# Uniform Design: Theory and Application

**Kai-Tai FANG**

Department of Mathematics
Hong Kong Baptist University
Kowloon Tong
Hong Kong
(*ktfang@hkbu.edu.hk*)

**Dennis K. J. LIN**

Department of Management Science and Information Systems
The Pennsylvania State University
University Park, PA 16802
(*dkl5@psu.edu*)

**Peter WINKER**

Department of Economics
University of Mannheim
D-68131 Mannheim
Germany
(*peter.winker@vwl.uni-mannheim.de*)

**Yong ZHANG**

Mechanical Engineering Department
Worcester Polytechnic Institute
Worcester, MA 01609
(*yzh@wpi.edu*)

A uniform design (UD) seeks design points that are uniformly scattered on the domain. It has been popular since 1980. A survey of UD is given in the first portion: The fundamental idea and construction method are presented and discussed and examples are given for illustration. It is shown that UD's have many desirable properties for a wide variety of applications. Furthermore, we use the global optimization algorithm, threshold accepting, to generate UD's with low discrepancy. The relationship between uniformity and orthogonality is investigated. It turns out that most UD's obtained here are indeed orthogonal.

KEY WORDS: Computer experiment; Discrepancy; Orthogonal design; Threshold accepting.

## 1. INTRODUCTION

Classical experimental designs are mostly based on (analysis of variance) ANOVA-type models that typically involve main effects, interactions, and random error. A two-way ANOVA model with two factors $A$ and $B$, for example, can be expressed as

$$Y_{ijk} = \mu + \alpha_i + \beta_j + (\alpha\beta)_{ij} + \varepsilon_{ijk}, \tag{1.1}$$

where $\alpha_i, \beta_j$, and $(\alpha\beta)_{ij}$ are the main effects of $A$ and $B$ and interaction between $A$ and $B$, respectively; $\mu$ is the grand mean; and $\varepsilon_{ijk}$ is the random error. The objective of an experimental design is then to provide a good estimate for all parameters with a suitable number of experiments. When the number of factors increases, the number of parameters in the corresponding ANOVA model increases exponentially, as does the required number of experiments. A common approach to this problem is to assume that the high-order interactions are negligible. Thus, a fractional factorial design, which allows estimation of all main effects and low-order interactions, can reduce the number of experiments significantly.

The optimal regression design (or optimal design, for short), on the other hand, is based on a prespecified regression model, such as

$$Y = \sum_{i=1}^{k} \beta_i g_i(x_1, \ldots, x_s) + \varepsilon, \tag{1.2}$$

where $x_1, \ldots, x_s$ are $s$ input factors, $g_i$'s are known functions, $\beta_i$'s are unknown parameters, and $\varepsilon$ is the random error. Different criteria of optimality may imply different optimal designs; see, for example, Pukelsheim (1993).

In many circumstances, the function $g_i$'s are unknown, in which case Model (1.2) can be represented as

$$Y = h(x_1, \ldots, x_s) + \varepsilon, \tag{1.3}$$

where the function $h$ is unknown. The goal here is mostly to estimate the average value $E(h(\mathbf{x}))$ over the experimental domain, where $h(\mathbf{x})$ is an output of the experiment. Without loss of generality, we assume that the experimental domain is the unit cube $C^s$, so

$$E(h(\mathbf{x})) = \int_{C^s} h(\mathbf{x})\, d\mathbf{x}. \tag{1.4}$$

This usually can be estimated by the mean

$$\bar{h} = \frac{1}{n} \sum_{\mathbf{x} \in \mathcal{P}} h(\mathbf{x}), \tag{1.5}$$

where $\mathcal{P}$ is a set of $n$ experimental points over the domain. We seek an experimental design that estimates $E(h(\mathbf{x}))$ in an efficient way.

McKay, Beckman, and Conover (1979) proposed a method of generating a set of experimental points $\mathcal{P} = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$ called *Latin hypercube sampling* (LHS). LHS provides a more efficient estimate of the overall mean of the

response than the estimate based on simple random sampling. Fang (1980) and Wang and Fang (1981), on the other hand, proposed the *uniform design* (UD) concept that allocates experimental points uniformly scattered on the domain. Both the LHS design and UD are "space filling" experimental designs—the LHS design in a *randomly uniform fashion* and the UD in a *deterministically uniform fashion.* Specifically, if the experimental domain is finite, LHS designs are similar to UD. When the experimental domain is continuous, the fundamental difference between these two designs is that, in LHS designs, points are selected at random from cells, whereas in UD points are selected from the center of cells. Furthermore, an LHS design requires one-dimensional balance of all levels for each factor, but a UD requires one-dimensional balance *and* $s$-dimensional uniformity. Thus, these designs are similar in one dimension but can be very different in higher dimensions.

The Koksma–Hlawka inequality (see Hua and Wang 1981) gives the upper error bounds of the estimate of $E(h(\mathbf{x}))$:

$$|E(h(\mathbf{x})) - \bar{h}| \le D(\mathcal{P})V(h), \tag{1.6}$$

where $V(h)$ is a measure of the variation of $h$ and $D(\mathcal{P})$ is the discrepancy of $\mathcal{P}$, a measure of the uniformity of $\mathcal{P}$. The definition of $V(h)$ in the sense of Hardy and Krause was given by Niederreiter (1992, p. 19). Note that $V(h)$ is independent of the design points. Thus, given a bounded $V(h)$, Inequality (1.6) indicates that, the more uniform a set $\mathcal{P}$ of points is over the experimental region $C^s$, the more accurate $\bar{h}$ is as an estimator of $E(h(\mathbf{x}))$. Therefore, one should choose a set of experimental points with smallest discrepancy among all possible designs for a given number of factors and experimental runs. This is the fundamental idea of UD. Note that the UD is robust against changes of the function $h$ for which $V(h)$ remains unchanged. This fact indicates that the UD can provide a good estimate of $E(h(\mathbf{x}))$ for a very large class of $h(\mathbf{x})$. The key issue to be addressed then is how to find $n$ points in $C^s$ with minimum discrepancy.

This article is organized into two parts: The first part (Secs. 2 and 3) provides a brief survey of UD's. Existing designs are not listed; we only explain what they are and how they can be used. The second part (Secs. 4–6) provides some new research results on the construction of UD's that are based on an analysis of the relationship between uniformity and orthogonality. New designs obtained by this approach are tabulated. Specifically, Section 2 provides a brief and informative introduction to UD—its general properties, optimality, and construction method. A direct application to dynamic systems is discussed in Section 3. The relationship between uniformity and orthogonality is discussed in Section 4, followed by two construction algorithms in Section 5. Some numerical results obtained are presented in Section 6. Concluding remarks are given in Section 7.

## 2. UNIFORM DESIGNS

Suppose there are $s$ factors of interest over a standard domain $C^s$. The goal here is to choose a set of $n$ points $\mathcal{P}_n = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\} \subset C^s$ such that these points are uniformly scattered on $C^s$. Let $M(\mathcal{P}_n)$ be a measure of the nonuniformity of $\mathcal{P}_n$; we seek a set $\mathcal{P}_n^*$ that minimizes $M$ or, equivalently, maximizes the uniformity over all possible $n$ points on $C^s$.

### 2.1 Measures of Uniformity

From the Koksma–Hlawka inequality in (1.6), a natural choice of $M$ is the discrepancy $D(p)$. Let $F_n(\mathbf{x})$ be the empirical distribution function of $\mathcal{P}_n$:

$$F_n(\mathbf{x}) = \frac{1}{n}\sum_{i=1}^{n} I\{\mathbf{x}_i \le \mathbf{x}\}, \tag{2.1}$$

where $I\{\cdot\}$ is the indicator function and all inequalities are understood to be with respect to the componentwise order of $R^s$. Then the $L_p$ *discrepancy* can be defined as

$$D_p(\mathcal{P}_n) = \left[\int_{C^s} |F_n(\mathbf{x}) - F(\mathbf{x})|^p \, d\mathbf{x}\right]^{1/p}, \tag{2.2}$$

where $F(\mathbf{x})$ is the uniform distribution function on $C^s$. The popular $L_\infty$ discrepancy obtained by taking $p = \infty$ in (2.2) is called the star discrepancy, or discrepancy for simplicity. This is probably the most commonly used measurement for discrepancy and can be reexpressed as follows:

$$D(\mathcal{P}_n) = \sup_{\mathbf{x} \in C^s} |F_n(\mathbf{x}) - F(\mathbf{x})|. \tag{2.3}$$

The discrepancy has been universally accepted in quasi-Monte Carlo methods and number-theoretic methods. In fact, the discrepancy is the Smirnov–Kolmogorov statistic for goodness-of-fit tests. One disadvantage of the discrepancy is that it is expensive to compute. Attempts have been made to evaluate the discrepancy algorithmically (e.g., see Winker and Fang 1997). With the discrepancy criterion in mind, we next discuss how to construct a UD.

### 2.2 Construction Method

For the case $s = 1$, the UD under $D$ is

$$\mathcal{P}_n^* = \left\{\frac{1}{2n}, \frac{3}{2n}, \ldots, \frac{2n-1}{2n}\right\}, \tag{2.4}$$

with $D = 1/2n$ (see Fang and Wang 1994). For $s > 1$, the problem of finding a UD is much more difficult. One approach is to reduce the domain $C^s$ into a smaller subdomain $\mathcal{D}_s \subset C^s$. Obviously the quality of the $\mathcal{D}_s$ UD depends on the quality of the set of candidates $\mathcal{D}_s$.

