Uniform Designs and Their Combinatorial Constructions

Jianxing Yin[1], Kai-Tai Fang[2], Yu Tang[1,2]

[1]Department of Mathematics
Suzhou University
Suzhou 215006, P. R. China

[2]Department of Mathematics
Hong Kong Baptist University
Hong Kong, P. R. China

Abstract Uniform designs has been widely used in various fields. In this talk, two constructions for uniform designs from combinatorics are presented. One is obtained by resolvable PPBDs which serves to unify some known combinatorial constructions. The other provides a recursive method to obtain a new three-level uniform design from old one.

Keywords: combinatorial construction; discrepancy; uniform design

1. Introduction

Uniform design was motivated by three projects in system engineering in 1978 (see Fang (1980) and Wang and Fang (1981)). It has been widely used in various fields, such as industry, system engineering, pharmaceutics, and natural sciences (see Fang and Lin (2003) and Fang *et al.* (2000)). Generally speaking, uniform design is a type of "space filling" design for computer experiments (Bates *et al.* (1996)). However, If we restrict the domain to certain lattice points, then uniform design is also a fractional factorial design. Many criteria for measuring discrepancy of designs have been proposed in the literature. See, for example, Hickernell (1998a) and Hickernell (1998b). A fractional factorial design is referred to as a uniform design if it achieves the smallest value under a certain measure of discrepancy.

There are several methods to construct uniform designs such as *the good lattice method* (Wang and Fang (1981), Fang and Wang (1994)), *Latin square method* (Fang, Shiu and Pan (1999)), *expending orthogonal design method* (Fang (1995)), *optimization searching method* (Winker and Fang (1998), Fang, Ma and Winker (2002)). However, most of these methods are limited to obtain uniform designs with small number of runs. A relatively effective method for constructing uniform designs with modest and large scale is established via combinatorial configurations. The goal of this talk is to present two constructions for uniform designs from combinatorics. One is obtained by resolvable PPBDs which serves to unify some known combinatorial constructions. The other provides a recursive method to obtain a new three-level uniform design from old one.

2. The Construction via Resolvable PPBDs

To present our constructions we require some combinatorial terminology. Let us first define the notion of a partially pairwise balanced design (PPBD) which is resolvable.

Let K be a set of positive integers and I a set of nonnegative integers. By an (n, K, I)-partially pairwise balanced design, or a (n, K, I)-PPBD, we mean a pair $(V, \mathcal{A})$ such that the following properties are satisfied:

1. V is a set of n treatments called points;
2. $\mathcal{A}$ is a family of subsets of V called blocks;
3. each block has size $k \in K$;
4. any pair of distinct points is contained in exactly λ blocks for some $\lambda \in I$.

Suppose that $(V, \mathcal{A})$ is a (n, K, I)-PPBD. A parallel class in $(V, \mathcal{A})$ is a collection of disjoint blocks from $\mathcal{A}$ whose union is V. A partition of $\mathcal{A}$ into parallel classes is called a resolution, and $(V, \mathcal{A})$ is said to be resolvable, denoted by (n, K, I)-RPPBD, if $\mathcal{A}$ has at least one resolution.

In statistical experiment, it is hoped that a factorial design X should contain no fully aliased column, that is, each of its column cannot be obtained from another column by a permutation of levels. In view of this, we require an (n, K, I)-RPPBD to have no identical parallel classes. Such RPPBDs will be denoted by (n, K, I)-$\widetilde{\text{R}}$PPBD. For convenience, we also write $\mathcal{D}(n; m; q_1, q_2, \cdots, q_m)$ for the set of all factorial designs of n runs and m factors with $q_1, q_2, \cdots, q_m$ levels in turn. Obviously, any $X \in \mathcal{D}(n; m; q_1, q_2, \cdots, q_m)$ can be thought of as an $n \times m$ matrix with entries $1, 2, \cdots, q_i$ at the i-th column.

