Discrete Discrepancy and Its Application in Experimental Design

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Summary. Discrepancy is a kind of important measure used in experimental design. Recently, a so-called discrete discrepancy has been applied to evaluate the uniformity of factorial designs. In this paper, we review some recent advances on application of the discrete discrepancy to several common experimental designs and summarize some important results.

Key words: Block design; discrepancy; factorial design; generalized minimum aberration; minimum moment aberration; orthogonality; uniformity; uniform design; supersaturated design.

2000 Mathematics Subject Classification: 62K15, 62K05, 62K99.

1 Introduction

Discrepancy has been employed to many fields of statistics, in particular, to experimental design. Based on discrepancy, Wang & Fang (1981) and Fang & Wang (1994) proposed a kind of novel experimental design, called uniform design, which favors a design with the smallest discrepancy value. In view of geometry, a uniform design spreads its experimental points uniformly over the experimental domain. Uniformity is an important concept related to uniform designs. Several important and popular measures of uniformity are discrepancies, such as the star discrepancy

Contemporary Multivariate Analysis and Experimental Design—In Honor Celebration of Professor Kai-Tai Fang's 65th birthday. Edited by Jianqing Fan and Gang Li. The World Scientific Publisher, 2005.

and the L_p-star discrepancy, etc, in the Quasi-Monte Carlo methods. The star discrepancy, introduced by Weyl (1916), measures the difference between the empirical distribution $F_n(x)$ of the set of design points, $P = \{z_1, \ldots, z_n\}$ in the unit hypercube $C^m = [0,1]^m$, and the uniform distribution $F_*(x)$ on C^m, and has been used in goodness-of-fit test named as the Kolmogorov-Smirov statistic. However, the star discrepancy is not easy to compute. The *L_p-star discrepancy*, viewed as an extension of the star discrepancy, has been widely used in Quasi-Monte Carlo methods. The set P is associated with an $n \times m$ matrix, $X_P = (x_{ki})$. It is well known that the L_p-star discrepancy is invariant to the permutation of rows and columns of X_P, but it is not invariant if the hypercube C^m is rotated by mapping x_{ki} to $1 - x_{ki}$. When n is small, the star discrepancy is not sensitive enough while the L_p-star discrepancy ignores differences between $F_n(x)$ and $F_*(x)$ in any low dimensional manifold. Unreasonable results of the L_2-star discrepancy may be easy found through many sets of points. Therefore, by using reproducing kernels in Hilbert space, Hickernell (1998a), Hickernell (1998b) proposed several modified versions of the L_p-star discrepancy, such as the centered L_p-discrepancy and the wrap-around L_p-discrepancy. These discrepancies can overcome the weakness of the L_p-star discrepancy mentioned above. In particular, when $p = 2$, analytical expressions of the centered L_2-discrepancy (CD, for short) and the wrap-around L_2-discrepancy (WD, for short) have also been obtained by Hickernell (1998a), Hickernell (1998b). The statistical justification for the CD/WD serving as a measure of uniformity for fractional factorial designs with two- or three-level has been interpreted by Fang & Mukerjee (2000), Fang, Lin, Winker & Zhang (2000), Ma & Fang (2001), Fang (2002), Fang & Ma (2002), Fang, Ma & Mukerjee (2002), Fang, Lin & Qin (2003), Ma, Fang & Lin (2003), Qin (2003), Fang & Qin (2004), Chatterjee, Fang & Qin (2004a) and Chatterjee, Fang & Qin (2004b).

Note that the above discrepancies are defined in a unite hypercube domain and used for measuring the uniformity of points corresponding to continuous variables. However, for factorial designs the number of possible levels for each factor may be restricted to a finite number. For example, a factor may have only two values (low and high) or three values (low, medium and high). In these situations it is reasonable to represent the experimental domain $\mathcal{X}$ as a discrete set, e.g., $\mathcal{X} = \{0, 1, \ldots, q_1 - 1\} \times \cdots \times \{0, 1, \ldots, q_m - 1\}$ for mixed levels. Liu & Hickernell (2002b) provided some justification for directly using the discrepancy defined on a discrete domain instead of on a continuous domain as a measure of uniformity of such design points. By using a reproducing kernel in Hilbert space, the so-called *discrete discrepancy* (DD, for short) was directly defined on such a discrete domain by Hickernell & Liu (2002), Liu & Hickernell (2002a), Liu (2002) and Fang, Lin & Liu (2003). Comparing with other discrepancies mentioned above, the DD not only enormously reduces the computational cost, particularly in constructing uniform designs, but also has itself statistical properties.