Here, we introduce the most popular UD, called a U UD. An $n \times s$ matrix $\mathbf{U}_{n,s} = (u_{ij})$, where each column is a permutation of $\{1, 2, \ldots, n\}$, is called a U-type design. Its induced matrix, $\mathbf{X}_{n,s} = (x_{ij})$, is defined as

$$x_{ij} = (u_{ij} - .5)/n, \qquad i = 1, \ldots, n; j = 1, \ldots, s. \tag{2.5}$$

A U-type design $\mathbf{U}_{n,s}$ provides an $n$-run experimental design for $s$ factors, each having $n$ levels, if the rank of $\mathbf{U}_{n,s}$ is $s$. The matrix $\mathbf{X}_{n,s}$ can be considered as $n$ points on $C^s$. Let $\mathcal{U}_{n,s}$ denote the set of all $\mathbf{U}_{n,s}$ designs and $\mathcal{X}_{n,s}$ be the set of all $\mathbf{X}_{n,s}$. There is a one-to-one correspondence between $\mathbf{U}_{n,s}$ and $\mathbf{X}_{n,s}$ so that they can be used interchangeably.

Useful U UD's were constructed and tabulated by Fang (1994).

*Definition 1.* A U-type design $U_{n,s}$ with rank $s$ whose induced matrix has the smallest discrepancy over $\mathcal{X}_{n,s}$ is called a U UD and is denoted by $U_n(n^s)$.

The notation $U_n(n^s)$ is purposely chosen to mimic that commonly used for orthogonal designs $L_n(q^s)$, where $n$ is the number of experiments, $s$ the number of factors, and $q$ the number of levels for each factor. The first column of $U_n(n^s)$ can always be taken as $(1, 2, \ldots, n)'$. There are $n! - 1$ possible permutations of $\{1, 2, \ldots, n\}$ for the second column, $n! - 2$ choices for the third column, and so on. Table 1 shows an example of a $U_7(7^3)$ UD.

### 2.3 Properties of U-Type Uniform Designs

The aim of the UD is to choose a set of $n$ points $\mathcal{P}_n \in C^s$ with smallest discrepancy value $D(\mathcal{P}_n)$. A conjecture in number theory states that

$$D(\mathcal{P}_n) \geq c(s)\,\frac{(\log n)^{s-1}}{n}, \quad \text{for any } \mathcal{P}_n,$$

where the constant $c(s)$ depends on $s$ only. This conjecture is clearly true for $s = 2$ (Hua and Wang 1981). If we can find a sequence $\mathcal{P}_n$ with $D(\mathcal{P}_n)$ having order $O(n^{-1}(\log n)^{s-1})$ as $n \to \infty$, we can consider $\mathcal{P}_n$ to be uniformly scattered over $C^s$ at least for large $n$. If $\mathcal{P}_n$ is generated by the Monte Carlo method, its discrepancy has order $O_p(n^{-1/2})$, independent of $s$.

The good-lattice-point method (Fang and Wang 1994) produces $\mathcal{P}_n$ with order $O(n^{-1}(\log n)^{s-1})$. Any set $\mathcal{P}_n$ generated by the good-lattice-point method forms the induced matrix of a U-type design. Therefore, the UD generated from a U-type design resulting from the good-lattice-point method has order $O(n^{-1}(\log n)^{s-1})$. With numerical comparisons for $s \leq 12$, we find that a UD generated by a U-type design has lower discrepancy than one generated by the Monte Carlo method.

### 2.4 Further Remarks on Uniformity

Most statistical experimental designs are based on model assumptions. It is desirable to have a design that is insensitive to the assumptions. That is, a change in the underlying distribution or model should cause only a small change in the performance of the design. As previously mentioned, the UD is robust to certain changes of the function $h$ over the domain $\{h: V(h) < c\}$ for a given $c > 0$ [cf. (1.4)–(1.6)]. Consider a nonparametric regression model (1.3). When $h(x_1, \ldots, x_s)$ can be expressed as $\sum_{i=1}^{k} \beta_i g_i(x_1, \ldots, x_s)$, optimal design theory can provide the most efficient design. If Model (1.3) cannot be expressed as (1.2), an approximately linear regression model may be considered:

$$Y(x_1, \ldots, x_s) = \sum_{i=1}^{k} \beta_i g_i(x_1, \ldots, x_s) + \psi(x_1, \ldots, x_s) + \varepsilon, \quad (2.6)$$

where $\psi(\mathrm{x})$, with $\mathrm{x} = (x_1, \ldots, x_s)$, is an unknown bias. Under certain conditions on $\psi(\mathrm{x})$, Wiens (1991) showed that the uniform measure design is the best design in the sense of the power of the $F$ test.

The UD is based on a nonparametric regression model. Therefore, the UD can be considered as a nonparametric experimental design. That is, we do not need precise knowledge of the model to select a reasonable design. A natural approach is to find a suitable $k, g_1, \ldots, g_k$ to approximate Model (1.2). Xie and Fang (1996) used decision theory to define a risk function under which they proved that the uniform measure design is an admissible minimax design. Fourier regression models have been used in problems with a periodic response, such as in circuits. A Fourier regression model with one factor is of the form

$$E(Y(x)) = \beta_0 + \sum_{i=1}^{m} \beta_i \sin(2\pi i x) + \sum_{i=1}^{m} \phi_i \cos(2\pi i x), \qquad x \in [0, 1). \quad (2.7)$$

A $D$-optimal design under this model is an equidistant grid with at least $2m + 1$ supporting points. That is, the uniform design is $D$-optimal under this model. Riccomagno, Schwabe, and Wynn (1997) extended Model (2.7) to the multiple-factor case and gave a necessary and sufficient condition for U-type designs to be $D$-optimal, where the U-type designs are generated by the *good-lattice-point* method and their induced matrix is defined as $x_{ij} = (u_{ij} - 1)/n$, replacing (2.5).

Table 1. $U_7(7^3)$ Table

| No. | 1 | 2 | 3 |
|---|---|---|---|
| 1 | 1 | 2 | 3 |
| 2 | 2 | 4 | 6 |
| 3 | 3 | 6 | 2 |
| 4 | 4 | 1 | 5 |
| 5 | 5 | 3 | 1 |
| 6 | 6 | 5 | 4 |
| 7 | 7 | 7 | 7 |

## 3. A DYNAMIC SYSTEM EXAMPLE

This section presents a case study of launching a dynamic system for a one-off ship-based flight detector. The launching parameters are determined by a combination of several factors—the motion of wave and wind, the rock of the ship, the relative motion between the detector and launching support, the direction of launching support relative to the base (ship as well as launching device) system, plus other factors. For this problem, a series of coordinate systems are set up as illustrated in Figure 1. This system has the following characteristics:

1. Six degrees of freedom ship rock, including three degrees of freedom positional rock and three degrees of freedom angular rock;
2. Two degrees of freedom circumgyration launching system, with circumgyration axes not intersecting each other;

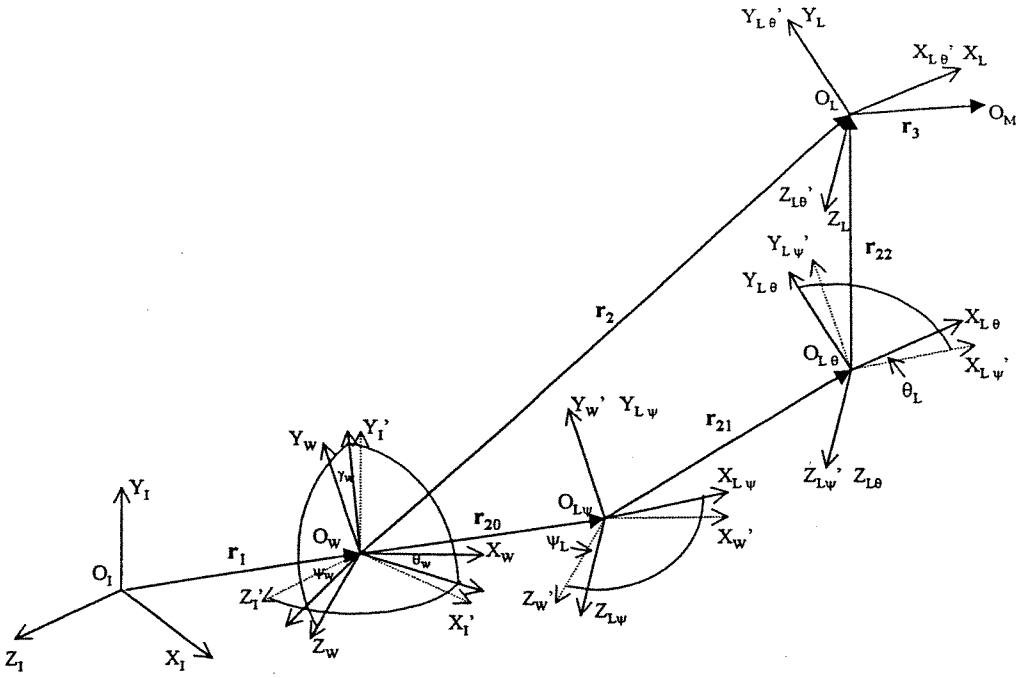


*Figure 1. The Coordinate Systems.*

3. The guide launching mode;
4. Choice-permitted launching position;
5. Two-period launching procedure; that is, the one-degree-of-freedom motion of the detector with respect to launching support in the former part (major part) of the launching procedure and the multidegree-of-freedom motion of the detector with respect to launching support in the later part of the launching procedure;
6. Large-range direction of the launching support composed with the no-limitation azimuth and wide-range elevation angle.