Consider an (n, K, I)-$\widetilde{\text{R}}$PPBD, $(V, \mathcal{A})$. Let V be $\mathrm{I}_n = \{1, 2, \ldots, n\}$. Assume that $\mathcal{A}$ can be partitioned into m parallel classes $\mathcal{A}_1, \mathcal{A}_2, \cdots, \mathcal{A}_m$ where the j-th class contains q_j blocks. Then we can construct a factorial design $X \in \mathcal{D}(n;\, m; q_1, \cdots, q_m)$ from $(V, \mathcal{A})$ in the following way:

1. For each parallel class $\mathcal{A}_j$ $(1 \leq j \leq m)$, assign a natural order $1, 2, \cdots, q_j$ to its q_j blocks in an arbitrary order.
2. For $1 \leq j \leq m$, associate $\mathcal{A}_j$ with a vector of length n, X_j, in such a way that its i-th coordinate $(1 \leq i \leq n)$ has value $w \in \{1, 2, \ldots, q_j\}$ if and only if point i is contained in the w-th block in $\mathcal{A}_j$.

3. Take $X = (X_1^T, X_2^T, \cdots, X_m^T)$, where X_j^T is the transpose of X_j.

Moreover, the inner structure of the $\widetilde{\text{R}}$PPBD ensures that the derived fractional factorial design is uniform. To be precise, if we use the "Discrete Discrepancy" (see, Hickernell (1998a)) as the measure of uniformity, we then have the following theorem. The proof of this theorem was developed in Fang, Tang and Yin (2002).

Theorem 2.1 Let $(V, \mathcal{A})$ be an $(n, K, \{\lambda_1, \lambda_2\})$-$\widetilde{\text{R}}$PPBD satisfying $|\lambda_1 - \lambda_2| \leq 1$. Then the factorial design X derived from $(V, \mathcal{A})$ is a uniform design under "Discrete Discrepancy".

We give a simple example to illustrate the above construction.

Example 2.2 Let $V = \{1, 2, 3, 4, 5, 6\}$. Then the following 4 classes of blocks form a $(6, \{2, 3\}, \{1, 2\})$-$\widetilde{\text{R}}$PPBD:

$$\begin{array}{cccc} \{1,2,3\} & \{1,2,4\} & \{1,5\} & \{1,6\} \\ \{4,5,6\} & \{3,5,6\} & \{2,6\} & \{2,5\} \\ & & \{3,4\} & \{3,4\} \end{array}$$

The derived uniform design is as follows:

row	1	2	3	4
1	1	1	1	1
2	1	1	2	2
3	1	2	3	3
4	2	1	3	3
5	2	2	1	2
6	2	2	2	1

Recent years it has been received much attention the relationship between optimal factorial designs or uniform designs under certain criteria and combinatorial configurations such as pairwise balanced designs (PBDs) and balanced incomplete block designs (BIBDs). Vital papers in this area include Nguyen (1996), Cheng (1997), Liu and Zhang (2000), Lu, Hu and Zheng (2003), Fang et al. (2003a, 2003b) and the references therein.

$\widetilde{\text{R}}$PPBDs are related to many well-known combinatorial configurations which are resolvable. Clearly, if $I = \{\lambda\}$, then an (n, K, I)-RPPBD is nothing else than a resolvable PBD (or RPBD for short). In this case, it is often written as RB$(K, \lambda; n)$. Further, if $K = \{k\}$, it is well-known as a resolvable BIBD (RBIBD) or an RB$(k, \lambda; n)$. Also, if $\lambda_2 = \lambda_1 + 1$, a $(n, K, \{\lambda_1, \lambda_2\})$-RPPBD can be viewed as a resolvable (n, K, λ_2) packing, as well as a resolvable (n, K, λ_1) covering. Therefore, the construction described above serves to unify many known constructions for uniform designs via combinatorial configurations.

It is worth mentioning that a (n, K, I)-RPPBD can exist without any numerical restriction on its parameters, while other combinatorial designs such as RPBDs and RBIBDs are generally restricted by certain congruence conditions on their parameters. Therefore, the construction described above makes also a relaxation of the parameters regarding the existing constructions for uniform designs via combinatorial configurations.