The main purpose of this paper is to review some recent developments on the application of the discrete discrepancy to experimental design.

2 Discrete discrepancy

We begin with a brief review of the discrete discrepancy. Let $\mathcal{X}$ be a measurable subset of $\boldsymbol{R}^m$. A kernel function $K(\boldsymbol{x}, \boldsymbol{w})$ is any real-valued function defined on $\mathcal{X} \times \mathcal{X}$, and is symmetrical in its arguments and non-negative definite, i.e.,

$$K(\boldsymbol{x}, \boldsymbol{w}) = K(\boldsymbol{w}, \boldsymbol{x}), \text{ for any } \boldsymbol{x}, \boldsymbol{w} \in \mathcal{X} \quad \text{and} \tag{1}$$

$$\sum_{i,j=1}^{n} a_i a_j K(\boldsymbol{x}^i, \boldsymbol{x}^j) \geq 0, \text{ for } a_i \in R, \ \boldsymbol{x}^i \in \mathcal{X}, \ i = 1, \ldots, n. \tag{2}$$

Let F_* denote the uniform distribution function on $\mathcal{X}$, $P = \{\boldsymbol{z}_1, \ldots, \boldsymbol{z}_n\} \subseteq \mathcal{X}$ be a set of design points and F_n denote the empirical distribution of P, where

$$F_n(\boldsymbol{x}) = \frac{1}{n} \sum_{\boldsymbol{z} \in P} 1_{\{\boldsymbol{z} \leq \boldsymbol{x}\}}.$$

Here $\boldsymbol{z} = (z_1, \ldots, z_m) \leq \boldsymbol{x} = (x_1, \ldots, x_m)$ means that $z_j \leq x_j$ for all j, 1_A is the indicator function of A. For a given kernel function $K(\boldsymbol{x}, \boldsymbol{w})$, the discrepancy of P is defined as

$$\begin{aligned} D(P; K) &= \left\{ \int_{\mathcal{X}^2} K(\boldsymbol{x}, \boldsymbol{w}) d[F_*(\boldsymbol{x}) - F_n(\boldsymbol{x})] d[F_*(\boldsymbol{w}) - F_n(\boldsymbol{w})] \right\}^{\frac{1}{2}} \\ &= \left\{ \int_{\mathcal{X}^2} K(\boldsymbol{x}, \boldsymbol{w}) dF_*(\boldsymbol{x}) dF_*(\boldsymbol{w}) - \frac{2}{n} \sum_{\boldsymbol{z} \in P} \int_{\mathcal{X}} K(\boldsymbol{x}, \boldsymbol{z}) dF_*(\boldsymbol{x}) \right. \\ &\quad \left. + \frac{1}{n^2} \sum_{\boldsymbol{z}, \boldsymbol{z}' \in P} K(\boldsymbol{z}, \boldsymbol{z}') \right\}^{\frac{1}{2}}. \end{aligned}$$

From the above definition, it is clear that the discrepancy measures how far apart the empirical distribution F_n is from the population distribution F_*. Consequently, for a fixed number of points, n, a design with low discrepancy is preferred. Several kernel functions were proposed and discussed by Hickernell (1998a,b; 2000).

Let d denote a factorial design with n runs and m factors, where the ith factor has q_i levels. The experimental domain $\mathcal{X} = \{0, 1, \ldots, q_1 - 1\} \times \cdots \times \{0, 1, \ldots, q_m - 1\}$ is formed by all possible $\prod_{i=1}^{m} q_i$ level-combinations of the m factors, F_* is the discrete uniform distribution on $\mathcal{X}$. For notational convenience in this paper we define for given $a > 0, \rho > 1$,

$$\widetilde{K}(x_j, w_j) = \begin{cases} a\rho & \text{if } x_j = w_j, \\ a & \text{if } x_j \neq w_j, \end{cases} \quad \text{for } x_j, w_j \in \{0, 1, \ldots, q_j - 1\}, \tag{3}$$

and

$$K(\boldsymbol{x}, \boldsymbol{w}) = \prod_{j=1}^{m} \widetilde{K}(x_j, w_j), \tag{4}$$

for any $\boldsymbol{x} = (x_1, \ldots, x_m)$ and $\boldsymbol{w} = (w_1, \ldots, w_m) \in \mathcal{X}$. Then $K(\boldsymbol{x}, \boldsymbol{w})$ is a kernel function. In particular, it satisfies conditions (1) and (2). The corresponding *discrete discrepancy*, denoted by $D(d; a, \rho)$, can be used for measuring the uniformity of design points over the domain $\mathcal{X}$ (Hickernell & Liu (2002); Liu & Hickernell (2002a)).