A set of equations was thus formulated as follows.

*The motions of wind and ocean wave, which are the environments of the operation of the system:*

$$S(w) = \frac{A}{w^p} \exp\left(-\frac{B}{w^q}\right), \tag{3.1}$$

where $w$ is the frequency, $p$ and $q$ are the numerical constants, and parameters $A$ and $B$ reflect the effects of wind and wave. The values of these parameters depend on the ocean zone.

*The angular motion of the base system, which is composed of the ship and the launching system:*

$$\vec{\omega}_{MW} = f_\omega(\vec{\omega}_W, \vec{\omega}_{ML}), \tag{3.2}$$

where $\vec{\omega}_{MW}$ is the angular velocity of the detector in the ship coordinate system and $f_\omega$ is the matrix transformation based on the angular velocity of the ship rock $\vec{\omega}_W$ and the angular velocity of the detector in the launching coordinate system $\vec{\omega}_{ML}$.

*Displacement equations of the detector:*

$$m \begin{bmatrix} \ddot{x}_L \\ \ddot{y}_L \\ \ddot{z}_L \end{bmatrix} = \begin{bmatrix} \sum F_{L_x} \\ \sum F_{L_y} \\ \sum F_{L_z} \end{bmatrix}, \tag{3.3}$$

where $m$ is the mass of the detector; $x_L, y_L$, and $z_L$ are the displacements of the centroid of the detector in the launching coordinate system; and $\sum F_{L_x}, \sum F_{L_y}$, and $\sum F_{L_z}$ are the three components of the total forces acting on the detector in the launching coordinate system.

*Rotation equations of the detector:*

$$\begin{bmatrix} \dot{\omega}_{M_x} \\ \dot{\omega}_{M_y} \\ \dot{\omega}_{M_z} \end{bmatrix} = \begin{bmatrix} \sum M_{M_x}/J_{x1} \\ \sum M_{M_y}/J_{y1} \\ \sum M_{M_z}/J_{z1} \end{bmatrix}, \tag{3.4}$$

where $\omega_{M_x}, \omega_{M_y}$, and $\omega_{M_z}$ and $\sum M_{M_x}, \sum M_{M_y}$, and $\sum M_{M_z}$ are the three components of the detector angular velocity and the total-moment-acted-on detector in the detector coordinate system, respectively; $J_{x1}, J_{y1}$, and $J_{z1}$ are the three components of the rotation inertia of the detector.

*Centroid position, velocity, and acceleration of the detector:*

$$\vec{r}_{MI} = f_r(\vec{r}_1 + \vec{r}_2 + \vec{r}_3), \tag{3.5}$$

$$\vec{v}_{MW} = f_v(\dot{\vec{r}}_{1W}, \dot{\vec{r}}_{2W}, \dot{\vec{r}}_{3W}, \vec{r}_{2W}, \vec{r}_{3W}, \vec{\omega}_W, \vec{\omega}_{MW}), \tag{3.6}$$

and

$$\vec{a}_{MW} = f_a(\ddot{\vec{r}}_{1W}, \ddot{\vec{r}}_{3W}, \dot{\vec{r}}_{1W}, \dot{\vec{r}}_{2W}, \dot{\vec{r}}_{3W}, \vec{r}_{2W}, \vec{r}_{3W}, \dot{\vec{\omega}}_W, \dot{\vec{\omega}}_{MW}, \vec{\omega}_W, \vec{\omega}_{MW}), \tag{3.7}$$

where $f_r, f_v$, and $f_a$ are corresponding vector operators. All notations were properly defined by Zhang (1996).

From these equations, the responses (outputs) can be calculated for any given set of input variables. Due to the complexity of the system, we wish to find a simpler model to replace Models (3.1)–(3.7). Because the range of the direction of the launching support relative to the base system (the azimuth and pitching angles) is very large, we have to

consider experimental points in a uniform fashion. Moreover, because of the high cost of the experiment, we specify other factors to have the characteristic values and only concentrate on two factors, azimuth angle ($\psi$) in $[-180°, 180°]$ and pitching angle ($\theta$) in $[-10°, 70°]$. A $U_{17}(17^2)$ design is chosen for the experiment. Two responses, $\omega_1$ and $\omega_2$, are considered and calculated for these 17 points by Equations (3.1)–(3.7) and are listed in Table 2.

Based on subject-matter knowledge and the model-selection techniques in regression analysis, we find the following regression models:

$$\begin{aligned}\omega_1 &= 217.5842 - 105.7505\psi^2 + 7.3675\psi^4 \\ &\quad - .0130\psi^8 - 95.3594\theta^2 + 30.1229\psi^2\theta^2 \\ &\quad + 10.2364\psi^2\theta^3 - .5653\psi^6\theta^5 + .0399\psi^8\theta^8 \qquad (3.8)\end{aligned}$$

and

$$\begin{aligned}\omega_2 &= -.0862 + 219.5894\psi - 36.8394\psi^3 + 1.8644\psi^5 \\ &\quad - .0398\psi^7 - .5590\theta + 1.6468\psi\theta - .0320\psi^5\theta^6. \qquad (3.9)\end{aligned}$$

The advantage of the fitted models (3.8) and (3.9) is that the responses can be determined quickly by the polynomial calculation. This avoids the complexity of solving the system of ordinary differential equations, which is time consuming and impractical to implement in the launching control systems.

For assessing performance of these two models, we calculate $\omega_1$ and $\omega_2$ for $\psi$ from $-180$ to 180 in 10-unit increments and $\theta$ from $-10$ to 50 in 5-unit increments by both the original equations (3.1)–(3.7) and the approximation models (3.8) and (3.9). Figure 2, (a) and (b), shows $\omega_1$ and $\omega_2$ based on (3.1)–(3.7), and Figure 2, (c) and (d), shows $\omega_1$ and $\omega_2$ based on the approximation models. It is clear that panels (a) and (c) of Figure 2 have a similar shape, as do panels (b) and (d). Denote by $\Omega_i$ $(i = 1, 2)$ the preceding $\omega_i$ values obtained by Equations (3.1) and (3.7). The matrices $\Omega_1$ and $\Omega_2$ have size $37 \times 13$. Let $\hat{\Omega}_i$ stand for the preceding $\omega_i$ values calculated by the corresponding approximation model. We have $\mathrm{tr}(\Omega_1 - \hat{\Omega}_1)'(\Omega_1 - \hat{\Omega}_1) = 6.3590 \times 10^{-5}$, $\mathrm{tr}(\Omega_2 - \hat{\Omega}_2)'(\Omega_2 - \hat{\Omega}_2) = 4.2900 \times 10^{-6}$, which shows that the approximation models have good performance. More examples involving applications of UD (including computer experiments) were given by Fang, Lin, and Zhang (1998).

Table 2. Design and Data in Dynamic System

| No. | $\psi$ | $\theta$ | $10^4\omega_1$ | $10^4\omega_2$ |
|---|---|---|---|---|
| 1 | −180.0 | 20 | −206 | 0 |
| 2 | −157.5 | 55 | −118 | −86 |
| 3 | −135.0 | 0 | −155 | −155 |
| 4 | −112.5 | 35 | −70 | −205 |
| 5 | −90.0 | 70 | 0 | −222 |
| 6 | −67.5 | 15 | 81 | −203 |
| 7 | −45.0 | 50 | 101 | −157 |
| 8 | −22.5 | −5 | 202 | −84 |
| 9 | .0 | 30 | 190 | 0 |
| 10 | 22.5 | 55 | 87 | 86 |
| 11 | 45.0 | 10 | 153 | 155 |
| 12 | 67.5 | 45 | 69 | 203 |
| 13 | 90.0 | −10 | 0 | 219 |
| 14 | 112.5 | 25 | −76 | 203 |
| 15 | 135.0 | 60 | −78 | 155 |
| 16 | 157.5 | 5 | −202 | 84 |
| 17 | 180.0 | 40 | −168 | 0 |

Certainly, the model-selection methods in regression have their flaws, as pointed out by one referee. The regression method is used here to demonstrate the use of UD. It is believed that better data-analysis methods (sometimes with suitable assumptions) can extract more useful information from the data. In fact, the associate editor suggested the use of stochastic modeling (e.g., see Sacks, Welch, Mitchell, and Wynn 1989) as an alternative data-analysis method here (especially when the experiment is costly, only a few observations are feasible). This seems to be a sensible direction for future study.

