1}\mathbf{1}.$$

When q is odd, from (3) of Lemma 2 we have $\mathbf{b}_s = (1/q^s)A_s\mathbf{1}$ and $\mathbf{y} = nA_s^{-1}\mathbf{b}_s = (n/q^s)\mathbf{1}$. When $q = 2$, it is easy to find

$$\mathbf{b}_0 = \frac{35}{32}\mathbf{1}, \quad A_0 = \begin{pmatrix} \frac{5}{4} & 1 \\ 1 & \frac{5}{4} \end{pmatrix}, \quad A_0^{-1} = \begin{pmatrix} \frac{20}{9} & -\frac{16}{9} \\ -\frac{16}{9} & \frac{20}{9} \end{pmatrix}$$

and

$$\mathbf{b}_s = \left(\frac{35}{32}\right)^s \mathbf{1}, \quad A_s^{-1}\mathbf{b}_s = \left(\frac{35}{32}\right)^s \otimes^s (A_0^{-1}\mathbf{1}) = \left(\frac{35}{32}\frac{4}{9}\right)^s \mathbf{1}.$$

By straightforward algebra, it follows that $\mathbf{y} = (n/2^s)\mathbf{1}_{2^s}$. When q is even, the assertion (2) follows by a similar approach.

(3) Denote by $\boldsymbol{t}^k$ the k-order Kronecker product of a vector $\boldsymbol{t}$. Let

$$L(\boldsymbol{y},\lambda,\lambda_1,\ldots,\lambda_s)=\left(\frac{13}{12}\right)^s-\frac{2}{n}\boldsymbol{b}_s'\boldsymbol{y}+\frac{1}{n^2}\boldsymbol{y}'\boldsymbol{A}_s\boldsymbol{y}+\lambda(\boldsymbol{y}'\mathbf{1}-n)$$
$$+\sum_{i=1}^{s}\left(\boldsymbol{y}'G_i-\frac{n}{q}\mathbf{1}'\right)\lambda_i,$$

where $G_i=\mathbf{1}^{i-1}\otimes I_q\otimes\mathbf{1}^{s-i}$, and λ_i ($q\times 1$ vector) satisfies $\mathbf{1}'\boldsymbol{A}_0^{-1}\lambda_i=\mathbf{1}'\boldsymbol{A}_0^{-1}\mathbf{1},\ i=1,\ldots,s$. Then

$$\frac{\partial L}{\partial\lambda}=\boldsymbol{y}'\mathbf{1}-n=0, \tag{3.1}$$

$$\frac{\partial L}{\partial \boldsymbol{y}}=-\frac{2}{n}\boldsymbol{b}_s+\frac{2}{n^2}\boldsymbol{A}_s\boldsymbol{y}+\lambda\mathbf{1}+\sum_{i=1}^{s}G_i\lambda_i=\mathbf{0}, \tag{3.2}$$

$$\frac{\partial L}{\partial\lambda_i}=G_i'\boldsymbol{y}-\frac{n}{q}\mathbf{1}=\mathbf{0},\quad i=1,\ldots,s. \tag{3.3}$$

(In fact, Eq. (3.3) indicate that the design is a U-type design.) From (3.2),

$$-\frac{2}{n}\boldsymbol{A}_s^{-1}\boldsymbol{b}_s+\frac{2}{n^2}\boldsymbol{y}+\lambda\boldsymbol{A}_s^{-1}\mathbf{1}+\sum_{i=1}^{s}(\boldsymbol{A}_0^{-1}\mathbf{1})^{i-1}\otimes(\boldsymbol{A}_0^{-1}\lambda_i)\otimes(\boldsymbol{A}_0^{-1}\mathbf{1})^{s-i}=\mathbf{0}. \tag{3.4}$$

Multiplying $\mathbf{1}_{q^s}$ to both sides in (3.4),

$$-\frac{2}{n}\mathbf{1}'\boldsymbol{A}_s^{-1}\boldsymbol{b}_s+\frac{2}{n^2}\mathbf{1}'\boldsymbol{y}+\lambda\mathbf{1}'\boldsymbol{A}_s^{-1}\mathbf{1}$$
$$+\sum_{i=1}^{s}(\mathbf{1}'\boldsymbol{A}_0^{-1}\mathbf{1})^{i-1}\otimes(\mathbf{1}'\boldsymbol{A}_0^{-1}\lambda_i)\otimes(\mathbf{1}'\boldsymbol{A}_0^{-1}\mathbf{1})^{s-i}=\mathbf{0}$$

gives

$$\lambda=\frac{2(\mathbf{1}'\boldsymbol{A}_s^{-1}\boldsymbol{b}_s-1)}{n\mathbf{1}'\boldsymbol{A}_s^{-1}\mathbf{1}}-s. \tag{3.5}$$

