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Uniform Experimental Designs and their Applications in Industry*

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The uniform experimental design is one kind of space filling designs that can be used for computer experiments and also for industrial experiments when the underlying model is unknown. The uniform design seeks its design points to be uniformly scattered on the experimental domain. In this chapter we shall introduce the theory and method of the uniform design and related data analysis and modelling methods. Applications of the uniform design to industry and other areas are discussed.

1. Introduction

Consider the simple fact that where there is an effect, there is a cause. Engineers are constantly faced with the problem of distinguishing between the effects that are caused by particular factors and those are due to random error, or specifically building an empirical model between the input (experimental) variables and the output (response) variables.

Industrial management is becoming increasingly aware of the benefits of running statistically designed experiments. Statistical designs, developed by Sir R. A. Fisher in the 1920s, largely originated from agricultural problems. Designing experiments for industrial problems and designing experiments for agricultural problems are similar in their basic concerns. There are, however, many differences (see Lin, 2000). Many new types of designs have been proposed in the recent years for solving industrial problems. A comprehensive introduction to these designs can be found in *Handbook of Statistics*, Vol. 13 (edited by Ghosh and Rao, 1996). This chapter introduces an important class of designs, called *Uniform Design*.

Most experimental designs, like orthogonal and optimal designs, assume that the underlying model is known with some unknown parameters such as main effects, interactions, regression coefficients and choose a design such that estimation of the parameters has the highest efficiency. However, the experimenter in many experiments

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does not know the underlying model. A space filling design becomes the best choice in this case. In computer experiments, the underlying model is known, but too complicated. In this case we can treat the model as a black box or unknown. Both cases need a space filling design. The uniform design (UD) is one of space filling designs and it seeks experimental points to be uniformly scattered on the domain. The UD was proposed by Fang and Wang (Fang, 1980; Wang and Fang, 1981) and has been popularly used since 1980. The UD has several advantages. It can explore relationships between the response and the factors with a reasonable number of runs and is shown to be robust to the underlying model specifications. For practical ease, most uniform designs have been constructed and tabulated for the practitioners. In the past decade there were a lot of UD publications in theory and applications, for example, Fang and Wang (1994), Fang and Hickernell (1995), Hickernell (1999), Fang and Mukerjee (2000), Xie and Fang (2000), Fang and Lin (2000), Fang, Lin, Winker and Zhang (2000), Hickernell and Liu (2002), Fang and Ma (2000) and Fang (2002).

This chapter is organized as follows. Section 2 gives a background for understanding the uniform design. In Section 3, we describe how to implement the uniform design in practice, illustrated by a real life example. It is hoped that the practitioner will know how to implement uniform design from reading this section. Section 4 discusses how to apply the uniform design in other environments, such as mixed level problems, categorical factors and mixture experiments. The construction methods of uniform designs are introduced in Section 5. The related theory and algorithms are reviewed and discussed. Most uniform design tables are available on the website at `http://www.math.hkbu.edu.hk/UniformDesign`, called as **UD-web** for short. Section 6 focuses on the important problem of computer experiments. The role of uniform design in computer experiments is investigated. It is found that the uniformity is also an important criterion in other type of experimental designs. Section 7 discusses the connections between uniformity and other popular design criteria, such as isomorphism, resolution, aberration, orthogonality, and confounding. The applications of uniform design in construction of supersaturated designs and in modern quality engineering are given at the end.

2. Preliminaries

Suppose that there are s factors in a factorial experiment; each factor has q levels. The total number of level-combinations is then q^s. This is too large to be implemented even when s and q are moderate. Therefore, two-level and three-level factorial designs are commonly used. If the higher-order interactions of the factors can be ignored, a fractional factorial design with a smaller run size can be used. Among all types of fractional factorial designs, orthogonal array is probably the most efficient and popular one.

In many experiments one wishes to explore relationship between the response and factors and to predict the response at any point in the experimental domain. Regression models can be used for fitting the experimental data resulted from a factorial plan. When the relationship between the response and factors is nonlinear or when the experimental

domain is large, two-level designs are shown to be insufficient. Often the experimenter does not know the model between the response (y) and the factors ($x_1, \ldots, x_s$, say) in the process. One wishes that the design is robust against different model assumptions. Suppose that the response and the factors in an experiment have a regression model

$$y = g(x_1, \ldots, x_s) + \varepsilon, \tag{2.1}$$

where the function g is unknown and ε is the random error. When the function g is a polynomial (of first-order or second-order, say), the corresponding model (2.1) is called a response surface model (see, for example, Box and Draper, 1987; Myers and Montgomery, 1995; Draper and Lin, 1996).

When the underlying mathematical function g in (2.1) is complex and nonlinear, one can use an approximately linear model to replace the original model (2.1)

$$y = \sum_{i=1}^{m} g_i(x_1, \ldots, x_s) + h(x_1, \ldots, x_s) + \varepsilon, \tag{2.2}$$

where all the functions g_i's are known and the function h denotes the departure of the model (2.2) from the true one (2.1). A robust design is useful in this case (Hickernell, 1999). In fact, the experimenter may not know all the g_i's due to lack of knowledge about the process. In this case the model (2.1) is called a *nonparametric regression model*, for which the best design should be a space-filling design (Doehlert, 1970; Hickernell, 1999; Xie and Fang, 2000). As we shall see that the uniform design is a good choice. Computer models are often used in science and engineering fields to describe complicated physical phenomena which is governed by a set of equations, including linear, nonlinear, ordinary, and partial differential equations. The equations are often too difficult to be solved simultaneously, but can be simulated by the computer modelling program. We can express the relationship between the input $(x_1, \ldots, x_s)$ and the output y as

$$y = f(x_1, \ldots, x_s), \tag{2.3}$$

where the function f has no analytic expression. One may wish to do simulation on a computer to simulate the behavior of the device/process and to find an approximate model that is much simpler than the true one (cf. Fig. 1). These programs, due to the number and complexity of the equations, require special designs. Designing computer

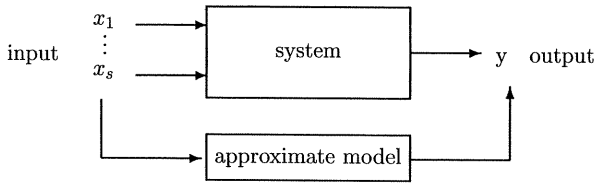

Fig. 1. Computer experiments.

experiments has received a great deal of attention in the recent literature. See, for example, Bates, Buck, Riccomagno and Wynn (1996) and Koehler and Owen (1996). The later gave a comprehensive review on designs of computer experiments. The uniform design was in fact motivated by three system engineering projects in 1978 (see Fang, 1980; Wang and Fang, 1981). In the past two decades, the uniform design has been successfully applied in other areas, such as industry, system engineering, pharmaceutics, and natural sciences.