## 4. UNIFORMITY AND ORTHOGONALITY

The orthogonal design is one major kind of fractional factorial experimental design. It has been widely used in various problems of industry, agriculture, quality control, and the natural sciences. Orthogonal designs can be regarded as a special case of orthogonal arrays. An orthogonal array (OA) of strength $r$ and size $n$ with $s$ constraints is given by an $n \times s$ matrix $\mathbf{O}$ with entries from a set of $q \geq 2$ symbols, where each $n \times r$ submatrix of $\mathbf{O}$ contains all possible $1 \times r$ row vectors with the same frequency $\lambda$. In practice, OA's of strength 2 are extremely important because they exhibit good properties for specific applications of experimental designs. OA's of strength 2 are called orthogonal designs (OD's) and will be the center of our interest for the rest of this article. A formal definition of an OD can be given as follows:

*Definition 2.* An $n \times s$ matrix, denoted by $L_n(q_1 \times \cdots \times q_s)$ with entries $1, 2, \ldots, q_j$ at the $j$th column is called an OD if it satisfies the following conditions:

1. Each entry in each column occurs the same number of times.
2. In any two columns, each pair $(1,1), \ldots, (1, q_j), (2,1), \ldots, (2, q_j), \ldots, (q_i, q_j)$ occurs the same number of times for any $1 \leq i \leq j \leq s$.

If some of the $q_j$ are the same, the matrix is denoted $L_n(q_1^{t_1} \times \cdots \times q_m^{t_m}), t_1 + \cdots + t_m = s$; in particular, $L_n(q^s)$ has $s$ columns, each having the same number of levels $q$.

The value of $n$ has to be a multiple of $q_j^2$ for $t_j \geq 2$ and a multiple of $q_j$ for $t_j = 1$. An OD for given parameters $(n, s; q_1, \ldots, q_s)$ is not unique. Table 3 shows an OD $L_9(3^4)$ (e.g., see Dehnad 1989, p. 63). By exchanging rows and columns of an OD, we can obtain many other *equivalent* OD's. Here, we choose the representation with all entries in the first row equal to 1 and call it the canonical form. The design given in Table 3 is in canonical form.

If we relabel the three levels 1, 2, and 3 of this design to be symmetric around 0—for example, $-1, 0$, and 1—and denote this design matrix by $\mathbf{L}$, then it is easy to see that the columns of the design are orthogonal to each other; that is, $\mathbf{L}'\mathbf{L} = 2\mathbf{I}_4$, where $\mathbf{I}_4$ is the $4 \times 4$ identity matrix. Although

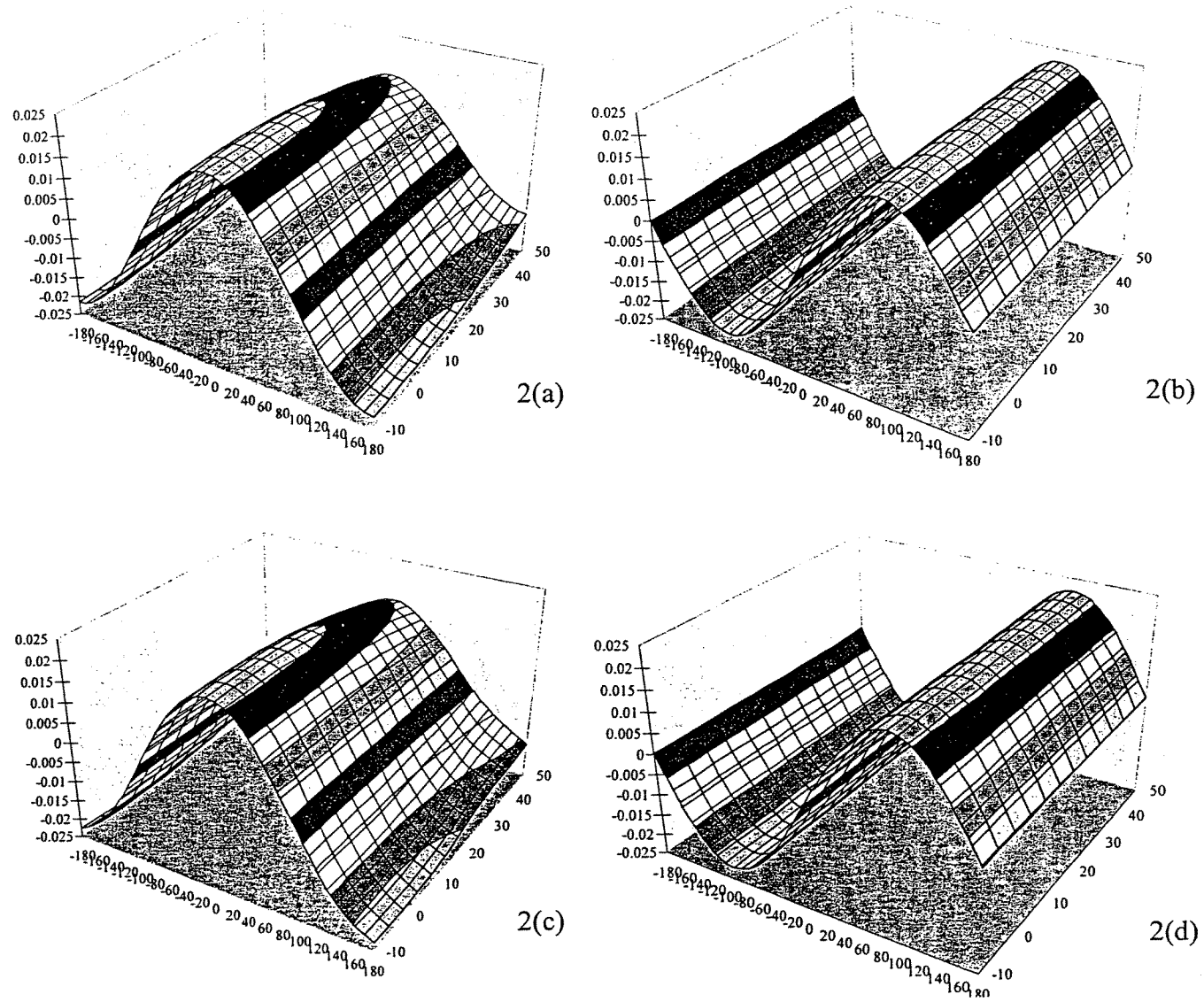


*Figure 2. Performance Comparison.*

necessary, the condition of column orthogonality (CO) is not sufficient for design orthogonality (DO) introduced by Definition 2.

In past decades, much effort has been devoted to the generation of OD's, including the following:

1. Orthogonal Latin squares for the construction of $L_9(3^4), L_{16}(4^5), L_{25}(5^6), L_{49}(7^8), \ldots, L_{t^2}(t^{t+1})$;

*Table 3. Orthogonal Design $L_9(3^4)$*

| | Column | | | |
|---|---|---|---|---|
| Row | 1 | 2 | 3 | 4 |
| 1 | 1 | 1 | 1 | 1 |
| 2 | 1 | 2 | 2 | 2 |
| 3 | 1 | 3 | 3 | 3 |
| 4 | 2 | 1 | 2 | 3 |
| 5 | 2 | 2 | 3 | 1 |
| 6 | 2 | 3 | 1 | 2 |
| 7 | 3 | 1 | 3 | 2 |
| 8 | 3 | 2 | 1 | 3 |
| 9 | 3 | 3 | 2 | 1 |

2. Hadamard matrices for $L_4(2^3), L_8(2^7), L_{16}(2^{15}), \ldots, L_{4t}(2^{4t-1})$;

3. Group theory (difference sets) for $L_{18}(2 \times 3^7), L_{36}(4 \times 3^{13}), L_{54}(2 \times 3^{25})$, and so forth;

4. Finite fields for designs of type $L_{t^m}(t^q)$.

The reader can refer to, for example, Bose and Bush (1952), Raghavarao (1971), and Bose, Chakravarti, and Knuth (1960, 1961). All of these approaches strongly depend on pure mathematics. Consequently, they are not easy for nonmathematicians to understand. Furthermore, how to construct particular OD's for practical uses remains an open question in most instances. It is known that an OD is uniform in any one- and two-dimensional projection in the sense of Definition 2. Therefore, points of an OD are uniformly scattered over the domain in a certain sense to be defined later. This fact gives a link between OD and UD. We next introduce some improved measurements of uniformity as the major optimality criteria to be used in our construction algorithms.

### Improved Measurements of Uniformity

Warnock (1972) gave an analytic formula for calculating the $L_2$ discrepancy:

$$(D_2(\mathcal{P}_n))^2 = 3^{-s} - \frac{2^{1-s}}{n}\sum_{k=1}^{n}\prod_{l=1}^{s}(1-x_{kl}^2) + \frac{1}{n^2}\sum_{k=1}^{n}\sum_{j=1}^{n}\prod_{i=1}^{s}[1-\max(x_{ki},x_{ji})], \quad (4.1)$$

where $\mathbf{x}_k = (x_{k1},\ldots,x_{ks})$. Obviously, the $L_2$ discrepancy is much easier to calculate numerically than the $L_\infty$ discrepancy (see also Heinrich 1995). Unfortunately, the $L_2$ discrepancy exhibits some disadvantages, as pointed out by Hickernell (1998). For example, it suffers from the projection uniformity over all subdimensions. To overcome these disadvantages, Hickernell proposed three new measures of uniformity that are also related to the $L_2$ norm—namely, the symmetric $L_2$ discrepancy ($SL_2$), the centered $L_2$ discrepancy ($CL_2$), and the modified $L_2$ discrepancy ($ML_2$). All three discrepancies satisfy a Koksma–Hlawka type inequality; that is, each discrepancy has its corresponding measure of variation replacing $V(f)$ in (1.6).