Multiplying G_k' to both sides in (3.4),

$$-\frac{2}{n}(\mathbf{1}'\boldsymbol{A}_0^{-1}\boldsymbol{b}_0)^{s-1}\boldsymbol{A}_0^{-1}\boldsymbol{b}_0+\frac{2}{n^2}G'\boldsymbol{y}+\lambda(\mathbf{1}'\boldsymbol{A}_0^{-1}\mathbf{1})^{s-1}\boldsymbol{A}_0^{-1}\mathbf{1}$$
$$+\sum_{i=1,i\neq k}^{s}(\mathbf{1}'\boldsymbol{A}_0^{-1}\mathbf{1})^{s-1}(\boldsymbol{A}_0^{-1}\mathbf{1})+(\mathbf{1}'\boldsymbol{A}_0^{-1}\mathbf{1})^{s-1}(\boldsymbol{A}_0^{-1}\lambda_k)=\mathbf{0}.$$

From (3.3)–(3.5),

$$\lambda_k=\frac{2}{nq}\frac{(\mathbf{1}'\boldsymbol{A}_0^{-1}\boldsymbol{b}_0)^{s-1}-1}{(\mathbf{1}'\boldsymbol{A}_0^{-1}\mathbf{1})^{s-1}}\boldsymbol{A}_0\mathbf{1}+\frac{2}{n}\left[\frac{1}{\mathbf{1}'A_s^{-1}\mathbf{1}}-\frac{8q^2+2q}{8q^2+2q-1}\frac{\mathbf{1}'\boldsymbol{A}_s^{-1}\boldsymbol{b}_s}{\mathbf{1}'\boldsymbol{A}_s^{-1}\mathbf{1}}\right]\mathbf{1}+\mathbf{1}$$

Table 1
The number of level-combinations

$n(1,i,j)$				$n(2,i,j)$				$n(3,i,j)$				$n(4,i,j)$			
68	67	67	68	67	70	70	67	67	70	70	67	68	67	67	68
67	70	70	67	70	65	65	70	70	65	65	70	67	70	70	67
67	70	70	67	70	65	65	70	70	65	65	70	67	70	70	67
68	67	67	68	67	70	70	67	67	70	70	67	68	67	67	68

and

$$\boldsymbol{y} = n\boldsymbol{A}_s^{-1}\boldsymbol{b}_s - \frac{n^2\lambda}{2}\boldsymbol{A}_s^{-1}\mathbf{1} - \frac{n^2}{2}\sum_{i=1}^{s}(\boldsymbol{A}_0^{-1}\mathbf{1})^{i-1}\otimes(\boldsymbol{A}_0^{-1}\lambda_i)\otimes(\boldsymbol{A}_0^{-1}\mathbf{1})^{s-i}$$

$$= n\boldsymbol{A}_s^{-1}\boldsymbol{b}_s - n\left[\frac{\mathbf{1}'\boldsymbol{A}_s^{-1}\boldsymbol{b}_s}{\mathbf{1}'\boldsymbol{A}_s^{-1}\mathbf{1}}\left(1-\frac{s(8q^2+2q)}{8q^2+2q-1}\right)+\frac{s-1}{\mathbf{1}'\boldsymbol{A}_s^{-1}\mathbf{1}}\right]\boldsymbol{A}_s^{-1}\mathbf{1}$$

$$-\frac{n}{q}\frac{(\mathbf{1}'\boldsymbol{A}_0^{-1}\boldsymbol{b}_0)^{s-1}-1}{(\mathbf{1}'\boldsymbol{A}_0^{-1}\mathbf{1})^{s-1}}\sum_{i=1}^{s}(\boldsymbol{A}_0^{-1}\mathbf{1})^{i-1}\otimes\mathbf{1}\otimes(\boldsymbol{A}_0^{-1}\mathbf{1})^{i-1}.$$