3. Implementation of the uniform design in industrial experiments

The uniform design employs many terminologies form the factorial design such as level, level-combination, etc., but the underlying model is (2.1) for industrial experiment and is (2.3) for computer experiments. Uniform designs have been tabulated. Each uniform design table has a notation $U_n(q^s)$, where 'U' stands for UD, n for the number of runs, s for the number of factors and q for the number of levels. For implementing the uniform design in industrial experiments the following steps are necessary:

1. Choose factors and experimental domain as well as determine suitable number of levels for each factor.
2. Choose a suitable UD table to accommodate the number of factors and levels. This can be easily done by visiting the UD-web.
3. From the uniform design table, randomly determine the run order of experiments and conduct the experiments.
4. Find a suitable model to fit the data. Regression analysis, neural networks, wavelets, multivariate splines, sliced inverse regression and principal Hessian direction are useful in modelling.
5. Knowledge discovery from the built model. Find the 'best' combination of the factor-values that maximizes/minimizes the response and verify the prediction with further follow-up experiments.

We next illustrate the procedure of implementing uniform design, step by step. A chemical experiment is conducted in order to find the best setup to increase the yield. Three factors are under consideration: the ratio of raw materials (X_1), the amount of pyridine (X_2), and the time length of the reaction (X_3). The response variable is designated as the yield (Y). Unfortunately, the experimenter does not know the underlying relationship between y and (X_1, X_2, X_3).

The experimental domain is chosen to be $[1, 3.4] \times [10, 28] \times [0.5, 3.5]$ and each factor takes 7 levels in this domain as follows:

X_1, the ratio of raw materials (in %): 1.0, 1.4, 1.8, 2.2, 2.6, 3.0, 3.4;
X_2, the amount of pyridine (in ml): 10, 13, 16, 19, 22, 25, 28;
X_3, the time length of reaction (in hours): 0.5, 1.0, 1.5, 2.0, 2.5, 3.0, 3.5.

This experiment could be arranged with a UD table of the form $U_n(7^3)$, meaning an n-run uniform design for three factors, each at seven levels (see next section for the formal definition). It turns out that the experimenter chose $U_7(7^3)$ design that

Table 1
$U_7(7^3)$ and related design

No.	**1**	**2**	**3**	x_1	x_2	x_3	Y
1	1	5	4	1.0	22	2.0	0.6146
2	2	2	2	1.4	13	1.0	0.3506
3	3	7	6	1.8	28	3.0	0.7537
4	4	3	7	2.2	16	3.5	0.8195
5	5	6	1	2.6	25	0.5	0.0970
6	6	1	5	3.0	10	2.5	0.7114
7	7	4	3	3.4	19	1.5	0.4186

is listed in the left portion of Table 1. The seven levels marked by $1, 2, \ldots, 7$ are transformed into the real levels of the factors. Randomize the order of these 7 level-combinations, implement the experiments, and record the corresponding yield Y (see Table 1). Specifically, the heading of **(1, 2, 3)** in Table 1 represents the uniform design table for three factors in seven runs. Such a table can be easily found from the UD-web. The heading of (x_1, x_2, x_3) in Table 1 represents the actual experimental values for these three factors. The very last column Y gives the responses of the experimental results.

The major goal of the data analysis is to establish a suitable model. The best result among the seven responses is $y_4 = 81.95\%$ at $X_1 = 2.2$, $X_2 = 16$ and $X_3 = 3.5$. This can be served as a benchmark. We wish to know whether there is any level-combination to produce a better yield. The simplest model is the first-order regression:

$$E(Y) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3.$$

Based on the data in Table 1 and by model selection techniques in regression analysis, the resulting model turns out to be

$$E(Y) = 0.0713 + 0.2333 x_3$$

with $R^2 = 93.96\%$ and $s^2 = 0.381$. This model is not satisfactory to the engineers. Therefore, a more complicated second-order centered quadratic regression is considered,

$$\begin{aligned} E(Y) = {} & \beta_0 + \beta_1(x_1 - \bar{x}_1) + \beta_2(x_2 - \bar{x}_2) + \beta_3(x_3 - \bar{x}_3) + \beta_{11}(x_1 - \bar{x}_1)^2 \\ & + \beta_{22}(x_2 - \bar{x}_2)^2 + \beta_{33}(x_3 - \bar{x}_3)^2 + \beta_{12}(x_1 - \bar{x}_1)(x_2 - \bar{x}_2) \\ & + \beta_{13}(x_1 - \bar{x}_1)(x_3 - \bar{x}_3) + \beta_{23}(x_2 - \bar{x}_2)(x_3 - \bar{x}_3). \end{aligned}$$

In this data set, $\bar{x}_1 = 2.2$, $\bar{x}_2 = 19$ and $\bar{x}_3 = 2.0$. Once again, by using model selection techniques, the final model is

$$\begin{aligned} E(Y) = {} & 0.595 + 0.232(x_3 - 2) - 0.054(x_3 - 2)^2 \\ & + 0.0547(x_1 - 2.2)(x_3 - 2) \end{aligned} \tag{3.1}$$

with $R^2 = 99.83\%$ and $s^2 = 0.00023$. The corresponding ANOVA table is given in Table 2.

Statistical diagnostics such as residual plots, partial residual plots, and normal plots indicate that Model (3.1) is acceptable. Note that Model (3.1) does not include factor X_2. This indicates that factor X_2 has less influence on Y within the experimental domain. Furthermore, contours of Y against (x_1, x_3) in Figure 2 show that (i) there are interactions between factors X_1 and X_3; and (ii) the maximum value of the response is located at the boundary of the domain.