Consider the set, denoted by $\mathcal{D}(n; q_1 \cdots q_m)$, of asymmetrical factorials with n runs and m factors, where the ith factor has q_i levels, q_i is any positive integer ($\geq$ 2) and the n level-combinations are not necessarily distinct. If some q_i's are equal, we denote it by $\mathcal{D}(n; q_1^{s_1} \cdots q_r^{s_r})$, where $\sum_{i=1}^{r} s_i = m$. U-type designs play a key role in construction of uniform designs. A design d is called *U-type* if levels of each factor appear equally often (Fang, Lin, Winker & Zhang (2000)). Following Fang, Lin & Liu (2003) and Qin & Fang (2004), the squared DD-value, $(D(d; a, b))^2$, can be calculated as follows:

$$(D(d; a, b))^2 = -\prod_{i=1}^{m} \frac{(\rho + q_i - 1)a}{q_i} + \frac{(a\rho)^m}{n} + \frac{2a^m}{n^2} \sum_{k=1}^{n} \sum_{l=k+1}^{n} \rho^{\sigma_{kl}},$$

where σ_{ij} is the coincidence number between the ith and jth rows of d.

A lower bound of $D(d; a, b)$ over U-type designs in $\mathcal{D}(n; q_1 \cdots q_m)$ is given in the following theorem. A necessary and sufficient condition for a design reaching this lower bound is obtained also.

Theorem 1. *Let $d \in \mathcal{D}(n; q_1 \cdots q_m)$ be a U-type design. Then*

$$(D(d; a, \rho))^2 \geq L^A(d; a, \rho), \tag{5}$$

where

$$L^A(d; a, \rho) = -\prod_{i=1}^{m} \frac{(\rho + q_i - 1)a}{q_i} + \frac{(a\rho)^m}{n} + \frac{(n-1)[1 + (\rho - 1)(\sigma - \gamma)]a^m \rho^\gamma}{n},$$

$\sigma = \sum_{i=1}^{m} (n/q_i - 1)/(n-1)$ and γ is the integer part of σ. The lower bound of $L^A(d; a, \rho)$ can be achieved if and only if for any run d^k of d, among the $(n-1)$ values of σ_{kl} $(l \neq k)$, there are $(n-1)(\gamma+1-\sigma)$ with the value γ and $(n-1)(\sigma-\gamma)$ with the value $\gamma + 1$.

One lower bound of $D(d; a, \rho)$ for symmetrical design $d \in \mathcal{D}(n; q^m)$ can be obtained from Theorem 1. Recently, Qin & Li (2003) obtained the following lower bound of $D(d; a, \rho)$ for a design $d \in \mathcal{D}(n; q^m)$, which is sharper than the lower bound obtained from Theorem 1.

Theorem 2. *Let $d \in \mathcal{D}(n; q^m)$. Then*

$$(D(d; a, \rho))^2 \geq L^C(d; a, \rho),$$

where

$$L^C(d; a, \rho) = \frac{a^m}{n^2} \sum_{v=1}^{m} \binom{m}{v} (\rho - 1)^v R_{n,v,q} \left(1 - \frac{R_{n,v,q}}{q^v}\right),$$

$R_{n,v,q}$ is the residual of n (mod q^v).

Note that Theorems 1 and 2 hold for a wide range of DD measures in which the kernel satisfies (4), no matter what the values of a and ρ ($a > 0, \rho > 1$) are. The lower bound $L^A(d; a, \rho)$ or $L^C(d; a, \rho)$ can be used as a benchmark for searching uniform designs. A design $d \in \mathcal{D}(n; q_1 \cdots q_m)$ is called a *uniform design* under $D(d; a, \rho)$ if its DD value $D(d; a, \rho)$ achieves the minimum value over $\mathcal{D}(n; q_1 \cdots q_m)$. Based on Theorem 1 or 2, a design $d \in \mathcal{D}(n; q_1 \cdots q_m)$ or $\mathcal{D}(n; q^m)$ in which the squared DD-value equals the lower bound $L^A(d; a, \rho)$ or $L^C(d; a, \rho)$ is obvious a uniform design. In this paper, the uniformity criterion favors designs with the smallest discrete discrepancy.