When $s=1,2$, from Lemma 2, $\boldsymbol{y}=n/q^s\mathbf{1}$. □

Note that Theorem 1 does not require $\mathscr{P}$ to be a U-type design in the first two assertions. When q is odd or 2 and n is a multiple of q^s, Theorem 1 shows that a complete design is a $\mathscr{P}$-uniform design for the cases of $q=2$, odd q and even q only for $s=1,2$. For these cases the conjecture is true. $\mathscr{P}$ is complete. The conjecture in the case of even q and $s>2$ is more complicated. First, a $\mathscr{P}$-uniform design is not necessary a U-type design. For example, when $n=1088$, $q=4$ and $s=2$, the $n(i,j)$ elements of the $\mathscr{P}$-uniform design are given by

$$\boldsymbol{N} \equiv (n(i,j)) = \begin{pmatrix} 68 & 67 & 67 & 68 \\ 67 & 70 & 70 & 67 \\ 67 & 70 & 70 & 67 \\ 68 & 67 & 67 & 68 \end{pmatrix}.$$

Second, if the design $\mathscr{P}$ is a U-type, the assertion (3) shows that the complete design for $s=1,2$ is a $\mathscr{U}$-uniform design and orthogonal design. Third, the conjecture is not true for the cases of even q and $s>2$. For example, the case of $n=4352$, $q=4$, $s=3$, the $n(i,j,k)$ elements of the $\mathscr{P}$-uniform design given in Table 1 show that the design is U-type, but not orthogonal.

Note that calculation of the CL_2-value for any complete design is a rather easy task.

Theorem 2. *For a complete design* $\mathscr{P}$ *in* $\mathscr{P}(n, q^s)$ *with* $n = rq^s$ *runs where* r *is a positive integer,*

$$[CL_2(\mathscr{P})]^2 = \left(\frac{13}{12}\right)^s - \left(\frac{13}{12} - \frac{1}{12q^2}\right)^s, \quad \text{if } q \text{ is odd};$$

$$= \left(\frac{13}{12}\right)^s - 2\left(\frac{13}{12} + \frac{1}{24q^2}\right)^s + \left(\frac{13}{12} + \frac{1}{6q^2}\right)^s, \quad \text{if } q \text{ is even}$$

which is independent of r.

Proof. As $\mathscr{P}$ is complete, it follows $\boldsymbol{y}(\mathscr{P}) = r\mathbf{1}_{q^s}$. From Lemma 1 we have

$$[CL_2(\mathscr{P})]^2 = \left(\frac{13}{12}\right)^s - \frac{2}{n} r \otimes^s (\boldsymbol{b}_0'\mathbf{1}) + \frac{1}{n^2} r^2 \otimes^s (\mathbf{1}'\boldsymbol{A}_0\mathbf{1}).$$

When q is odd, from (2) and (3) of Lemma 2 we have

$$\frac{2}{n} r \otimes^s (\boldsymbol{b}_0'\mathbf{1}) = \frac{2}{n} r q^s \left(\frac{13}{12} - \frac{1}{12q^2}\right)^s = 2\left(\frac{13}{12} - \frac{1}{12q^2}\right)^s$$

and

$$\frac{1}{n^2} r^2 \otimes^s (\mathbf{1}'\boldsymbol{A}_0\mathbf{1}) = \frac{r^2}{n^2}(q\boldsymbol{b}_0'\mathbf{1})^s = \left(\frac{13}{12} - \frac{1}{12q^2}\right)^s.$$

The assertion follows immediately. The assertion for the even case can be proven in a similar manner. □

When a lattice design $\mathscr{P}$ is not complete, does the conjecture still hold? Note that $[CL_2(\mathscr{P})]^2 = \sum_{u \neq \emptyset} I_u(\mathscr{P})^2$, where $I_u(\mathscr{P}) = I_{|u|}(\mathscr{P}^u)$, $\mathscr{P}^u$ is the projection of $\mathscr{P}$ onto C^u and

$$I_s(\mathscr{P})^2 = \int_{C^s} \left(\frac{N(\mathscr{P}, J_{\boldsymbol{x}})}{n} - \mathrm{Vol}(J_{\boldsymbol{x}})\right)^2 \mathrm{d}\boldsymbol{x}.$$