Table 2
ANOVA table (SAS output)

Source	DF	Sum of Squares	Mean Square	F Value	Prob>F
Model	3	0.40488	0.13496	595.722	0.0001
Error	3	0.00068	0.00023		
C Total	6	0.40556			
Root MSE	0.01505	R-square	0.9983	C.V.	2.79813
Dep Mean	0.53791	Adj R-sq	0.9966		

Parameter Estimates

Variable	DF	Parameter Estimate	Standard Error	T for H0: Parameter = 0	Prob > |T|
INTERCEPT	1	0.595071	0.00871685	68.267	0.0001
$x_3 - 2$	1	0.231759	0.00569920	40.665	0.0001
$(x_3 - 2)^2$	1	−0.054033	0.00670981	−8.053	0.0040
$(x_1 - 2.2)(x_3 - 2)$	1	0.054669	0.01196354	4.570	0.0197

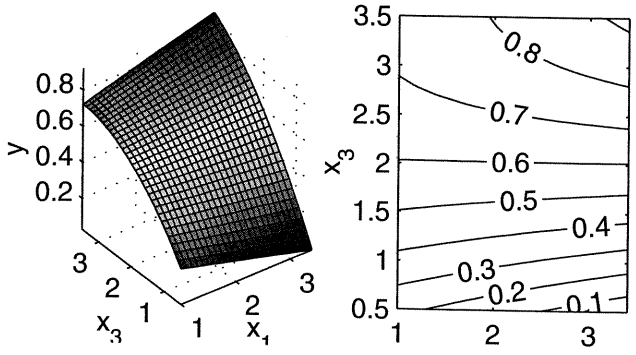

Fig. 2. Contours of Y against x_1 and x_2.

For searching the 'best' combination of the factor-value we maximize Y with respect to x_1 and x_3 under the model (3.1) over the domain $D = \{(x_1, x_3)\colon 1 \leqslant x_1 \leqslant 3.4,\ 0.5 \leqslant x_3 \leqslant 3.5\}$, that is to find (x_1^*, x_3^*) such that

$$\widehat{Y}(x_1^*, x_3^*) = \max_D \widehat{Y}(x_1, x_2),$$

where $\widehat{Y}(x_1, x_2)$ is given by (3.1). By any optimization algorithm, it is easily found that $x_1^* = 3.4, x_3^* = 3.5$ and the corresponding response $\widehat{Y}(3.4, 3.5) = 91.87\%$ is the maximum. However, this is only a statistical prediction and further verification with confirmatory experiment is needed.

The simplest way for additional experiments is to run a few experiments at $x_1 = 3.4, x_3 = 3.5$ and $x_2 = 19$. As factor X_2 does not appear in the model, we take its average value 19. The experimenter ran three such additional experiments and found the corresponding responses as 91.05%, 92.11% and 91.53%, respectively. The mean of these three responses is 91.56% that is close to the prediction 91.87%. Thus, one can conclude the best combination is $x_1 = 3.4, x_2 = 19, x_3 = 3.5$ indeed.

Since the best combination is on the boundary, it is wise to expand the experimental domain. For example, an additional 2-factor experiment with levels

$$x_1\colon 3.0, 3.4, 3, 8, 4.2; \qquad x_3\colon 3.0, 3.5, 4.0, 4.5$$

using the UD table $U_4(4^2)$ is recommended for such an additional experiment.

Besides the polynomial regression model, there are many other methods for modelling such as wavelets, B-spline function, spatial modelling techniques and Kriging (see Koehler and Owen, 1996; Sacks, Welch, Mitchell and Wynn, 1989 for details). We shall discuss the B-spline function and related modelling techniques in Section 6.

4. Uniform design in other environments

Suppose that there are s factors in an experiment and the experimental domain is a hyper-rectangle. The UD arranges experimental points to be uniformly scattered on the domain. Finding the most uniform design is a very difficult optimization problem, i.e., a NP hard problem. Therefore, a reasonable structure for UDs is needed. The so-called U-type design gives a good structure. A detailed discussion will be given in Section 5.2. Suppose that there are s factors each having q levels in an experiment. There are q^s level-combinations.

DEFINITION 1. A U-type design denoted by $U(n; q^s)$ is a matrix of n rows and s columns with entries $\{1, \ldots, q\}$ such that q entries in each column appear equally often.

A U-type design $U(n; q^s)$ can be utilized as a design with n runs and s factors each having q levels. Obviously, the number of levels q should be a divisor of n. Note that a U-type table may have a poor uniformity. Let $\mathcal{U}(n; q^s)$ be the set of all U-type designs

$U(n; q^s)$ and M be a measure of uniformity over $\mathcal{U}(n; q^s)$ such that the smaller value of M, the better the uniformity of the design. See Section 5 for a formal definition on uniformity measure M.

DEFINITION 2. A design $\boldsymbol{U} \in \mathcal{U}(n; q^s)$ is called a uniform design under the measure M if

$$M(\boldsymbol{U}) = \min_{V \in \mathcal{U}(n;q^s)} M(\boldsymbol{V}) \tag{4.1}$$

and is denoted by $U_n(q^s)$.

The Uniform design is often displayed as a table, called a UD table. As examples, Tables 3 and 4 give two uniform designs $U_7(7^3)$ and $U_{12}(12^4)$, respectively. A number of UD tables can be found on the UD-web. Note that given (n, q, s), the corresponding uniform design is not unique. Two U-type design are called *equivalent* if one can be obtained from another by permuting rows and columns.

Table 3
$U_7(7^3)$

No.	**1**	**2**	**3**
1	1	5	4
2	2	2	2
3	3	7	6
4	4	3	7
5	5	6	1
6	6	1	5
7	7	4	3

Table 4
$U_{12}(12^4)$

No.	**1**	**2**	**3**	**4**
1	1	10	4	7
2	2	5	11	3
3	3	1	7	9
4	4	6	1	5
5	5	11	10	11
6	6	9	8	1
7	7	4	5	12
8	8	2	3	2
9	9	7	12	8
10	10	12	6	4
11	11	8	2	10
12	12	3	9	6

4.1. Experiment with mixed levels

The number of levels for different factors may not be the same, due to the need of the experiment or due to limitation of the experimental environment. The uniform design is also available for such a situation with mixed levels (see Fang, 1994). We next extend the definition of the uniform design to the case of mixed levels.