3 Statistical inference for uniform designs measured by DD

3.1 Robustness of uniform designs measured by DD

At the initial stage of an experiment, it is often the case that a practitioner does not have enough information about models concerning the response and factors. Therefore, it is important to use a factorial design that is robust against the underlying model specifications. Since the uniform design spreads the design points evenly in the design space, it usually has robust performance with different modelling methods. Wiens (1991) gave two optimality properties of uniform designs. Hickernell (1999) and Yue & Hickernell (1999) proved that the uniform design is optimal and robust for approximate linear regression methods. Moreover, Xie & Fang (2000) proved that the uniform design is admissible and minimax under a certain sense in nonparametric regression model. Recently, Hickernell & Liu (2002) reported that although it is rare for a single design to be both maximally efficient and robust, uniform designs may limit the effects of aliasing to yield reasonable efficiency and robustness together.

3.2 Connections between DD and GMA/MMA

Minimum aberration (Fries & Hunter (1980); Franklin (1984)) and generalized minimum aberration (GMA, for short) (Tang & Deng (1999); Ma & Fang (2001); Xu & Wu (2001)) have become the popular and standard criteria for optimal factor assignment. Recently, Xu (2003) proposed the minimum moment aberration (MMA, for short) criterion to evaluate optimal factor assignment. Relationship between uniformity and aberration, which may raise the hope of improving the connection between uniform design theory and factorial design theory, has received a great deal of attention. The work of Fang & Mukerjee (2000) was a first attempt towards providing an analytic link between uniformity measured by CD and the word-length pattern of regular 2^{s-k} factorials. Fang & Ma (2002) and Fang, Ma & Mukerjee (2002) gave extensions of previous works for three- and higher-level factorials, respectively. For the discrete discrepancy, Qin & Fang (2004) obtained similar conclusions as follows.

Theorem 3. *Let $d \in \mathcal{D}(n; q_1 \cdots q_m)$. Then*

$$(D(d; a, \rho))^2 = \prod_{i=1}^{m} \frac{(\rho + q_i - 1)a}{q_i} \sum_{(j_1,\ldots,j_m)\in\mathcal{S}} \prod_{i=1}^{m} \left(\frac{\rho - 1}{\rho + q_i - 1}\right)^{j_i} \cdot C^*_{j_1\cdots j_m}(d),$$

where $C^*_{j_1\cdots j_m}(d)$'s are the MacWilliams transforms of the distance distribution of d, $\mathcal{S} = \{(j_1, \ldots, j_m) : 0 \le j_i \le 1, 1 \le i \le m, (j_1, \ldots, j_m) \ne (0, \ldots, 0)\}$.

Corollary 1. *Let $d \in \mathcal{D}(n; q^m)$. Then*

$$(D(d; a, b))^2 = \left(\frac{(\rho + q - 1)a}{q}\right)^m \sum_{j=1}^{m} \left(\frac{\rho - 1}{\rho + q - 1}\right)^j A_j^{xw}(d),$$

where $A_j^{xw}(d) = \sum_{j_1+\cdots+j_m=j} C^*_{j_1\cdots j_m}(d)$, $(A_1^{xw}(d), \ldots, A_m^{xw}(d))$ is called the generalized word-length pattern by Xu & Wu (2001).

From Theorem 3 noting that the coefficient of $C^*_{j_1\cdots j_m}(d)$ in $(D(d; a, \rho))^2$ decreases exponentially with $(j_1, \ldots, j_m)$, we anticipate that factorials which keep $A^{xw}_{j_1+\cdots+j_m}(d)$ small for small values of $j_1 + \cdots + j_m$, that is those having less aberration, should behave well in terms of uniformity in the sense of keeping $(D(d; a, \rho))^2$ small. This shows that uniform designs under the DD and GMA designs are strongly related to each other, and provides a justification for the criterion of GMA by consideration of uniformity measured by the DD. Theorem 3 also shows us that the uniformity criterion does not completely agree with the GMA criterion. However, Qin & Fang (2004) indicated that for asymmetrical factorials, a special kind of uniform design has MMA, and uniform designs, MMA designs and GMA designs are equivalent in a special class of symmetrical factorials.