Obviously, the $I_s(\mathscr{P})^2$ can be considered as a measure of uniformity and can be expressed as a similar formula to (2.2) and (2.6), respectively

$$I_s(\mathscr{P})^2 = \left(\frac{1}{12}\right)^s - \frac{2}{n} \sum_{k=1}^{n} \prod_{j=1}^{s} \left(\frac{1}{2}|x_{kj} - 0.5| - \frac{1}{2}|x_{kj} - 0.5|^2\right)$$

$$+ \frac{1}{n^2} \sum_{k=1}^{n} \sum_{j=1}^{n} \prod_{i=1}^{s} \left[\frac{1}{2}|x_{ki} - 0.5| + \frac{1}{2}|x_{ji} - 0.5| - \frac{1}{2}|x_{ki} - x_{ji}|\right]$$

$$= \left(\frac{1}{12}\right)^s - \frac{2}{n}\boldsymbol{f}_s'\boldsymbol{y} + \frac{1}{n^2}\boldsymbol{y}'\boldsymbol{E}_s\boldsymbol{y}, \tag{3.6}$$

where $\boldsymbol{f}_s = \otimes^s \boldsymbol{f}_0$, $\boldsymbol{E}_s = \otimes^s \boldsymbol{E}_0$, $\boldsymbol{f}_0 = (f_1, \ldots, f_q)'$, and $\boldsymbol{E}_0 = (e_{ij},\ i,j = 1, \ldots, q)$ with

$$f_i = \frac{1}{2}\left|\frac{2i-1-q}{2q}\right| - \frac{1}{2}\left|\frac{2i-1-q}{2q}\right|^2,$$

$$e_{ij} = \frac{1}{2}\left|\frac{2i-1-q}{2q}\right| + \frac{1}{2}\left|\frac{2j-1-q}{2q}\right| - \frac{1}{2}\left|\frac{i-j}{q}\right|.$$

Similar to Lemma 2 we have the following results:

(1) $|\boldsymbol{E}_0| = \begin{cases} 0, & q \text{ is odd}, \\ \left(\frac{1}{q}\right)^{q-2} \frac{1}{4q^2}, & q \text{ is even}, \end{cases}$

(2) $\boldsymbol{E}_0 \mathbf{1} - q\boldsymbol{f}_0 = \begin{cases} \mathbf{0}, & q \text{ is odd}, \\ \frac{1}{8q}\mathbf{1}, & q \text{ is even}. \end{cases}$

(3) When $q = 2$, $\boldsymbol{E}_0 = 1/4\boldsymbol{I}_2$, $E_s = 1/4^s \boldsymbol{I}_{2^s}$, $\boldsymbol{f}_0 = \frac{3}{32}\mathbf{1}$, $\boldsymbol{f}_s = (\frac{3}{32})^s \mathbf{1}$, and

$$I_s(\mathscr{P})^2 = \left(\frac{1}{12}\right)^s - 2\left(\frac{3}{32}\right)^s + \frac{1}{n^2 4^s}\boldsymbol{y}'\boldsymbol{y}. \tag{3.7}$$

Based on the measure of uniformity $I_s(\mathscr{P})$ we have

Lemma 3. *Let $\mathscr{P}$ be a lattice design in $\mathscr{P}(n; 2^s)$.*

(1) *If $n = r2^s$ is a multiple of 2^s, then $\mathscr{P}$ minimizes $I_s(\mathscr{P})$ over $\mathscr{P}(n; 2^s)$ if it is complete, in this case the minimum $I_s(\mathscr{P})^2$ is $1/n^2 2^s + (\frac{1}{12})^s - 2(\frac{3}{32})^s$.*

(2) *If $n < 2^s$, then $\mathscr{P}$ minimizes $I_s(\mathscr{P})$ over $\mathscr{P}(n; 2^s)$ if there are no duplicates at any level-combination, in this case the minimum $I_s(\mathscr{P})^2$ is $1/n^2 2^s + (\frac{1}{12})^s - 2(\frac{3}{32})^s$. As a consequence, the components of $\boldsymbol{y}(\mathscr{P})$ are n 1's and $(2^s - n)$ 0's.*

Proof. From (3.7) we have

$$\begin{aligned} I_s(P)^2 &= \left(\frac{1}{12}\right)^s - 2\left(\frac{3}{32}\right)^s + \frac{1}{n^2 4^s}[(\boldsymbol{y} - r\mathbf{1})'(\boldsymbol{y} - r\mathbf{1}) + 2r\boldsymbol{y}'\mathbf{1} - r^2\mathbf{1}'\mathbf{1}] \\ &= \left(\frac{1}{12}\right)^s - 2\left(\frac{3}{32}\right)^s + \frac{1}{n^2 4^s}[(\boldsymbol{y} - r\mathbf{1})'(\boldsymbol{y} - r\mathbf{1}) + 2rn - r^2\mathbf{1}'\mathbf{1}] \end{aligned}$$

that achieves its minimum at $\boldsymbol{y} = r\mathbf{1}$ and the first assertion follows.