Let us introduce these three discrepancies more precisely. Let $N(\mathbf{x},\mathcal{P}_n)$ denote the number of points of $\mathcal{P}_n$ falling into the region $[\mathbf{0},\mathbf{x}) = \{y \in C^s | 0 \le y_i < x_i, 1 \le i \le s\}$ and $v(B)$, the volume of $B \subset C^s$. Now, we can rewrite (2.2) as

$$D_p(\mathcal{P}_n) = \left[\int_{C^s}\left|\frac{N(\mathbf{x},\mathcal{P}_n)}{n} - v([\mathbf{0},\mathbf{x}))\right|^p d\mathbf{x}\right]^{1/p}. \quad (4.2)$$

The modified $L_p$ discrepancy is then defined by

$$D_p(\mathcal{P}) = \left[\sum_{u\neq\emptyset}\int_{C^u}\left|\frac{N(J_{\mathbf{x}_u},\mathcal{P})}{n} - v(J_{\mathbf{x}_u})\right|^p d\mathbf{x}_u\right]^{1/p}, \quad (4.3)$$

where $u$ is a nonempty subset of $S = \{1,\ldots,s\}$, $|u|$ denotes cardinality of $u$, $C^u$ is the $|u|$-dimensional unit cube involving the coordinates in $u$, $J_{\mathbf{x}}$ is a rectangle uniquely determined by $\mathbf{x}$, $J_{\mathbf{x}_u}$ is the projection of $J_{\mathbf{x}}$ on $C^u$, and $N(J_{\mathbf{x}_u},\mathcal{P})$ is the number of points of $\mathcal{P}$ falling in $J_{\mathbf{x}_u}$. Obviously, for the original discrepancy the origin $\mathbf{0}$ plays a specific role in the set of all vertices of $C^s$. The *centered* $L_p$ discrepancy puts all vertices into the same situation. Consequently, this discrepancy and its measure of variation are obtained from (4.3) by a modification such that it becomes invariant under reflections of $\mathcal{P}_n$ around any plane $x_j = .5$. In its definition [cf. (4.3)] and in the definition of $N(\mathbf{x},\mathcal{P}_n)$, we replace $[\mathbf{0},\mathbf{x})$ by

$$J(\mathbf{a},\mathbf{x}) = \{\mathbf{y} \in C^s | \min(a_j,x_j) \le y_j < \max(a_j,x_j), \quad \text{for } 1 \le j \le s\},$$

where $\mathbf{a} = (a_1,\ldots,a_s)$ is a vertex of $C^s$. For the centered $L_2$ discrepancy, Hickernell (1998) gave an analytical expression similar to (4.1) as follows:

$$(CL_2(\mathcal{P}_n))^2 = \left(\frac{13}{12}\right)^s - \frac{2}{n}\sum_{k=1}^{n}\prod_{j=1}^{s}\left(1+\frac{1}{2}|x_{kj}-.5| - \frac{1}{2}|x_{kj}-.5|^2\right) + \frac{1}{n^2}\sum_{k=1}^{n}\sum_{j=1}^{n}\prod_{i=1}^{s}\left[1+\frac{1}{2}|x_{ki}-.5| + \frac{1}{2}|x_{ji}-.5| - \frac{1}{2}|x_{ki}-x_{ji}|\right]. \quad (4.4)$$

The *symmetric* $L_p$ discrepancy and its measure of variation are modified such that they are invariant if $x_{kj}$ is replaced by $1-x_{kj}$ for any $j, 1 \le j \le s$. The construction is based on reproducing kernel Hilbert spaces and results in the following computational formula for the symmetric $L_2$ discrepancy:

$$(SL_2(\mathcal{P}_n))^2 = \left(\frac{4}{3}\right)^s - \frac{2}{n}\sum_{k=1}^{n}\prod_{j=1}^{s}(1+2x_{kj}-2x_{kj}^2) + \frac{2^s}{n^2}\sum_{k=1}^{n}\sum_{j=1}^{n}\prod_{i=1}^{s}[1-|x_{ki}-x_{ji}|]. \quad (4.5)$$

Finally, the *modified* $L_p$ discrepancy and its measure of variation are modified from (4.2) to (4.3) with $J_{\mathbf{x}} = [\mathbf{0},\mathbf{x})$ such that the projection uniformity over all subdimensions can be considered. The modified $L_2$ discrepancy also has a formula similar to (4.1):

$$(ML_2(\mathcal{P}_n))^2 = \left(\frac{4}{3}\right)^s - \frac{2^{1-s}}{n}\sum_{k=1}^{n}\prod_{l=1}^{s}(3-x_{kl}^2) + \frac{1}{n^2}\sum_{k=1}^{n}\sum_{j=1}^{n}\prod_{i=1}^{s}[2-\max(x_{ki},x_{ji})]. \quad (4.6)$$

## 5. CONSTRUCTION ALGORITHMS

The concept of U-type designs can be straightforwardly generalized to the case in which the number of experiments $n$ is a multiple of the number of levels $q$. Then, the notation $U_n(q^s)$ is used. Our conjecture is that uniform designs for a suitable measure of uniformity will be orthogonal. Hence, after introducing some measures of nonuniformity, we turn to the problem of finding a uniform design $U_n(q^s)$ under some measure of nonuniformity $M$ given the parameters $(n,q)$. We choose the discrepancy (2.3), the common $L_2$ discrepancy (4.1), the centered $L_2$ discrepancy (4.3), the symmetric $L_2$ discrepancy (4.4), and the modified $L_2$ discrepancy (4.5) as measures of nonuniformity $M$ to be considered. We shall denote them by $D, D_2, CL_2, SL_2$, and $ML_2$, respectively.

First, we describe a deterministic and constructive algorithm, the forward procedure (FP), which gives some insight into the computational problem. Then, the application of the threshold-accepting (TA) algorithm for the purpose of

finding UD's is introduced. It does not rely on constructive principles but represents a purely global optimization technique on a discrete space. As the results in Section 6 will show, however, it is much more powerful for this problem than the forward procedure.

### 5.1 The Forward Procedure

For illustration we employ $U_{16}(4^5)$. Without loss of generality, we can always choose the first column to be $(1\ 1\ 1\ 1\ 2\ 2\ 2\ 2\ 3\ 3\ 3\ 3\ 4\ 4\ 4\ 4)'$. Now, the algorithm proceeds along the following steps:

*Step 1.* Find the second column with four 1s, 2s, 3s, and 4s such that the design formed by these two columns has the minimum $M$ value. Let $t = 2$.

*Step 2.* For fixed first $t$ columns find the $(t+1)$st column with four 1s, 2s, 3s, and 4s such that the design formed by all $t+1$ columns has the minimum $M$ value. Let $t = t + 1$.

*Step 3.* If $t = 6$, the procedure is finished and the design obtained in the previous step is the final solution; otherwise go back to Step 2.

Note that the value $t$ is always one more than the number of design columns. It is easy to extend this algorithm to the general case $U_n(q_1 \times \cdots \times q_s)$. This algorithm gives a local minimum solution and provides a nearly uniform design in most cases.

### 5.2 The Threshold-Accepting Heuristic

Because a detailed description of the TA heuristic and its implementation and tuning for problems similar to the one of finding UD's can be found elsewhere (see Dueck and Scheuer 1991; Winker 1995; Winker and Fang 1997, 1998), we will sketch the central ideas and a few hints on the interpretation of the results presented in Section 6 and by Fang and Winker (1998, appendix).

TA is a refined local search algorithm sharing some common features with the more widely used simulated annealing algorithm. In our application it acts on the set of all U-type designs for the given parameter values $(n, s; q_1, \ldots, q_s)$, which we denote by $\mathcal{U}_{n,s;q_1,\ldots,q_s}$ or $\mathcal{U}$ for simplicity. Some local structure is introduced on this set by the definition that two U-type designs are close to one another (belong to a common neighborhood) if and only if the second can be obtained from the first by exchanging a maximum of $\lambda$ elements, where $\lambda$ is some fixed positive integer. Thereby only elements within the same column can be exchanged to stay within $\mathcal{U}$. Now, the algorithm can be described as follows:

*Step 1.* Choose randomly any U-type design $X_c \in \mathcal{U}$ and set the threshold parameter $T$ to its start value $T_0$.

*Step 2.* Choose randomly any U-type design $X_n$ close to $X_c$ in the sense just defined (for given $\lambda$) and calculate $\Delta M = M(X_n) - M(X_c)$ for the given measure of nonuniformity $M$.

*Step 3.* If $\Delta M \leq T$, set $X_c = X_n$, else leave $X_c$ unchanged.

*Step 4.* Repeat Step 2 and Step 3 a fixed number of times.

*Step 5.* If the given threshold sequence is not yet exhausted, take the next threshold value and repeat Step 2 to Step 4.