Recently, Hickernell & Liu (2002) defined a *projection discrepancy pattern* and proposed a *minimum projection uniformity* (MPU, for short) criterion in terms of this pattern, which considers the uniformity of low-dimensional projections of a design. Based on a specific kernel $K(x, w)$ raised for asymmetrical factorial designs, the t-dimensional projection discrepancy $D_{(t)}(d; K)$ of a design $d = (d_{ij})$ is defined as

$$(D_{(t)}(d; K))^2 = \frac{1}{n^2} \sum_{|u|=t} \sum_{i,j=1}^{n} \prod_{l\in u} \left(-1 + q_l \delta_{d_{il} d_{jl}}\right), \tag{6}$$

where u is any subset of the set $\{1, \ldots, m\}$, $|u|$ denotes the cardinality of u, δ_{xw} denotes the Kronecker delta function, i.e., $\delta_{xw} = 1$ if $x = w$ and $\delta_{xw} = 0$ otherwise. The vector

$$\mathrm{PD}(d; K) = (D_{(1)}(d; K), \ldots, D_{(m)}(d; K))$$

is called the projection discrepancy pattern, and the MPU criterion is to sequentially minimize $D_{(t)}(d; K)$ for $t = 1, \ldots, m$. Based on (6), Hickernell & Liu (2002) showed that

Theorem 4. *Let $d \in \mathcal{D}(n; q_1 \cdots q_m)$, then $(D_{(t)}(d; K))^2 = A_t^{xw}(d)$, i.e. the MPU is equivalent to the GMA defined by Xu & Wu (2001). For the case of 2-level designs, the MPU is equivalent to the* minimum G_2-aberration *of Tang & Deng (1999).*

And their results show that the MPU criterion may be further generalized to cover designs that are not fractional factorials by using the discrepancy. It is also shown that minimum aberration designs and minimum discrepancy designs are equivalent in a certain limit.

3.3 Connection between DD and orthogonality

We know that strength is a good measure of orthogonality for factorial designs. Liu (2002) studied the connection between uniformity and strength. Taking $a = 1+\tau\beta$ and $a\rho = 1 + \beta$, where $\beta > 0$ and $-1/(q-1) < \tau < 1$ in (3), Liu (2002) obtained the following relation between discrepancies of an orthogonal array (Hedayat, Sloane & Stufken (1999)) on its low-dimensional projections and its strength.

Theorem 5. *Let $d = (d_{ij}) \in \mathcal{D}(n; q^m)$, then*
(i) $D_{(t)}(d; a, \rho) = 0$ if and only if d is an $OA(n, m, q, t)$, where

$$(D_{(t)}(d; a, \rho))^2 = -\left[\frac{\beta(1+(q-1)\tau)}{q}\right]^t + \frac{\beta^t}{n^2} \sum_{|u|=t} \sum_{i,j=1}^{n} \prod_{l \in u} \tau^{1-\delta_{d_{il}d_{jl}}}.$$

(ii) $D(d; a, \rho) = 0$ if and only if d is an $OA(n, m, q, m)$ (here n must be a multiple of q^m).

Liu (2002) also showed that symmetrical saturated orthogonal arrays are the most uniform one among all the saturated factorial designs with the same parameters.

Recently, some new criteria, such as the B-criterion (Fang, Lu & Winker (2003)) and O-criterion (Fang, Ma & Mukerjee (2002)), have been utilized to measure and evaluate the orthogonality of factorial designs. These criteria can be viewed as extensions of the concept of strength in orthogonal array. For any t columns of $d \in \mathcal{D}(n; q^m)$, say $c_{l_1}, \ldots, c_{l_t}$, let $n_{\alpha_1 \cdots \alpha_t}^{(l_1 \cdots l_t)}$ be the number of runs in which $(c_{l_1}, \ldots, c_{l_t})$ takes the level-combination $(\alpha_1 \cdots \alpha_t)$, let