Our construction translates essentially an $(n, K, \{\lambda_1, \lambda_2\})$-$\widetilde{\text{R}}$PPBD with $|\lambda_1 - \lambda_2| \leq 1$ to a uniform design under Discrete Discrepancy. Though research on RPPBDs has mainly concentrated on certain special cases in combinatorial theory, numerous existence results and techniques can be modified to produce a large number of such $\widetilde{\text{R}}$PPBDs which create uniform designs. Here we do not go much deeper. Instead, we will give some examples. Let us first make an example for some small values of n.

Example 2.3 For any $n \in \{4, 5, 6, 7, 8, 9\}$, there exists an $(n, \{2, 3\}, \{1, 2\})$-$\widetilde{\text{R}}$PPBD.

Notes: For these stated values of n, an $(n, \{2, 3\}, \{1, 2\})$-$\widetilde{\text{R}}$PPBD can be constructed directly. For instance, take the set of treatments as Z_8. Then the following 4 parallel classes of blocks form a $(8, \{2, 3\}, \{1, 2\})$-$\widetilde{\text{R}}$PPBD:

$$\begin{array}{llll}
\{0,2,4\} & \{0,1,2\} & \{2,3,6\} & \{1,3,7\} \\
\{1,3,5\} & \{3,4,5\} & \{0,5,7\} & \{0,4,6\} \\
\{6,7\} & \{6,7\} & \{1,4\} & \{2,5\}
\end{array}$$

To make more examples, we need a few auxiliary designs which we define now.

Definition 2.4 A group divisible design (k, λ)-GDD of type g^u is a triple $(V, \mathcal{G}, \mathcal{B})$ which satisfies the following properties:

1. V is a set of cardinality gu called points;
2. $\mathcal{G}$ is a partition of V into u g-subsets called groups;
3. $\mathcal{B}$ is a collection of k-subsets of V (called blocks) such that a group and a block contain at most one common point;
4. every pair of points from distinct groups occurs in exactly λ blocks.

A (k, λ)-GDD is said to be resolvable (RGDD) if its blocks can be partitioned into parallel classes, each of which partitions the point set V.

A (k, λ)-frame of type g^u is a (k, λ)-GDD of type g^u whose blocks can be partitioned into partial parallel classes, each partitioning $V \backslash G$ for some $G \in \mathcal{G}$.

Remarks: It is easy to construct a $(n, \{2, 3\}, \{1, 2\})$-$\widetilde{\text{R}}$PPBD for any integers $n \geq 10$ by the $\widetilde{\text{R}}$PPBDs given in Example 2.2, in conjunction with the existence of a $(3, 1)$-frame of type 6^u (Stinson (1987)), a $(3, 2)$-frame of type 1^u without identical blocks (Shen (1990)) and a $(\{2, 3\}, 1)$-RGDD of type 2^3 with 3 parallel classes of blocks.

Example 2.5 Both an $(n, \{3, 4\}, \{0, 1\})$-$\widetilde{\text{R}}$PPBD with $n \geq 36$ and an $(n, \{2, 3\}, \{0, 1\})$-$\widetilde{\text{R}}$PPBD with $n \geq 18$ exist.

Notes: It is known (see Ling and Ge (2003)) that a $(4, 1)$-RGDD of type 12^u exists for all integers $u \geq 4$ and $u \neq 27$. Delete e $(1 \leq e \leq 12)$ points from a certain group of such a

RGDD. This produces an $(n,\{3,4\},\{0,1\})$-$\widetilde{\text{R}}$PPBD with $n \geq 36$ and $n \notin \{12\cdot 26,\cdots,12\cdot 27\}$. For the outstanding values of n, the $\widetilde{\text{R}}$PPBD can be constructed directly. Start with a $(3,1)$-RGDD of type 6^u with $u \geq 4$ (see Rees (1993)). and employ the same technique as above to get an $(n,\{3,4\},\{0,1\})$-$\widetilde{\text{R}}$PPBD with $n \geq 18$.