DEFINITION 3. A U-type design denoted by $U(n; q_1, \ldots, q_s)$ is a $n \times s$ matrix with elements $\{1, \ldots, q_j\}$ at the jth columns such that $\{1, \ldots, q_j\}$ appear in this column equally often. When some q_j are equal, we denote it by $U(n; q_1^{r_1} \times \cdots \times q_m^{r_m})$ with $r_1 + \cdots + r_m = s$.

Obviously, all $q_j (j = 1, \ldots, s)$ should be a divisor of n. Let $\mathcal{U}(n; q_1 \times \cdots \times q_s)$ be the set of all U-type designs $U(n; q_1 \times \ldots \times q_s)$. Similar to Definition 2, we have

DEFINITION 4. A design $\boldsymbol{U} \in \mathcal{U}(n; q_1, \ldots, q_s)$ is called a uniform design under the measure M if

$$M(\boldsymbol{U}) = \min_{V \in \mathcal{U}(n;q_1 \times \cdots \times q_s)} M(\boldsymbol{V})$$

and is denoted by $U_n(q_1 \times \cdots \times q_s)$.

For example, the $U_6(3^2 \times 2)$ design in Table 5 can be used for conducting an experiment with two 3-level factors and one 2-level factor.

There are situations where one cannot find an existing UD table to suitably fit the underlying experiment. In this case, the *pseudo-level* technique can be helpful. We explain the *pseudo-level* technique via the following example. Suppose that there are two 4-level factors and two 2-level factors in an experiment and one can not find any UD table in the literature. There are, however, many $U_{4m}(4^4)$ tables available. The left portion of Table 6 lists $U_8(4^4)$. Suppose that the first two columns of $U_8(4^4)$ are used for the two 4-level factors. We then merge the original levels in columns 3 and 4 by $(1, 2) \Rightarrow 1$ and $(3, 4) \Rightarrow 2$. By this process a U-type design $U(8; 4^2 \times 2^2)$ is generated (see the right-hand portion of Table 6). The new UD table with mixed levels may have a good uniformity. More discussion can be found in Section 5.3.

Table 5
$U_6(3^2 \times 2)$

No.	**1**	**2**	**3**
1	1	1	1
2	2	1	2
3	3	2	1
4	1	2	2
5	2	3	1
6	3	3	2

Table 6
$U_8(4^2 \times 2^2)$

No.	1	2	3	4	1	2	3	4
1	1	2	1	2	1	2	1	1
2	1	4	2	3	1	4	1	2
3	2	1	3	4	2	1	2	2
4	2	3	4	1	2	3	2	1
5	3	1	2	1	3	1	1	1
6	3	3	1	4	3	3	1	2
7	4	2	4	3	4	2	2	2
8	4	4	3	2	4	4	2	1

Table 7
$U_{12}(12^3 \times 3)$

No.	1	2	3	4
1	1	10	4	2
2	2	5	11	1
3	3	1	7	3
4	4	6	1	2
5	5	11	10	3
6	6	9	8	1
7	7	4	5	3
8	8	2	3	1
9	9	7	12	2
10	10	12	6	1
11	11	8	2	3
12	12	3	9	2

4.2. *Experiment with categorical factors*

The factors in factorial experiments can be quantitative or qualitative. The qualitative factors are also known as *categorical* or *indicator* factors. The uniform design can deal with categorical factors as well. The generalized linear model can be used for the data analysis and modelling.

Suppose that there are 3 quantitative factors X_1, X_2, X_3 each having 12 levels and one qualitative factor 'catalyst' X_4 with 3 catalysts c_1, c_2 and c_3. There is no existing UD table $U_{12}(12^3 \times 3)$. By the pseudo-level technique introduced in Section 4.1 we can construct a UD table $U_{12}(12^3 \times 3)$ from $U_{12}(12^4)$ as listed in Table 4. We have to choose one column of $U_{12}(12^4)$ to merge its 12 levels into 3 levels. There are four choices. The best of which is given in Table 7. Obviously, the factor 'catalyst' is put in the last column with 3 levels c_1, c_2 and c_3 and the three quantitative factors are put in the first three columns of the table.

For $i = 1, 2$, let $z_i = 1$ if $X_4 = c_i$ else $z_i = 0$. The z_1 and z_2 are called *dummy variables* that are used to describe which catalyst appear in the model. The simplest

linear model for this experimental data is

$$E(Y) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \gamma_1 z_1 + \gamma_2 z_2 \tag{4.2}$$

that also can be written as

$$E(Y) = \begin{cases} \beta_0 + \gamma_1 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3, & \text{if } X_4 = c_1, \\ \beta_0 + \gamma_2 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3, & \text{if } X_4 = c_2, \\ \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3, & \text{if } X_4 = c_3. \end{cases}$$

A quadratic model (or its centered version) would then be

$$E(Y) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{11} x_1^2 + \beta_{22} x_2^2 + \beta_{33} x_3^2 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta 23 x_2 x_3 + \gamma_1 z_1 + \gamma_2 z_2$$

and the model selection techniques in regression analysis can then be applied.

4.3. *Experiments with mixtures*

Many products are formed by mixtures of several ingredients, for example, building construction concrete consists of sand, water and one or more types of cement. Designs for deciding how to mix the ingredients are called *experimental designs with mixtures* that have played an important role in various fields such as chemical engineering, rubber industry, material and pharmaceutical engineering. A design of n runs for mixtures of s ingredients is a set of n points in the domain

$$T_s = \{(x_1, \ldots, x_s): x_j \geqslant 0,\ j = 1, \ldots, s,\ x_1 + \cdots + x_s = 1\}. \tag{4.3}$$