$$B_{l_1 \cdots l_t}(d) = \sum_{\alpha_1, \ldots, \alpha_t} \left(n_{\alpha_1 \cdots \alpha_t}^{(l_1 \cdots l_t)} - \frac{n}{q^t}\right)^2,$$

where the summation is taken over all possible level-combinations, and define

$$B_t(d) = \sum_{1 \le l_1 < \cdots < l_t \le m} B_{l_1 \cdots l_t}(d) \Big/ \binom{m}{t},$$

the *B-criterion* is to minimize $B_t(d)$ for $t = 1, \ldots, m$ sequentially. For symmetrical designs, Qin & Chen (2004) showed that B-criterion is equivalent to GMA. Qin & Li (2003) indicated that B-criterion and O-criterion are mutually equivalent, and gave the following connection between DD and B-criterion.

Theorem 6. *Let $d \in \mathcal{D}(n; q^m)$. Then*

$$(D(d; a, \rho))^2 = \frac{(a\rho)^m}{n^2} \sum_{v=1}^{m} \binom{m}{v} (\rho - 1)^v B_v(d).$$

3.4 Connection between DD and CD/WD

As mentioned in Section 1, usefulness of uniformity measured by the CD/WD in two- or three-level factorials has been discussed. The definitions and computation formulas for the CD and WD can refer to Hickernell (1998a) and Hickernell (1998b). For $d \in \mathcal{D}(n; q^m)$, its CD and WD are denoted by $CD(d)$ and $WD(d)$ respectively. Recently, Qin & Fang (2004) gave the following result, which connect the DD with the CD and WD.

Theorem 7. *For any design $d \in \mathcal{D}(n; q^m)$, we have the following equations:*
(i) when $q = 2$, $\rho = 5/4$ and $a = 1$,

$$(D(d; a, \rho))^2 = (CD(d))^2 + 2(35/32)^m - (13/12)^m - (9/8)^m;$$

(ii) when $q = 2$, $\rho = 6/5$ and $a = 5/4$,

$$(D(d; a, \rho))^2 = (WD(d))^2 + (4/3)^m - (11/8)^m;$$

(iii) when $q = 3$, $\rho = 27/23$ and $a = 23/18$,

$$(D(d; a, \rho))^2 = (WD(d))^2 + (4/3)^m - (73/54)^m.$$

It is well known that there is yet an open problem whether uniformity measured by the CD/WD may be utilized as a criterion for assessing factorials with high levels. However, the DD can be used to compare symmetrical and asymmetrical factorials with high levels. Hence, the DD can be regarded as a kind of generalization of the CD and WD. We strongly recommend to use the discrete discrepancy as a measure of uniformity for comparing fractional factorials in most cases.

3.5 Connection between DD and balance

Block design is an important kind of experimental design. Its basic ideas come from agricultural and biological experiments. But now the applications of these ideas are found in many areas of sciences and engineering. The most widely-used one is the balanced incomplete block (BIB, for short) design in which every pair of treatments occurs altogether in exact the same number of blocks. Another important one is the resolvable incomplete block (RIB, for short) design. For a thorough discussion of block designs, please refer to Dey (1986).

As we know the definitions in block designs reflect some "*balance*" among the treatments, the blocks, or the parallel classes. This kind of balance is easy to be accepted intuitively. While in existed works on block designs the criterion of balance is introduced from the estimation point of view. In fact the balance criterion can be regarded as a kind of *uniformity*. Recently, Liu & Chan (2004) and Liu & Fang (2004) studied the uniformity of block designs and obtained some satisfactory results. Liu & Chan (2004) used the DD measure to prove theoretically that BIB designs are the most uniform ones among all binary incomplete block designs. This is an important characteristic of BIB designs in terms of uniformity. While Liu & Fang (2004) obtained a sufficient and necessary condition under which a certain kind of RIB design is the most uniform one in the sense of the DD measure, and showed that this uniform design is connected. They also proposed a construction method for such designs via a kind of U-type designs. This method sets up an important bridge between this kind of RIB designs and U-type designs. All these results confirm our judgement that the "*balance*" criterion can be regarded as a kind of *uniformity*. Note that these results are obtained in the sense of the DD measure, but they also holds for any of the modified L_2-discrepancies proposed by Hickernell (1998a) and Hickernell (1998b).