As $I_s^2(\mathscr{P})$ is a linear function of $\boldsymbol{y}'\boldsymbol{y} = \sum_{(i_1,\ldots,i_s)\in\mathscr{G}} n^2(i_1, \ldots, i_s)$ from (3.7), and

$$\sum n^2(i_1, \ldots, i_s) \geqslant \sum n(i_1, \ldots, i_s) = n,$$

$I_s(\mathscr{P})$ achieves its minimum at $\mathscr{P}$ with components of $\boldsymbol{y}(\mathscr{P})$ being 1 or 0. The assertion follows. □

Theorem 3. *Let $\mathscr{P}$ be a set in $\mathscr{P}(n; 2^s)$ with $n = 2^{s-1}$ and $s \geqslant 3$. Then $\mathscr{P}$ is a $\mathscr{U}$-uniform design if and only if it is an orthogonal array* OA$(n; 2^s; s-1)$.

Proof. Note

$$(CL_2(\mathscr{P}))^2 = \sum_{|u|<s, u\neq\emptyset} I_u(\mathscr{P})^2 + I_s(\mathscr{P})^2.$$

Sufficiency: If the design $\mathscr{P}$ is an $\mathrm{OA}(n; 2^s; s-1)$, its projection onto any $|u|$-dimensional space with $|u| < s$ is a complete design and its $I_u(\mathscr{P})$ achieves its minimum from Lemma 3. Furthermore, the components of $\boldsymbol{y}(\mathscr{P})$ are different from each other and $I_s(\mathscr{P})$ achieves its minimum from Lemma 3. Thus, $\mathscr{P}$ is a $\mathscr{U}$-uniform design.

Necessarity: Suppose that $\mathscr{P}$ is a $\mathscr{U}$-uniform design. Its projection onto any $|u|$-dimensional space with $|u| < s$ must be a complete design, otherwise we can find another design (for example, take an $\mathrm{OA}(n; 2^s; s-1)$) such that the latter has a smaller CL_2-value than $\mathscr{P}$ from Lemma 3. The orthogonality of $\mathscr{P}$ follows. □

Theorem 3 indicates that the conjecture is true when $q=2$, $s \geqslant 3$ and $n=q^{s-1}$. However, defining a new measure of uniformity as

$$[CL_{2,t}(\mathscr{P})]^2 = \sum_{0<|u|\leqslant t} I_u(\mathscr{P})^2,$$

we have

Theorem 4. *A $\mathscr{U}$-uniform design $U_n(q^s)$ under $CL_{2,t}$, where $t < s, n$ is a multiple of q^t and q equals 2 or q is odd, is an orthogonal array $\mathrm{OA}(n; q^s; t)$, if the latter exists.*

The proof of this theorem is based on the following Lemma whose proof is similar to that of Theorem 1.

Lemma 4. *Under the assumption of Theorem 1, when $q=2$ or q is odd, $\mathscr{P}$ minimizes $I_s(\mathscr{P})$ over $\mathscr{P}(n, q^s)$ if and only if $\boldsymbol{y}(\mathscr{P}) = (n/q^s)\mathbf{1}$.*

4. Conclusion and discussion

In this paper, we have shown that the conjecture proposed by FLWZ is true if the lattice design is complete and the number of levels is 2 or odd or if the lattice design has $n=2^{s-1}$ runs with each factor having 2 levels. The conjecture is also true for even q and $s=1,2$. The conjecture is not true when the design is complete with even number of levels (with the exception of 2) and $s>2$. In fact, all the above cases produce OA of strength s or $s-1$. So the question is: is there a discrepancy function that yields an OA of strength 2? The answer in this note is yes — the function $CL_{2,t}(\mathscr{P})$ with $t=2$. We also show that the conjecture is true in the cases of $q=2$ or q odd, if we choose $CL_{2,t}$ as the measure of uniformity.

The conjecture also opens a number of further research problems. First, there are many useful measures of uniformity in the literature (see Hickernell, 1998). We might choose another measure such that a close relationships between orthogonality and uniformity can be obtained. Second, Ma and Fang (1998) proposed a new concept of *uniformly orthogonal design*: a design that is both orthogonal and uniform (under a given measure of uniformity). They found that the uniformly orthogonal design has good properties in confounding and estimation. A further study on uniformly orthogonal designs is currently under investigation by the authors.

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