Cornell (1990) and references therein give a comprehensive review on designs of experiments with mixtures. Wang and Fang (1990), however, proposed the uniform design for experiments with mixtures that seeks experimental points to be uniformly scattered in the domain T_s. They employed the transformation method for construction of such uniform designs. Let $\boldsymbol{U} = (u_{ki})$ be a uniform design $U_n(n^{s-1})$ on C^{s-1}. Calculate $c_{ki} = (u_{ki} - 0.5)/n$ and

$$x_{ki} = \left(1 - c_{ki}^{1/(s-i)}\right) \prod_{j=1}^{i-1} c_{kj}^{1/(s-j)}, \quad i = 1, \ldots, s-1,$$

$$x_{ks} = \prod_{j=1}^{s-1} c_{kj}^{1/(s-j)}, \quad k = 1, \ldots, n.$$

Then $\{\boldsymbol{x}_k = (x_{k1}, \ldots, x_{ks}),\ k = 1, \ldots, n\}$ is a uniform design on T_s. However, in most experiments with mixtures some constraints have to be placed on the ingredients. For example, in making a cake, water and flour should be the major ingredients while sugar

and milk have a small percentage. The constraints may be $0 \leqslant a_i \leqslant x_i \leqslant b_i \leqslant 1$, $i = 1 \ldots, s$, or $\mathbf{0} \leqslant \boldsymbol{a} \leqslant \boldsymbol{x} \leqslant \boldsymbol{b} \leqslant \mathbf{1}$ where $\boldsymbol{a} = (a_1, \ldots, a_s)$, $\boldsymbol{b} = (b_1, \ldots, b_s)$ and $\mathbf{0}$ and $\mathbf{1}$ are vectors of 0's and 1's, respectively. In this case the experimental domain becomes

$$T_s(\boldsymbol{a}, \boldsymbol{b}) = \{\boldsymbol{x}\colon \mathbf{0} \leqslant \boldsymbol{a} \leqslant \boldsymbol{x} \leqslant \boldsymbol{b} \leqslant \mathbf{1}\}. \tag{4.4}$$

The domain $T_s(\boldsymbol{a}, \boldsymbol{b})$ is not empty if and only if

$$a \equiv \sum_{i=1}^{n} a_i < 1 < \sum_{i=1}^{n} b_i \equiv b.$$

Wang and Fang (1996) applied the transformation method for construction of uniform designs on $T_s(\boldsymbol{a}, \boldsymbol{b})$, but their method can not give a good design when some $d_i = b_i - a_i$ are very small. Later Fang and Yang (2000) employed the conditional method to propose an alternative method that can construct uniform designs for all cases.

5. Construction of uniform designs

In this section, we discuss measures of uniformity, the construction methods and algorithms for UD. The uniform design seeks its design points to be uniformly scattered on the domain. Suppose that there are s factors in an experiment. Without loss of generality we can assume that the experimental domain is the unit cube $C^s = [0, 1]^s$ (after making a suitable linear transformation). The aim is to choose a set of n experiment points $\mathcal{P} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n\} \subset C^s$ that is uniformly scattered on C^s. Let M be a measure of uniformity of $\mathcal{P}$ such that the smaller M corresponds to better uniformity. Let $\mathcal{Z}(n, s)$ be the set of sets of n points on C^s. A set $\mathcal{P}^* \in \mathcal{Z}(n, s)$ is called a uniform design if it has the minimum M-value over $\mathcal{Z}(n, s)$, i.e.,

$$M(\mathcal{P}^*) = \min_{\mathcal{P} \in \mathcal{Z}(n,s)} M(\mathcal{P}). \tag{5.1}$$

The following three subjects are the key for the construction of UDs:

(1) define a suitable measure of uniformity;
(2) reduce the complexity of the computation of searching UDs;
(3) apply a powerful optimization algorithm to find a UD.

5.1. Measure of uniformity

Let $\mathcal{P} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n\}$ be a set of n points in the s-dimensional unit cube $C^s = [0, 1)^s$. Many different measures of uniformity of $\mathcal{P}$ have been defined (cf. Fang and Wang, 1994; Hickernell, 1998a, 1998b; Hickernell, Liu and Yam, 2000). A reasonable measure should be invariant under reordering the runs and relabeling factors. The most popular

measure of uniformity in quasi-Monte-Carlo methods is the star L_p-discrepancy (or L_p-discrepancy for short) (see Hua and Wang, 1981; Niederreiter, 1992)

$$D_p(\mathcal{P}) = \left\{ \int_{C^s} \left| \frac{N(\mathcal{P}, [\mathbf{0}, \boldsymbol{x}))}{n} - \mathrm{Vol}\big([\mathbf{0}, \boldsymbol{x})\big) \right|^2 \mathrm{d}\boldsymbol{x} \right\}^{1/p}, \tag{5.2}$$

where $[\mathbf{0}, \boldsymbol{x})$ denotes the interval $[0, x_1) \times \cdots \times [0, x_s)$, $N(\mathcal{P}, [\mathbf{0}, \boldsymbol{x}))$ is the number of points of $\mathcal{P}$ falling in $[\mathbf{0}, \boldsymbol{x})$, and $\mathrm{Vol}(A)$ is the volume of A. The L_∞-discrepancy is called *star discrepancy* (or discrepancy for short) and can be expressed as

$$D(\mathcal{P}) = \max_{\boldsymbol{x} \in C^s} \left| \frac{N(\mathcal{P}, [\mathbf{0}, \boldsymbol{x}))}{n} - \mathrm{Vol}\big([\mathbf{0}, \boldsymbol{x})\big) \right|. \tag{5.3}$$

Let $F(\boldsymbol{x})$ be the uniform distribution on C^s and $F_{\mathcal{P}}(\boldsymbol{x})$ be the empirical distribution function of $\mathcal{P}$, i.e.,

$$F_{\mathcal{P}}(\boldsymbol{x}) = \frac{1}{n} \sum_{i=1}^{n} I\{\boldsymbol{x}_i \leqslant \boldsymbol{x}\},$$

where $I\{A\} = 1$ if A occurs, otherwise 0. The star discrepancy is the norm

$$\big\| F_{\mathcal{P}}(\boldsymbol{x}) - F(\boldsymbol{x}) \big\| = \max_{\boldsymbol{x} \in C^s} \big| F_{\mathcal{P}}(\boldsymbol{x}) - F(\boldsymbol{x}) \big|$$

that is the Kolmogorov–Smirnov statistics in goodness-of-fit test. The star discrepancy has played an important role in high-dimensional integration, but it is hard to calculate (Winker and Fang, 1997). Suppose we want to numerically calculate an integral

$$I(f) = \int_{C^s} f(x_1, \ldots, x_s)\, \mathrm{d}x_1 \cdots \mathrm{d}x_s = \int_{C^s} f(\boldsymbol{x})\, \mathrm{d}\boldsymbol{x}$$