The result of this algorithm is the design with the minimum value of the discrepancy measure $M$. Of course, the performance of this algorithm depends on the choice of a specific local structure by the value of $\lambda$, the predefined sequence of threshold values $T_i$, and the total number of iterations (iterations in Step 4 times the number of different threshold values). For the application to $U_{16}(4^5)$, we found $\lambda = 3$ (in fact, admitted exchanges were restricted to a subset of all possible cases) and a total number of iterations of 500,000 to be reasonable values. The threshold sequence was generated from a first exploratory data analysis as described by Winker and Fang (1997). In particular, the threshold sequence is monotonically decreasing to 0 as the algorithm proceeds. Thus, in the beginning, a temporary increase of $M$ is accepted to escape local minima corresponding to designs with high discrepancy, but at the end only improvements (i.e., a reduction of the discrepancy) are accepted.

Before turning to the results, two final remarks on the TA are in order. First, the natural restriction on the first or even the first two columns of the design as depicted in Tables 4 and 5 were not imposed because they did not improve

*Table 4. $L_{16}(4^5)$ and $U_{16}(4^5)$ Designs Generated by Forward Procedure*

| Row | (1) | (2) | (L3) | (L4) | (L5) | ($D_2^3$) | ($D_2^4$) | ($D_2^5$) | (S, C, M3) | (C, S4) | (S5) | (C5) | (M4) | (M5) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 1 | 1 | 1 | 1 | 1 | 4 | 3 | 3 | 4 | 4 | 3 | 3 | 4 | 2 |
| 2 | 1 | 2 | 2 | 2 | 2 | 2 | 1 | 2 | 2 | 2 | 4 | 4 | 1 | 3 |
| 3 | 1 | 3 | 3 | 3 | 3 | 1 | 4 | 4 | 3 | 1 | 2 | 1 | 2 | 1 |
| 4 | 1 | 4 | 4 | 4 | 4 | 3 | 3 | 3 | 1 | 3 | 3 | 2 | 3 | 4 |
| 5 | 2 | 1 | 2 | 3 | 4 | 1 | 2 | 3 | 1 | 1 | 2 | 4 | 2 | 3 |
| 6 | 2 | 2 | 1 | 4 | 3 | 3 | 4 | 1 | 3 | 3 | 2 | 3 | 3 | 2 |
| 7 | 2 | 3 | 4 | 1 | 2 | 3 | 2 | 4 | 2 | 4 | 1 | 2 | 4 | 4 |
| 8 | 2 | 4 | 3 | 2 | 1 | 4 | 4 | 1 | 4 | 2 | 1 | 1 | 1 | 1 |
| 9 | 3 | 1 | 3 | 4 | 2 | 2 | 4 | 4 | 3 | 2 | 1 | 2 | 1 | 4 |
| 10 | 3 | 2 | 4 | 3 | 1 | 4 | 1 | 2 | 1 | 4 | 4 | 1 | 4 | 1 |
| 11 | 3 | 3 | 1 | 2 | 4 | 2 | 3 | 1 | 4 | 3 | 4 | 4 | 3 | 3 |
| 12 | 3 | 4 | 2 | 1 | 3 | 1 | 1 | 2 | 2 | 1 | 4 | 3 | 2 | 2 |
| 13 | 4 | 1 | 4 | 2 | 3 | 3 | 1 | 2 | 2 | 3 | 3 | 1 | 3 | 1 |
| 14 | 4 | 2 | 3 | 1 | 4 | 1 | 3 | 4 | 4 | 1 | 3 | 2 | 2 | 4 |
| 15 | 4 | 3 | 2 | 4 | 1 | 4 | 2 | 1 | 1 | 2 | 1 | 3 | 1 | 2 |
| 16 | 4 | 4 | 1 | 3 | 2 | 2 | 2 | 3 | 3 | 4 | 2 | 4 | 4 | 3 |

Table 5. $U_{16}(4^5)$ Designs Generated by Threshold Accepting

| Row | (1) | (2) | $(D_2^3)$ | $(D_2^4)$ | $(D_2^5)$ | (S3) | (C, S4) | (S5) | (C3) | (C4) | (C5) | (M3) | (M4) | (M5) |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 1 | 1 | 4 | 3 | 3 | 2 | 1 | 2 | 3 | 1 | 2 | 2 | 3 | 3 |
| 2 | 1 | 2 | 2 | 1 | 2 | 1 | 3 | 4 | 4 | 4 | 4 | 4 | 4 | 1 |
| 3 | 1 | 3 | 1 | 4 | 4 | 4 | 4 | 3 | 2 | 2 | 1 | 3 | 2 | 2 |
| 4 | 1 | 4 | 3 | 3 | 3 | 3 | 2 | 1 | 1 | 3 | 3 | 1 | 1 | 4 |
| 5 | 2 | 1 | 1 | 2 | 3 | 3 | 4 | 2 | 1 | 2 | 4 | 4 | 2 | 4 |
| 6 | 2 | 2 | 3 | 4 | 1 | 4 | 1 | 3 | 2 | 3 | 2 | 2 | 1 | 2 |
| 7 | 2 | 3 | 3 | 2 | 4 | 1 | 3 | 1 | 4 | 1 | 3 | 1 | 3 | 1 |
| 8 | 2 | 4 | 4 | 4 | 1 | 2 | 2 | 4 | 3 | 4 | 1 | 3 | 4 | 3 |
| 9 | 3 | 1 | 2 | 4 | 4 | 3 | 2 | 4 | 4 | 3 | 1 | 3 | 1 | 1 |
| 10 | 3 | 2 | 4 | 1 | 2 | 4 | 3 | 1 | 3 | 2 | 3 | 1 | 2 | 3 |
| 11 | 3 | 3 | 2 | 3 | 1 | 1 | 1 | 3 | 1 | 4 | 2 | 2 | 4 | 4 |
| 12 | 3 | 4 | 1 | 1 | 2 | 2 | 4 | 2 | 2 | 1 | 4 | 4 | 3 | 2 |
| 13 | 4 | 1 | 3 | 1 | 2 | 2 | 2 | 1 | 2 | 4 | 3 | 1 | 4 | 2 |
| 14 | 4 | 2 | 1 | 3 | 4 | 1 | 4 | 3 | 1 | 1 | 1 | 3 | 3 | 4 |
| 15 | 4 | 3 | 4 | 2 | 1 | 4 | 3 | 4 | 3 | 3 | 4 | 4 | 1 | 3 |
| 16 | 4 | 4 | 2 | 2 | 3 | 3 | 1 | 2 | 4 | 2 | 2 | 2 | 2 | 1 |

the efficiency of the implementation. Second, although it is an optimization heuristic, TA will eventually—that is, with the number of iterations going to infinity—converge with a probability as close to 1 as one likes and to a solution as close to the global optimum as one needs. For a proof of this global convergence property, see Althöfer and Koschnick (1991).

## 6. NUMERICAL RESULTS

As a first instance for a test of these two algorithms (FP and TA) and our hypothesis on the connection between uniformity and orthogonality, we use $U_{16}(4^5)$. The results are given in Tables 4 and 5. We denote the designs obtained by FP with F$D_2$, FS, F$C$, and F$M$, and the results obtained by TA with T$D_2$, T$S$, T$C$, and T$M$, respectively, where $D_2, S, C$, and $M$ stand for the different $L_2$ discrepancies $D_2, CL_2, SL_2$, and $ML_2$ introduced in Section 4.

Table 4 presents the designs obtained by FP, and the results for TA are contained in Table 5. By rearranging rows and columns, the first two columns can be made identical for all cases that we have listed in columns (1) and (2). Columns $(L3), (L4)$, and $(L5)$ in Table 4 show the last three columns of the canonical orthogonal design $L_{16}(4^5)$ given in many textbooks. Columns $(D_2^3), (D_2^4)$, and $(D_2^5)$ give the last three columns of the design obtained by FP under $D_2$. The third columns of $U_{16}$ under $SL_2, CL_2$, and $ML_2$ are the same and are given by the column with heading $(S, C, M3)$. Similarly, column $(C, S4)$ gives the fourth column of $U_{16}$ under $CL_2$ and $SL_2$. The other columns of Table 4 show the fourth and fifth columns of $U_{16}$ under $CL_2, SL_2$, and $ML_2$, respectively. In Table 5, corresponding notation is used for the designs obtained by TA under the preceding four $L_2$ discrepancies.

Tables 6 and 7 summarize the $D, D_2, SL_2, CL_2$, and $ML_2$ values for all the designs listed in Tables 4 and 5. Again, in the first column the letter F denotes designs obtained by the FP, and designs marked with T were generated by TA. Finally, the canonical orthogonal design given in Table 4 is labeled with an O. As before, $D_2, S, C$, and $M$ stand for the four $L_2$-type measures of nonuniformity $D_2, SL_2, CL_2$, and $ML_2$, respectively. The last figure indicates how many columns of the design have been considered. For example, F$D_2$5 means the design with five columns obtained by FP under $D_2$. T$S$5 is the design with five columns obtained by TA under $SL_2$. For each of these designs, the discrepancy $D$ and the four $L_2$-type discrepancies $(D_2, SL_2, CL_2$, and $ML_2)$ are calculated. The last two columns of the table indicate whether the corresponding design is DO or at least CO.