Example 2.6 Let $n \geq 5$ and $n \equiv 0 \bmod 12$. Then there exists an $(n,\{3,4\},\{1,2\})$-$\widetilde{\text{R}}$PPBD.

Notes: It was proved (see Ge (2001))that a $(4,1)$-frame of type 12^u exists for $u \geq 5$. Replacing each group of such an RGDD with a copy of a $\widetilde{\text{R}}\text{B}(3,2;12)$ gives us the $\widetilde{\text{R}}$PPBD, as desired.

3. The Recursive Construction

In this section, we present a recursive construction for three-level experimental designs, which are uniform in the sense of the wrap-around discrepancy (Hickernell (1998b)). This criterion is based on the coincide number between any two distinct runs. If we denote by $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$ the i-th and the j-th runs, then the coincide number between these two runs λ_{ij} is the number of positions where $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$ take the same value. Obviously, $\lambda_{ij} = \lambda_{ji}$ and λ_{ii} is the factor number. The following result can be found in Fang, Lu and Winker (2003).

Theorem 3.1 For a $\text{U}(n,3^m)$,

$$(WD_2(\mathcal{P}))^2 \geq -(\frac{4}{3})^m + \frac{1}{n}(\frac{3}{2})^m + \frac{n-1}{n}(\frac{23}{18})^m(\frac{27}{23})^\lambda, \tag{1}$$

where $\lambda = \frac{m(n-3)}{3(n-1)}$. The lower bound can be achieved if and only if λ is an integer and for all $i \neq j$, $\lambda_{ij} = \lambda$.

It is not difficult to extend Theorem **??** to the case where $\lambda = \frac{m(n-3)}{3(n-1)}$ is not an integer. We state it in the following theorem.

Theorem 3.2 For a $\text{U}(n,3^m)$,

$$(WD_2(\mathcal{P}))^2 \geq -(\frac{4}{3})^m + \frac{1}{n}(\frac{3}{2})^m + \frac{n-1}{n}(\phi+1-\lambda)(\frac{23}{18})^m(\frac{27}{23})^\phi + \frac{n-1}{n}(\lambda-\phi)(\frac{23}{18})^m(\frac{27}{23})^{\phi+1}, \tag{2}$$

where $\lambda = \frac{m(n-3)}{3(n-1)}$ and $\phi = \lfloor \lambda \rfloor$. The lower bound can be achieved if and only if for all $i \neq j$, $\lambda_{ij} = \phi$ or $\phi + 1$.

Motivated by a construction for combinatorial configurations contained in Furino, Miao and Yin (1996), we found a recursive method to obtain a new uniform design under WD_2 from old one, which is stated in the following way.

Theorem 3.3 Let $t \geq 2$ be a positive integer. If a uniform design $\mathrm{U}_{3p}(3^{3p-1})$ achieving the lower bound (**??**) in Theorem **??** exists, then so does a uniform design $\mathrm{U}_{3^t p}(3^{3^t p-2})$ achieving the lower bound (**??**) in Theorem **??**.

What Theorem **??** says is that if we happen to have a uniform design $\mathrm{U}_{3p}(3^{3p-1})$ under WD_2 achieving the lower bound (**??**) in Theorem **??**, then we can recursively obtain an infinite class of uniform designs of the form $\mathrm{U}_{3^t p}(3^{3^t p-2})$ under WD_2 which achieves the lower bound (**??**) in Theorem **??**. To describe the recursive procedure of Theorem **??**, we use the notation $Q^m = \{1, 2, \cdots, q\}^m$ to indicate the experimental points of designs.

Consider a $\mathrm{U}_{3p}(3^{3p-1})$ achieving the low bound (**??**) in Theorem **??**, $X = (x_{ij})_{3p \times (3p-1)}$, over Q. We have $\lambda_X = \frac{(3p-1)(3p-3)}{3(3p-1)} = p-1$, and $\lambda_{ij} = \lambda_X$ for all $1 \leq i \neq j \leq n$ by Theorem **??**.