that can be approximated by

$$\widehat{I}(\mathcal{P}_n) = \frac{1}{n} \sum_{k=1}^{n} f(\boldsymbol{x}_k),$$

where $\mathcal{P}_n = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n\}$ is a set of n points on C^s. The error upper bound of this approximation is given by the Koksma–Hlawka inequality

$$\big| I(f) - \widehat{I}(\mathcal{P}_n) \big| \leqslant V(f) D(\mathcal{P}_n), \tag{5.4}$$

where $V(f)$ is the variation of the integrand (Niederreiter, 1992, Theorem 2.11). The upper bound suggests to find a set with minimum discrepancy. If the set $\mathcal{P}_n$ is chosen by the Monte-Carlo method, i.e., $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n$ are i.i.d. each being uniformly distributed on C^s, then $D(\mathcal{P}_n) = \mathrm{O}_p(\frac{1}{\sqrt{n}})$ as $n \to \infty$. However, the quasi-Monte-Carlo methods

can find sequences $\mathcal{P}_n$ such that $D(\mathcal{P}_n) = O(\frac{1}{n}(\log(n))^s)$ as $n \to \infty$. The virtue of quasi-Monte-Carlo methods produces applications of quasi-Monte-Carlo methods to numerical analysis and statistics (see Hua and Wang, 1981; Fang and Wang, 1994) including experimental design.

The discrepancy was proposed by Weyl (1916). One disadvantage of the discrepancy is that it is expensive to compute. Warnock (1972) gave an analytic formula for calculating the L_2-discrepancy

$$\big(D_2(\mathcal{P})\big)^2 = 3^{-s} - \frac{2^{1-s}}{n}\sum_{k=1}^{n}\prod_{l=1}^{s}\big(1-x_{kl}^2\big) + \frac{1}{n^2}\sum_{k=1}^{n}\sum_{j=1}^{n}\prod_{i=1}^{s}\big[1-\max(x_{ki},x_{ji})\big], \tag{5.5}$$

where $\boldsymbol{x}_k = (x_{k1},\ldots,x_{ks})$. Obviously, the L_2-discrepancy is much easier to be calculated numerically. Fang, Lin, Winker and Zhang 2000) found that both discrepancy and L_2-discrepancy are not suitable for searching UDs. The discrepancy is not sensitive enough while the L_2-discrepancy ignores differences $|\frac{N(\mathcal{P},[\mathbf{0},\boldsymbol{x}))}{n} - \mathrm{Vol}([\mathbf{0},\boldsymbol{x}))|^2$ on any low-dimensional subspace. Therefore, they adopt three modified L_2-discrepancies proposed by Hickernell (1998a) for searching UDs: the symmetric L_2-discrepancy (SD), the centered L_2-discrepancy (CD) and the modified L_2-discrepancy (MD). These discrepancies are defined by

$$\big(D_2(\mathcal{P})\big)^2 = \sum_{u\neq\emptyset}\int_{C^u}\left|\frac{N(\mathcal{P}_u, J_{\boldsymbol{x}_u})}{n} - \mathrm{Vol}(J_{\boldsymbol{x}_u})\right|^2 \mathrm{d}u, \tag{5.6}$$

where u is a nonempty subset of the set of coordinate indices $S = \{1,\ldots,s\}$, $|u|$ denotes the cardinality of u, C^u is the $|u|$-dimensional unit cube involving the coordinates in u, $\mathcal{P}_u$ is the projection of $\mathcal{P}$ on C^u, $J_{\boldsymbol{x}}$ is a rectangle uniquely determined by $\boldsymbol{x}$ and is chosen with the geometric consideration, and $J_{\boldsymbol{x}_u}$ is the projection of $J_{\boldsymbol{x}}$ on C^u. The *centered L_2-discrepancy* (CD for short) is considered by an appealing property that it becomes invariant under reordering the runs, relabeling factors and reflections of the points about any plane passing through the center of the unit cube and parallel to its faces. The latter is equivalent to the invariance of replacing the ith coordinate x_i by $1-x_i$ for some $i = 1,\ldots,s$. For the CD, Hickernell (1998a) gave an analytical expression similar to (5.5) as follows:

$$\big(\mathrm{CD}(\mathcal{P})\big)^2 = \left(\frac{13}{12}\right)^s - \frac{2}{n}\sum_{k=1}^{n}\prod_{j=1}^{s}\left(1+\frac{1}{2}|x_{kj}-0.5| - \frac{1}{2}|x_{kj}-0.5|^2\right) + \frac{1}{n^2}\sum_{k=1}^{n}\sum_{j=1}^{n}\prod_{i=1}^{s}\left[1+\frac{1}{2}|x_{ki}-0.5| + \frac{1}{2}|x_{ji}-0.5| - \frac{1}{2}|x_{ki}-x_{ji}|\right]. \tag{5.7}$$

From the definition (5.6), the CD considers the uniformity not only of $\mathcal{P}$ over C^s, but also of all the projection uniformity of $\mathcal{P}$ over C^u. On the other hand, the L_2-discrepancy concerns with only the uniformity over C^s. The UD tables in the UD-web are all constructed under the CD. Ma (1997a, 1997b) proposed another symmetric version of the L_∞-discrepancy and discussed how to search UD under his discrepancy.

The wrap-around L_2-discrepancy (WD for short), proposed also by Hickernell (1998b), has other nice properties. Its analytical formula is given by

$$\big(\mathrm{WD}(\mathcal{P})\big)^2 = \left(\frac{4}{3}\right)^s + \frac{1}{n^2}\sum_{k=1}^{n}\sum_{j=1}^{n}\prod_{i=1}^{s}\left[\frac{3}{2} - |x_{ki}-x_{ji}|\big(1-|x_{ki}-x_{ji}|\big)\right]. \tag{5.8}$$

The above measures are defined only on C^s. For a U-type design $\boldsymbol{U} \in \mathcal{U}(n;q^s)$ we make the transformation from $\boldsymbol{U} = (u_{ij})$ to a set of n points on C^s, $\mathcal{P}_u = \{\boldsymbol{x}_1,\ldots,\boldsymbol{x}_n\}$ where $x_{ij} = (u_{ij}-0.5)/q$. Let M be a measure of uniformity on C^s. We can then define $M(\boldsymbol{U}) = M(\mathcal{P}_u)$.