Let us first look at the results in Table 6. We find the following:

1. All nine designs (from O5 to T$M$5) have the same discrepancy $(D)$. Only some of them are DO. That means that the discrepancy is not sensitive enough to distinguish different designs with regard to their orthogonality. There-

Table 6. Comparison Among $U_{16}(4^5)$ (full dimension)

| Meas. | $D$ | $D_2$ | $SL_2$ | $CL_2$ | $ML_2$ | DO | CO |
|---|---|---|---|---|---|---|---|
| O5 | .4871 | .00244 | .9807 | .0428 | .0944 | Y | Y |
| F$D_2$5 | .4871 | .00076 | 1.067 | .0515 | .1059 | N | N |
| F$S$5 | .4871 | .00093 | .8854 | .0447 | .0972 | N | Y |
| F$C$5 | .4871 | .00091 | .9523 | .0425 | .0928 | Y | Y |
| F$M$5 | .4871 | .00081 | .9524 | .0425 | .0921 | Y | Y |
| T$D_2$5 | .4871 | .00066 | .9843 | .0483 | .0999 | N | N |
| T$S$5 | .4871 | .00083 | .8389 | .0450 | .0979 | Y | Y |
| T$C$5 | .4871 | .00083 | .8822 | .0417 | .0916 | Y | Y |
| T$M$5 | .4871 | .00083 | .8962 | .0421 | .0914 | Y | Y |

Table 7. Comparison Among $U_{16}(4^5)$ (lower dimension)

| Meas. | $D$ | $D_2$ | $SL_2$ | $CL_2$ | $ML_2$ | DO | CO |
|---|---|---|---|---|---|---|---|
| 2-dim. | .2344 | .00357 | .0571 | .0114 | .0140 | Y | Y |
| O$D_2$3 | .3301 | .00211 | .1348 | .0189 | .0284 | Y | Y |
| O$S$3 | .3301 | .00211 | .1348 | .0189 | .0284 | Y | Y |
| O$C$3 | .3301 | .00211 | .1348 | .0189 | .0284 | Y | Y |
| O$M$3 | .3301 | .00211 | .1348 | .0189 | .0284 | Y | Y |
| F$D_2$3 | .3301 | .00209 | .1407 | .0192 | .0286 | N | N |
| F$S$3 | .3301 | .00211 | .1348 | .0189 | .0284 | Y | Y |
| F$C$3 | .3301 | .00211 | .1348 | .0189 | .0284 | Y | Y |
| F$M$3 | .3301 | .00211 | .1348 | .0189 | .0284 | Y | Y |
| T$D_2$3 | .3301 | .00237 | .1539 | .0202 | .0299 | N | N |
| T$S$3 | .3301 | .00227 | .1466 | .0195 | .0291 | Y | Y |
| T$C$3 | .3301 | .00216 | .1390 | .0190 | .0285 | Y | Y |
| T$M$3 | .3301 | .00223 | .1426 | .0190 | .0286 | Y | Y |
| O$D_2$4 | .4138 | .00144 | .3345 | .0285 | .0521 | Y | Y |
| O$S$4 | .4138 | .00144 | .3345 | .0285 | .0521 | Y | Y |
| O$C$4 | .4138 | .00144 | .3345 | .0285 | .0521 | Y | Y |
| O$M$4 | .4138 | .00144 | .3345 | .0285 | .0521 | Y | Y |
| F$D_2$4 | .4138 | .00119 | .3813 | .0309 | .0541 | N | N |
| F$S$4 | .4138 | .00128 | .3311 | .0284 | .0519 | N | Y |
| F$C$4 | .4138 | .00128 | .3311 | .0284 | .0519 | Y | Y |
| F$M$4 | .4138 | .00124 | .3311 | .0284 | .0519 | Y | Y |
| T$D_2$4 | .4138 | .00125 | .4380 | .0330 | .0573 | N | N |
| T$S$4 | .4138 | .00138 | .3523 | .0307 | .0550 | Y | Y |
| T$C$4 | .4138 | .00135 | .3531 | .0288 | .0524 | Y | Y |
| T$M$4 | .4138 | .00128 | .3584 | .0289 | .0524 | Y | Y |

fore, the discrepancy is not suitable for the purpose of this article.

2. The designs obtained by FP and TA under the standard $L_2$ discrepancy ($D_2$) and the symmetric $L_2$ discrepancy ($SL_2$) are not DO, the latter being CO, whereas the designs generated by both algorithms under $CL_2$ and $ML_2$ are DO.

3. If we look at the designs O5, F$S$5, T$S$5, T$C$5, and T$M$5 that are orthogonal, the canonical orthogonal design (O5) exhibits the largest $D_2$ value. Looking at the other three measures of nonuniformity, we might conclude that the canonical orthogonal design (O5) is not the best one. For example, the designs T$C$5 and T$M$5 have lower values than the orthogonal design under all measures. It is difficult to give a ranking of the other four orthogonal designs F$S$5, T$S$5, T$C$5, and T$M$5. The best value for each measure, however, is always related to a design generated by TA.

4. To summarize our comparison of the full-dimensional cases, we might say that TA beats FP.

Now, let us study the two-dimensional cases. In the two-dimensional case all the methods produce the same design that is orthogonal. The first row of Table 7 gives its discrepancies. Following this line, three blocks of Table 7 show three-dimensional results from the canonical orthogonal design, the FP and TA. We find that three different columns of the orthogonal design may have different discrepancies. For fair comparisons, we choose the best result of all six possible choices in Table 8 to put in Table 7. Similarly, we choose the best three columns of T$D_2$, T$S$, T$C$, and T$M$ and put their discrepancies into Table 7. The designs obtained by FP automatically give the required results. This is because in each step, FP only adds the column that results in minimum discrepancy. Similarly, we get another three blocks for the four-dimensional case. From these results we conclude the following:

1. In the low-dimensional cases, the FP very often gives better results than TA that is based on the full design. If we run TA directly on the low-dimensional problem, however,

Table 8. Discrepancies of Lower-Dimensional Projections of O5

| Columns | $D_2$ | $SL_2$ | $CL_2$ | $ML_2$ | DO | CO |
|---|---|---|---|---|---|---|
| O(1, 2, 3) | .00278 | .1778 | .01959 | .0291 | Y | Y |
| O(1, 2, 4) | .00223 | .1426 | .01904 | .0286 | Y | Y |
| O(1, 2, 5) | .00223 | .1426 | .01904 | .0286 | Y | Y |
| O(2, 3, 4) | .00211 | .1348 | .01892 | .0284 | Y | Y |
| O(2, 3, 5) | .00211 | .1348 | .01892 | .0284 | Y | Y |
| O(3, 4, 5) | .00211 | .1348 | .01892 | .0284 | Y | Y |
| O(1, 2, 3, 4) | .00174 | .3949 | .02940 | .0533 | Y | Y |
| O(1, 2, 3, 5) | .00174 | .3949 | .02940 | .0533 | Y | Y |
| O(1, 2, 4, 5) | .00174 | .3949 | .02940 | .0533 | Y | Y |
| O(2, 3, 4, 5) | .00144 | .3345 | .02846 | .0521 | Y | Y |

it can always provide designs with smaller discrepancy than FP. The reason is that FP searches only a small fraction of the possibilities, due to its sequential generation, whereas TA can freely move over all possible designs.

2. Comparing the standard OD and the new UD's we find that (a) O5 has a poor $L_2$ discrepancy, and (b) combining results on $SL_2, CL_2$, and $ML_2$ discrepancies, the performance of the standard OD is, in general, acceptable.

From the results on $U_{16}(4^5)$, we find that orthogonality of the design can be induced by uniformity. Is it true for other designs? Following our approach for $U_{16}(4^5)$, we applied the TA algorithm to several designs such as $U_4(2^3), U_8(2^7), U_{16}(2^{15}), U_{12}(2^{11}), U_9(3^4), U_{12}(3 \times 2^3), U_{16}(4 \times 2^{12}), U_{16}(4^2 \times 2^9), U_{16}(4^3 \times 2^6), U_{16}(4^4 \times 2^3), U_{18}(2 \times 3^7)$, and $U_{25}(5^6)$ under the three discrepancies $SL_2, CL_2$, and $ML_2$. The related results were given by Fang and Winker (1998). We can summarize our findings as follows:

1. Most (nearly) uniform designs obtained by TA under $SL_2, CL_2$, and $ML_2$ are orthogonal (at least CO) and are different from the standard orthogonal design, whose first row has all level 1s.

2. The three uniform designs obtained under the different measures of nonuniformity are often different, although they are all orthogonal. This fact raises the question of how to choose a suitable orthogonal design for a specific experiment.

Our initial guess that UD's under suitable measures of uniformity may be orthogonal is not contradicted by our findings for the problems we have studied so far. Hence, we will formulate our guess in the following conjecture.

*Conjecture.* For given parameters $(n, s; q_1, \ldots, q_s)$, the corresponding UD under one of the three discrepancies $SL_2, CL_2$, and $ML_2$ is also an OD, if the OD with $(n, s; q_1, \ldots, q_s)$ exists.

## 7. CONCLUDING REMARKS

A UD seeks design points that are uniformly scattered on the domain. It has been popularly used since 1980 (Fang 1980). Apart from the application examples given previously (mostly on computer experiments), the UD has been applied to other areas, as we shall discuss. We anticipate more UD applications in the future. As a summary, we list the following steps for the use of UD's.

1. Choose the factors and the experimental domain; determine a suitable number of levels for each factor.

2. Choose a suitable UD table related to the number of factors and levels.

3. Record the responses of experiments implemented according to the UD.

4. Use regression analysis to establish a regression model (1.3) that fits the experimental data well.

5. Find the "best" combination of the factor values that maximizes/minimizes the response and verify the claim with further experiments.