4 Application of the DD in supersaturated designs

In the context of factorial designs, there has been recent interest in the study of the *supersaturated design* (SSD, for short). Whenever the run size of a design is insufficient for estimating all the main effects represented by the columns of the design matrix, the design is called supersaturated. In industrial statistics and other scientific experiments, especially in their preliminary stages, very often there are a large number of factors to be studied and the run size is limited because of cost. However, in many situations only a few factors are believed to have significant effects. Under this assumption of *effect sparsity* (Box & Meyer (1986)), SSDs can be used effectively, allowing the simultaneous identification of the active factors.

4.1 Connection between DD and $E(s^2)$ in 2-level SSDs

Most studies on SSDs have focused on the 2-level case. Booth & Cox (1962), in the first systematic construction of SSDs, proposed the $E(s^2)$ *criterion*, which is a measure of *non-orthogonality* under the assumption that *only two out of the m* factors are active. After Booth & Cox (1962), there was not much work on the subject of SSDs until Lin (1993). Other recent work focusing on constructions of $E(s^2)$-optimal SSDs includes, e.g. Liu & Zhang (2000), Butler, Mead, Eskridge & Gilmour (2001), Liu & Dean (2004) and the references therein.

Recently, Liu & Hickernell (2002a) showed that the $E(s^2)$ criterion shares the same optimal designs with the DD criterion. They constructed a DD, i.e. taking $a = 1 + \tau\beta$ and $a\rho = 1 + \beta$ ($\beta > 0, -1 \leq \tau < 1$) in (3), and showed that for 2-level factorial designs both $E(s^2)$ and the DD can be expressed in terms of the *Hamming distances* (or the *coincidence numbers*) between any two runs of the design. These expressions in terms of Hamming distances lead to a lower bound on $E(s^2)$ and the lower bound of (5) on DD for 2-level SSDs. It is interesting to note that if a design d can attain one of these lower bounds, then it attains both of them. In other words, an $E(s^2)$-optimal design is also uniform (minimal discrepancy) for the DD. They further showed that in what cases these lower bounds can be achieved, even though the DD is *not* equivalent to the $E(s^2)$ criterion.

Theorem 8. *Let d be a 2-level design with n runs and m factors, where each column has the same number of ± 1 elements. Suppose that $\tau\beta > -1$, and that $m = c(n-1) + e$ for $e = -1, 0$ or 1. Also, suppose that either a) n is a multiple of 4 and there exists an $n \times n$ Hadamard matrix, or b) c is even and there exists a $2n \times 2n$ Hadamard matrix. Then the lower bounds of $E(s^2)$ and DD can be attained.*

Moreover, the DD is a more general, and thus more flexible criterion than $E(s^2)$. For example, $E(s^2)$ ignores possible interactions of more than one factor. However, the DD includes interactions of all possible orders, and their importance may be increased or decreased by changing the value of β.

4.2 Connection between DD and $E(f_{NOD})$ in mixed-level SSDs

Two-level SSDs can be used for screening the factors in simple linear models. When the relationship between a set of factors and a response is nonlinear, or approximated by a polynomial response surface model, designs with multi-level and mixed-level are often required, e.g., to exploring nonlinear effects of the factors. Recently, Fang, Lin & Liu (2003) proposed a new criterion, called the $E(f_{NOD})$ *criterion*, for comparing SSDs. For a design $d \in \mathcal{D}(n; q_1 \cdots q_m)$, the criterion is defined as minimizing

$$E(f_{NOD}) = \sum_{1 \le i < j \le m} f_{NOD}^{ij} \Big/ \binom{m}{2},$$

where

$$f_{NOD}^{ij} = \sum_{u=1}^{q_i} \sum_{v=1}^{q_j} \left(n_{uv}^{(ij)} - \frac{n}{q_i q_j} \right)^2,$$

$n_{uv}^{(ij)}$ is the number of (u, v)-pairs in the ith and jth columns. Here, the subscript NOD stands for *non-orthogonality* of the design. Fang, Lin & Liu (2003) obtained a lower bound for $E(f_{NOD})$ which can serve as a benchmark of design optimality. They also studied the connection between DD and $E(f_{NOD})$. Fang, Ge, Liu & Qin (2004a) provided the following lower bound and the sufficient and necessary condition to achieve it for $E(f_{NOD})$, which includes the bound and condition of Fang, Lin & Liu (2003) as a special case.