In the past, UD tables were constructed under the star discrepancy (Fang, 1980; Wang and Fang, 1981; Winker and Fang, 1998), under the centered L_2-discrepancy (Fang, Ma and Winker, 2001) and under wrap-around L_2-discrepancy (Fang and Ma, 2001a).

5.2. *Searching uniform designs*

In this subsection we introduce how to find UDs under centered L_2-discrepancy (CD). We shall omit "under CD" for simplicity. For one factor experiments ($s = 1$), Fang, Ma and Winker (2001) pointed out that the set of equidistant points is the unique UD on $[0, 1]$.

THEOREM 1. *For one factor experiment, the unique UD on* $[0, 1]$ *is*

$$\left\{\frac{2i-1}{2n},\ i = 1,\ldots,n\right\}$$

with $\mathrm{CD}^2 = \frac{1}{12n^2}$.

Clearly, the solution of (5.1) is not unique when $s > 1$. To search UDs for given n and s is an NP hard problem, as n and s increase. Furthermore, even for moderate values of n and s, it is an intractable problem to find a uniform design due to its complexity of the computation. We thus have to reduce the set of candidate designs. The set of U-type designs (cf. Definition 1) is one of such sets. The uniform design based on U-type designs for given n, is an approximation of the corresponding uniform design.

Figure 3 gives plots of UDs and UDs based on U-type designs (cf. Definition 2) for $s = 2$ and $n = 2, 3,\ldots, 9$. The lower plots on Figure 3 are of uniform designs and upper plots are of uniform designs based on U-type designs. The squared CD-value of each design is put on the top of its plot. The uniform designs are obtained by the Nelder–Mead simplex method built in MATLAB, which can be directly applied for

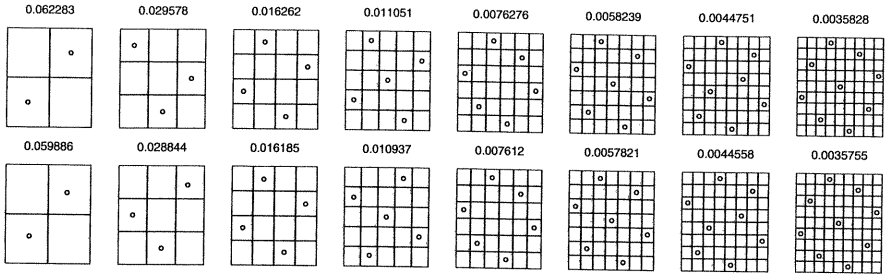

Fig. 3. Plots of uniform designs and their approximations.

$n \leqslant 6$. The Nelder–Mead simplex method did not perform well for $n > 7$. Therefore, for $n = 7, 8, 9$, we choose good UD as the initial values in order to converge to a low-discrepancy design. Comparing CD-value of two designs for $n = 2, \ldots, 9$ we find that the uniform designs based on U-type designs are very close to their corresponding uniform designs. However, when n and s increase, designs obtained by the use of the simplex method often exhibit poor uniformity, while designs based on U-type designs have a low-discrepancy. We shall *construct uniform designs based on U-type designs.*

Due to complexity of the computation for searching UDs, there are several methods such as the *good lattice method*, *Latin square method*, *expending orthogonal design method*, and *optimization searching* that can provide a good approximation to the uniform design. A good approximation uniform design is also called a nearly uniform design (Fang and Hickernell, 1995). We next describe these methods in details.

A. Good lattice point method

The good lattice point (*glp*) method is an efficient quasi-Monte-Carlo method, proposed by Korobov (1959), and discussed by many authors such as Hua and Wang (1981), Shaw (1988) and Fang and Wang (1994).

ALGORITHM 1 OF CONSTRUCTION OF A $U_n(n^s)$

Step 1. Find the candidate set of positive integers

$$\mathcal{H}_n = \{h\colon\ h < n,\ \text{the great common divisor of } n \text{ and } h \text{ is one}\}.$$

Step 2. For any s distinct elements of $\mathcal{H}_n$, $h_1, h_2, \ldots, h_s$, generate a $n \times s$ matrix $\boldsymbol{U} = (u_{ij})$ where $u_{ij} = ih_j \pmod{n}$ and the multiplication operation modulo n is modified as $1 \leqslant u_{ij} \leqslant n$. Denote $\boldsymbol{U}$ by $\boldsymbol{U}(n, \boldsymbol{h})$, where $\boldsymbol{h} = (h_1, \ldots, h_s)$ is called *generating vector* of the $\boldsymbol{U}$. Denote by $\mathcal{G}_{n,s}$ the set of all such matrices $\boldsymbol{U}(n, \boldsymbol{h})$.

Step 3. Find a generating vector $\boldsymbol{h}^*$ with $\boldsymbol{U}(n, \boldsymbol{h}^*) \in \mathcal{G}_{n,s}$ such that it has the best uniformity over the set $\mathcal{G}_{n,s}$. This $\boldsymbol{U}(n, \boldsymbol{h}^*)$ is a (nearly) uniform design $U_n(n^s)$.

EXAMPLE 1. For $n = 21$ and $s = 2$, we have

$$\mathcal{H}_{21} = \{1, 2, 4, 5, 8, 10, 11, 13, 16, 17, 19, 20\}.$$

If the CD is chosen as the measure of uniformity, the design matrix $\boldsymbol{U}(21, \boldsymbol{h}^*)$ with $\boldsymbol{h}^* = (1, 13)$ has the smallest CD-value over $\mathcal{G}_{21,2}$ and is a uniform design $U_{21}(21^2)$ that is given as follows

$$\begin{pmatrix} 1\,2 & 3 & 4\,5 & 6\,7 & 8 & 9\,10\,11\,12\,13\,14\,15\,16\,17\,18\,19\,20\,21 \\ 13\,5\,18\,10\,2\,15\,7\,20\,12 & 4\,17 & 9 & 1\,14 & 6\,19\,11 & 3\,16 & 8\,21 \end{pmatrix}'.$$

When the number of $\mathcal{H}_n$ is too small, the nearly uniform design obtained by the above *glp* method may be far from the uniform design. In this case some modification of the *glp* method can be applied. Instead of $\mathcal{H}_n$, we work on $\mathcal{H}_{n+1}$ in Steps 1 and 2 and delete the last row of $\boldsymbol{U}(n+1, h_1, \ldots, h_s)$ to form an $n \times s$ matrix, $\boldsymbol{U}$ say. All such matrices $\boldsymbol{U}$ form a set, denoted by $\mathcal{G}^*_{n,s}$. In Step 3, $\mathcal{G}_{n,s}$ is replaced by $\mathcal{G}^*_{n,s}$. This modification was suggested by Wang and Fang (1981) and Fang and Li (1995).