Each step may involve various difficulties. For example, finding a suitable regression model in Step 4 is a nontrivial problem.

Experiments with mixtures often appear in the design of food, chemical, and metallurgical products (e.g., see Cornell 1990). A design of experiments with mixtures is a set of points over the domain $T_s = \{(x_1, \ldots, x_s)\colon 0 \le x_j \le 1, j = 1, \ldots, s, x_1 + \cdots + x_s = 1\}$. The so-called UD of experiments with mixtures suggests uniformly scattering the experimental points on the simplex $T_s$. Fang and Wang (1994) proposed a method of generating UD of experiments with mixtures by the inverse transformation method.

One purpose of quality engineering is to produce a product that is *robust* with respect to noise factors. Robustness implies that the product's functional characteristics are not sensitive to variation caused by noise factors. Taguchi (1986) suggested two orthogonal designs, the *inner table* and the *outer table* for selecting the levels of the inner array factors to minimize the effect of the noise (outer array) factors. Let $L_n(p^r)$ and $L_m(q^s)$ be the inner and outer arrays in a parameter design. The total number of experiments required is $N = nm$. It is known that $n$ and $m$ are not small when $p$ and $q$ are moderate. As a result, the total number $N$ is large. This is one major weakness of Taguchi's approach (Taguchi 1986). Instead, we use two UD designs, $U_{n_*}(n_*^r)$ and $U_{m_*}(m_*^q)$, to replace $L_n(p^r)$ and $L_m(q^s)$, respectively. The total number of experiments becomes $N_* = n_* m_*$, which can be significantly smaller than $N$. Several authors have applied this idea to their work. Using UD to design outer-array points, in fact, was recommended by Wang, Lin, and Fang (1995).

In this article we also find that several orthogonal designs can be obtained by a unified method that minimizes a measure of nonuniformity over all related U-type designs. Definition 2 implies that the one- and two-dimensional projections of an orthogonal design are uniform in the sense that all elements appear the same number of times, whereby "elements" in the two-dimensional case means "pairs." Furthermore, UD's share the first property by Definition 2; that is, the one-dimensional projections are uniform in the sense that each element appears with the same frequency in each column. Instead of the second property, they exhibit $s$-dimensional uniformity. Hence, our results imply that the one-dimensional projection property and $s$-dimensional uniformity together may imply the two-dimensional projection property. We might expect to find new orthogonal designs by the proposed approach if the computer is powerful enough to generate uniform designs using the TA heuristic. The related theory will be investigated in the future.

A related problem consists of finding saturated (supersaturated) designs. These are designs for which the number of experiments equals (is less than) the number of parameters to be estimated. Several works, such as those of Lin (1993a,b, 1995) and Mukerjee and Wu (1995), have discussed how to find saturated and supersaturated designs. We believe that the approach given in this article can be applied to construct new and useful saturated (supersaturated) designs.

## ACKNOWLEDGMENTS

We thank the editor, an associate editor, and the referees for their constructive criticism. This work was partially supported by a Hong Kong UGC grant. Dennis Lin is partially supported by the National Science Foundation via grant DMS-9704711 and the National Science Council of the Republic of China via contract NSC 87-2119-M-001-007.

*[Received April 1998. Revised August 1999.]*

## REFERENCES

Althöfer, I., and Koschnick, K.-U. (1991), "On the Convergence of Threshold Accepting," *Applied Mathematics and Optimization*, 24, 183–195.

Bose, R. C., and Bush, K. A. (1952), "Orthogonal Arrays of Strength Two and Three," *The Annals of Mathematical Statistics*, 23, 508–524.

Bose, R. C., Chakravarti, I. M., and Knuth, D. E. (1960), "On Methods of Constructing Sets of Mutually Orthogonal Latin Squares Using a Computer, I," *Technometrics*, 2, 507–516.

——— (1961), "On Methods of Constructing Sets of Mutually Orthogonal Latin Squares Using a Computer, II," *Technometrics*, 3, 111–117.

Cornell, J. A. (1990), *Experiments With Mixtures: Design, Models, and the Analysis of Mixture Data* (2nd ed.), New York: Wiley.

Dehnad, K. (1989), *Quality Control, Robust Design, and the Taguchi Method*, Belmont, CA: Wadsworth & Brooks, Cole.

Dueck, G., and Scheuer, T. (1991), "Threshold Accepting: A General Purpose Algorithm Appearing Superior to Simulated Annealing," *Journal of Computational Physics*, 90, 161–175.

Fang, K. T. (1980), "The Uniform Design: Application of Number-Theoretic Methods in Experimental Design," *Acta Mathematicae Applagatae Sinica*, 3, 363–372.

——— (1994), *Uniform Design and Uniform Design Tables*, Beijing: Science Press.

Fang, K. T., Lin, D. K. J., and Zhang, Y. (1998), "Uniform Design: Theory and Applications," Working Paper, Series in Management Science 98-6, Pennsylvania State University, Dept. of Management Science and Information Systems.

Fang, K. T., and Wang, Y. (1994), *Number-Theoretic Methods in Statistics*, London: Chapman & Hall.

Fang, K. T., and Winker, P. (1998), "Uniformity and Orthogonality," Technical Report MATH-1176, Hong Kong Baptist University, Dept. of Mathematics.

Heinrich, S. (1995), "Efficient Algorithms for Computing the $L_2$-Discrepancy," Report 267/95, University of Kaiserslautern, Dept. of Computing.

Hickernell, F. J. (1998), "A Generalized Discrepancy and Quadrature Error Bound," *Mathematics of Computation*, 67, 299–322.

Hua, L. K., and Wang, Y. (1981), *Applications of Number Theory to Numerical Analysis*, Berlin: Springer-Verlag, and Beijing: Science Press.

Lin, D. K. J. (1993a), "A New Class of Supersaturated Designs," *Technometrics*, 35, 28–31.

——— (1993b), "Another Look at First-Order Saturated Designs: The *p*-Efficient Designs," *Technometrics*, 35, 284–292.

——— (1995), "Generating Systematic Supersaturated Designs," *Technometrics*, 37, 213–225.

McKay, M. D., Beckman, R. J., and Conover, W. J. (1979), "A Comparison of Three Methods for Selecting Values of Input Variables in the Analysis of Output From a Computer Code," *Technometrics*, 21, 239–245.

Mukerjee, R., and Wu, C. F. J. (1995), "On the Existence of Saturated and Nearly Saturated Asymmetrical Orthogonal Arrays," *The Annals of Statistics*, 23, 2102–2115.

Niederreiter, H. (1992), *Random Number Generation and Quasi-Monte Carlo Methods* (CBMS–NSF Regional Conference Series in Applied Mathematics), Philadelphia: Society of Industrial and Applied Mathematics.

Pukelsheim, F. (1993), *Optimal Design of Experiments*, New York: Wiley.

Raghavarao, D. (1971), *Constructions and Combinatorial Problems in Design of Experiments*, New York: Wiley.

Riccomagno, E., Schwabe, R., and Wynn, H. P. (1997), "Lattice-based *D*-Optimum Design for Fourier Regression," *The Annals of Statistics*, 25, 2313–2327.

Sacks, J., Welch, W. J., Mitchell, T. J., and Wynn, H. P. (1989), "Designs and Analysis of Computer Experiments," *Statistical Science*, 4, 409–435.

Taguchi, G. (1986), *Introduction to Quality Engineering*, Tokyo: Asian Production Organization.

Wang, Y., and Fang, K. T. (1981), "A Note on Uniform Distribution and Experimental Design," *KeXue TongBao*, 26, 485–489.

Wang, Y. J., Lin, D. K. J., and Fang, K. T. (1995), "Designing Outer Array Points," *Journal of Quality Technology*, 27, 226–241.

Warnock, T. T. (1972), "Computational Investigations of Low Discrepancy Point Sets," in *Applications of Number Theory to Numerical Analysis*, ed. S. K. Zaremba, New York: Academic Press, pp. 319–343.

Wiens, D. P. (1991), "Designs for Approximately Linear Regression: Two Optimality Properties of Uniform Designs," *Statistics & Probability Letters*, 12, 217–221.

Winker, P. (1995), "Identification of Multivariate AR-Models by Threshold Accepting," *Computational Statistics and Data Analysis*, 20, 295–307.

Winker, P., and Fang, K.-T. (1997), "Application of Threshold Accepting to the Evaluation of the Discrepancy of a Set of Points," *SIAM Journal on Numerical Analysis*, 34, 2028–2042.

——— (1998), *Optimal U-type Designs*, in *Monte Carlo and Quasi-Monte Carlo Methods 1996* (Lecture Notes in Statistics 127), eds. H. Niederreiter, P. Zinterhof, and P. Hellekalek, New York: Springer-Verlag, pp. 436–448.

Xie, M. Y., and Fang, K. T. (1996), "Admissibility and Minimaxity of the Uniform Design Measure in Nonparametric Regression Models," Technical Report MATH-136, Hong Kong Baptist University, Dept. of Mathematics.

Zhang, Y. (1996), "Modeling and Simulation for Launching Dynamics of Ship Based Vehicle," BSC report, Beijing Simulation Center, Beijing, China.