Theorem 9. *Let $d \in \mathcal{D}(n; q_1 \cdots q_m)$ be a U-type design, then*

$$E(f_{NOD}) \ge \frac{n(n-1)}{m(m-1)} \left[(\gamma + 1 - \sigma)(\sigma - \gamma) + \sigma^2 \right] + C(n, q_1, \ldots, q_m), \qquad (7)$$

where $C(n, q_1, \ldots, q_m) = \frac{nm}{m-1} - \frac{1}{m(m-1)}\left(\sum_{i=1}^m \frac{n^2}{q_i} + \sum_{1 \le i \ne j \le m} \frac{n^2}{q_i q_j}\right)$, σ, γ *and the sufficient and necessary condition for the lower bound to be achieved are the same as those of Theorem 1.*

Thus we conclude that

Theorem 10. *Let* $d \in \mathcal{D}(n; q_1 \cdots q_m)$ *be a U-type design, then* d *is a uniform design with its squared DD-value achieving the lower bound on the right hand side of (5) if and only if* d *is* $E(f_{NOD})$*-optimal with its* $E(f_{NOD})$ *achieving the lower bound on the right hand side of (7).*

Theorem 10 leads to a strong relation between $E(f_{NOD})$ optimality and uniformity measured by the DD of any SSD. The uniformity of $E(s^2)$- and ave χ^2-optimal (Yamada & Lin (1999)) SSDs can be obtained directly based on this theorem, as special cases of SSDs with equal-level factors.

4.3 Constructions of uniform SSDs measured by DD

To find uniform designs is an NP hard problem. There are several methods to construct uniform designs in literature, such as the good lattice method (Fang & Wang (1994)), Latin square method (Fang, Shiu & Pan (1999)) and optimization searching method (Fang, Ma & Winker (2002)). In these methods, computer algorithms play an important role to obtain uniform designs.

Recently, some combinatorial methods are introduced to construct uniform U-type designs in terms of DD as well as $E(f_{NOD})$. Note that in most cases, uniform U-type designs are supersaturated. So this kind of U-type designs are also called the *uniform SSDs*. Many infinite classes for the existence of uniform designs with the same Hamming distances between any distinct rows are also obtained simultaneously. These combinatorial approaches can be summarized as follows:

I. Constructing symmetrical uniform SSDs from

a. Resolvable balanced incomplete block designs, see Fang, Ge & Liu (2002b), Fang, Ge, Liu & Qin (2003);
b. Room squares, see Fang, Ge & Liu (2002a);
c. Resolvable packings and coverings, see Fang, Ge & Liu (2004) and Fang, Lu, Tang & Yin (2004);
d. Super-simple resolvable *t-designs*, see Fang, Ge, Liu & Qin (2004b).

II. Constructing asymmetrical uniform SSDs from

a. Resolvable group divisible designs, see Fang, Ge, Liu & Qin (2004a);
b. Latin squares, see Fang, Ge, Liu & Qin (2004a);
c. Resolvable partially pairwise balanced designs, see Fang, Tang & Yin (2004);
d. Other uniformly resolvable designs, see Fang, Ge, Liu & Qin (2004a).

In addition, Fang, Lin & Liu (2003) proposed a method by fractionalizing saturated orthogonal arrays for constructing asymmetrical uniform SSDs. The properties of the resulting uniform SSDs were also investigated in those papers.

5 Concluding remarks

Uniform experimental design has been widely used in many fields in the last two decades. Discrepancy is a measurement of the uniformity and is a criterion in experimental design. In this paper, we review the recent developments on the discrete discrepancy and summarize some important results. The uniformity of the common experimental designs, such as factorial design, orthogonal design, block design and supersaturated design, are also discussed in this paper. All these results show that orthogonality (non-orthogonality) and balance are strongly related to uniformity, and the discrete discrepancy plays an important role in evaluating such experimental designs.

Acknowledgements

The authors are grateful to Professors Kai-Tai Fang and Fred J. Hickernell for their helpful comments and suggestions. Thanks also go to the Editors and one anonymous Referee for their valuable comments. This work was partially supported by the National Natural Science Foundation of China (Grant Nos. 10171051, 10301015), the Outstanding Scholar Program of Nankai University, the Key Project of Chinese Ministry of Education, the Project-sponsored by SRF for ROCS (SEM) and the NSF of Hubei Province.

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