Now, for each column $x^{(j)} = (x_{1j}, x_{2j}, \cdots, x_{3pj})^T$ of X, define three vectors $y^{(jt)} = (y_{1,jt}, y_{2,jt}, \cdots, y_{9p,jt})^T$ $(t = 1, 2, 3)$, where

$$y_{i,jt} = \begin{cases} x_{ij} & if\ 1 \leq i \leq 3p, \\ x_{(i-3p)j} + t\ (mod\ 3) & if\ 3p < i \leq 6p, \\ x_{(i-6p)j} - t + 3\ (mod\ 3) & if\ 6p < i \leq 9p. \end{cases}$$

We then utilize these three vectors $y^{(jt)}$ $(j = 1, 2, \cdots, 3p-1,\ t = 1, 2, 3)$ to form a $9p \times (9p-3)$ matrix, and append a column $(\mathbf{1}_{3p}, \mathbf{2}_{3p}, \mathbf{3}_{3p})^T$ to this matrix. This produces a $9p \times (9p-2)$ matrix Y, where $\boldsymbol{x}_{3p} = (x, x, \cdots, x)_{1\times 3p}$ and $x = 1, 2, 3$.

We claim that Y is a uniform design $\mathrm{U}_{9p}(3^{9p-2})$ which achieves the lower bound in Theorem **??**. To see this, it is sufficient to show that all λ_{ij}'s $(i \neq j)$ for Y are equal to $3p-2$ or $3p-1$ by Theorem **??**, since $\lambda_Y = \frac{(9p-2)(9p-3)}{3(9p-1)} = 3p - 2 + \frac{6p}{9p-1}$, $\phi_Y = \lfloor \lambda_Y \rfloor = 3p-2$. To do this, we divide Y into three $3p \times (9p-2)$ matrices $Y_t^T (t = 1, 2, 3)$, that is, put $Y = (Y_1^T, Y_2^T, Y_3^T)^T$. Since the Hamming distance between any two distinct rows of X is $(3p-1) - (p-1) = 2p$, the Hamming distance between any two distinct rows i_1 and i_2 of Y is $3 \times 2p = 6p$, if row i_1 and row i_2 are in the same submatrix. When rows i_1 and i_2 are not in the same submatrix, then $\lambda_{i_1 i_2}$ is the number of the column of X which is equal to $3p-1$. Thus, all λ_{ij}'s $(i \neq j)$ of Y are $3p-2$ or $3p-1$.

We remark that the uniform design Y under WD_2 constructed from X contains a distinguished column $(\mathbf{1}_{3p}, \mathbf{2}_{3p}, \mathbf{3}_{3p})^T$. And it achieves the lower bound (**??**) in Theorem **??**.

Once we obtain a uniform design $\mathrm{U}_{9p}(3^{9p-2})$ Y as above, we can use it to create a $\mathrm{U}_{27p}(3^{27p-2})$ in the following steps.

1 On the distinguished column of Y, $(\mathbf{1}_{3p}, \mathbf{2}_{3p}, \mathbf{3}_{3p})^T$, define six column vectors $z^{(t)} = (z_{1t}, z_{2t}, \cdots, z_{27pt})^T$ $(t = 1, 2, \cdots, 6)$ such that
for $t = 1, 2, 3$,

$$z_{it} = \begin{cases} y_{i(27p-2)} & if\ 1 \leq i \leq 9p, \\ y_{(i-9p)(27p-2)} + t\ (mod\ 3) & if\ 9p < i \leq 18p, \\ y_{(i-18p)(27p-2)} - t + 3\ (mod\ 3) & if\ 18p < i \leq 27p; \end{cases}$$

for $t = 4, 5, 6$,

$$z_{it} = \begin{cases} y_{i(27p-2)} & if\ 1 \le i \le 9p, \\ y_{(i-9p)(27p-2)} + t\ (mod\ 3) & if\ 9p < i \le 18p, \\ y_{(i-18p)(27p-2)} - t + 4\ (mod\ 3) & if\ 18p < i \le 27p. \end{cases}$$

2 On any other column, define three column vectors $z^{(jt)} = (z_{1,jt}, z_{2,jt}, \cdots, z_{27p,jt})^T$ $(t = 1, 2, 3)$ such that

$$z_{i,jt} = \begin{cases} y_{ij} & if\ 1 \le i \le 9p, \\ y_{(i-9p)j} + t\ (mod\ 3) & if\ 9p < i \le 18p, \\ y_{(i-18p)j} - t + 3\ (mod\ 3) & if\ 18p < i \le 27p. \end{cases}$$

3 Append a column $(\mathbf{1}_{9p}, \mathbf{2}_{9p}, \mathbf{3}_{9p})^T$ to the matrix consisting of the above columns to form a new matrix Z.

It is readily checked that Z is the desired $\mathrm{U}_{27p}(3^{27p-2})$, whose λ_{ij}'s all equal $9p-2$ or $9p-1$. The design Z also contains a distinguished column $(\mathbf{1}_{9p}, \mathbf{2}_{9p}, \mathbf{3}_{9p})^T$ and achieves the lower bound (**??**) in Theorem **??**. Start with Z and employ the above steps recursively we can get a uniform design $\mathrm{U}_{3^t p}(3^{3^t p-2})$ for any $t \ge 4$.

Example 3.4 Start with the following uniform design $\mathrm{U}_6(3^5)$ which achieves (**??**) in Theorem **??**:

Table 1: $\mathrm{U}_6(3^5)$ under WD_2

row	1	2	3	4	5
1	1	1	1	1	1
2	1	2	2	2	2
3	2	1	2	3	3
4	2	3	3	2	1
5	3	3	1	3	2
6	3	2	3	1	3

Now apply our recursive method described above to get a uniform design $\mathrm{U}_{18}(3^{16})$ under WD_2 as follows.

In a similar vein, we can easily establish the following Theorem, which was stated under the name "Orthogonal Arrays" in Hedayat, Sloane and Stufken (1999) without proof.

Theorem 3.5 Let t be a positive integer. If a uniform design $\mathrm{U}_{3p}(3^{\frac{3p-1}{2}})$ achieving the lower bound (**??**) in Theorem **??** exists, then a uniform design $\mathrm{U}_{3^t p}(3^{\frac{3^t p-1}{2}})$ achieving (**??**) also exists.

Table 2: $U_{18}(3^{16})$ under WD_2

row	1	2	3	4	5	6	7	8	9	0	1	2	3	4	5	6
1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
2	1	1	1	2	2	2	2	2	2	2	2	2	2	2	2	1
3	2	2	2	1	1	1	2	2	2	3	3	3	3	3	3	1
4	2	2	2	3	3	3	3	3	3	2	2	2	1	1	1	1
5	3	3	3	3	3	3	1	1	1	3	3	3	2	2	2	1
6	3	3	3	2	2	2	3	3	3	1	1	1	3	3	3	1
7	2	3	1	2	3	1	2	3	1	2	3	1	2	3	1	2
8	2	3	1	3	1	2	3	1	2	3	1	2	3	1	2	2
9	3	1	2	2	3	1	3	1	2	1	2	3	1	2	3	2
10	3	1	2	1	2	3	1	2	3	3	1	2	2	3	1	2
11	1	2	3	1	2	3	2	3	1	1	2	3	3	1	2	2
12	1	2	3	3	1	2	1	2	3	2	3	1	1	2	3	2
13	3	2	1	3	2	1	3	2	1	3	2	1	3	2	1	3
14	3	2	1	1	3	2	1	3	2	1	3	2	1	3	2	3
15	1	3	2	3	2	1	1	3	2	2	1	3	2	1	3	3
16	1	3	2	2	1	3	2	1	3	1	3	2	3	2	1	3
17	2	1	3	2	1	3	3	2	1	2	1	3	1	3	2	3
18	2	1	3	1	3	2	2	1	3	3	2	1	2	1	3	3

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