EXAMPLE 2. The number of elements in $\mathcal{H}_6 = \{1, 5\}$ is 2. The nearly uniform design $U_6(6^2)$ is not uniform from its plot. Besides, it is impossible to obtain $U_6(6^s)$, $s > 2$, based on $\mathcal{H}_6$. Note $\mathcal{H}_7 = \{1, 2, 3, 4, 5, 6\}$. All nearly uniform designs $U_6(6^s)$, $s \leqslant 6$, can be generated based on $\mathcal{H}_7$.

The cardinality of $\mathcal{H}_n$ can be determined by the Euler function $\phi(n)$. Let $n = p_1^{r_1} \cdots p_t^{r_t}$ be the prime decomposition of n, where $p_1, \ldots, p_t$ are different primes and $r_1, \ldots, r_t$ are positive integers. Then $\phi(n) = n(1 - \frac{1}{p_1}) \cdots (1 - \frac{1}{p_t})$. For example, $\phi(n) = n - 1$ if n is a prime, and $\phi(n) < n/2$ if n is even. The number of columns of U-type designs generated by the *glp* method is limited to $\phi(n)/2 + 1$ or $\phi(n+1)/2 + 1$ (cf. Fang and Wang, 1994, p. 208). The maximum number of factors is less than $n/2 + 1$ if the UD is generated by the *glp* method. Therefore, we need other methods that can generating UD's with more columns.

B. Latin square method

An $n \times n$ matrix with n symbols as its elements is called a *Latin square* of order n if each symbol appears on each row as well as on each column once and only once. Any Latin square of order n is a U-type design $U(n; n^n)$ and any s columns of a Latin square form a U-type design $U(n; n^s)$. Given n, a Latin square is always available. A *left cyclic Latin square* of order n is an $n \times n$ Latin square such that

$$\boldsymbol{x}_{i+1} = L\boldsymbol{x}_i, \quad i = 1, \ldots, n-1,$$

where $\boldsymbol{x}_i$ is the ith row of the square and L is the left shift operator defined by

$$L(a_1, a_2, \ldots, a_n) = (a_2, a_3, \ldots, a_n, a_1).$$

For given n there are $n!$ left cyclic Latin squares. We want to find a left cyclic Latin square with the lowest discrepancy among all the $n!$ left cyclic Latin squares. The following algorithm was proposed by Fang, Shiu and Pan (1999).

ALGORITHM 2 OF CONSTRUCTION OF A $U_n(n^s)$

Step 1. Find a Latin square, $\boldsymbol{L} = (l_{ij}) = (\boldsymbol{l}_1, \ldots, \boldsymbol{l}_n)$ that has the smallest discrepancy among all $n!$ left cyclic Latin squares of order n.

Step 2. Search s of n columns of the square, $\boldsymbol{l}_{i_1}, \ldots, \boldsymbol{l}_{i_s}$, to form a U-type design $U(n; n^s)$ such that this design has the smallest discrepancy among all such $U(n; n^s)$ designs. This design is a nearly uniform design $U_n(n^s)$.

EXAMPLE 3. For $n = 8$ and $s = 3$ we find the cyclic Latin square

$$\begin{bmatrix} 1 & 2 & 5 & 4 & 7 & 3 & 8 & 6 \\ 2 & 5 & 4 & 7 & 3 & 8 & 6 & 1 \\ 5 & 4 & 7 & 3 & 8 & 6 & 1 & 2 \\ 4 & 7 & 3 & 8 & 6 & 1 & 2 & 5 \\ 7 & 3 & 8 & 6 & 1 & 2 & 5 & 4 \\ 3 & 8 & 6 & 1 & 2 & 5 & 4 & 7 \\ 8 & 6 & 1 & 2 & 5 & 4 & 7 & 3 \\ 6 & 1 & 2 & 5 & 4 & 7 & 3 & 8 \end{bmatrix}$$

with the smallest CD-value 0.4358. For $U_8(8^s)$, columns of the design are chosen from columns of the above Latin square

$s = 2$: columns 1 and 4 with CD-value 0.0696;
$s = 3$: columns 1, 2 and 6 with CD-value 0.1123;
$s = 4$: columns 1, 2, 5 and 6 with CD-value 0.1601;
$s = 5$: columns 1, 2, 3, 6 and 7 with CD-value 0.2207.

Many known properties of cyclic Latin squares help in saving computing times (Fang, Shiu and Pan, 1999).

C. Extending orthogonal design method

An *orthogonal design*, denote by $L_n(q^s)$, is a matrix of size $n \times s$ with q symbols such that each symbol in any column appears equally often and each pair of symbols in any two columns appear equally often. There are some relationships between orthogonal designs and uniform designs, such as

- Any orthogonal design, if it exists, can be obtained from a U-type design by the *pseudo-level technique*.
- Any orthogonal design $L_n(q^s)$ can be extended to a number of U-type designs. The design with the smallest discrepancy among these U-type designs is a nearly uniform design.

ALGORITHM 3 OF CONSTRUCTION OF A $U_n(n^s)$. Suppose that $L_n(q^s)$ exists and let $r = n/q$ be the replicates of each level.

Step 1. For each column, replace r 1's by a permutation of $\{1, \ldots, r\}$, replace r 2's by a permutation of $\{r + 1, \ldots, 2r\}$; ... ; and replace r q's by a permutation of $\{(q-1)r + 1, \ldots, qr\}$. This results a U-type design $U(n; n^s)$. Denote by $\mathcal{O}_{n,s,q}$ all such U-type designs.

Step 2. Find a $\boldsymbol{U}^* \in \mathcal{O}_{n,s,q}$ such that it has the best uniformity over the set $\mathcal{O}_{n,s,q}$. This $\boldsymbol{U}^*$ is a nearly uniform design $U_n(n^s)$.

The above algorithm was proposed by Fang (1995). The reader can refer Fang and Hickernell (1995) for discussion on the strength and weakness of these three methods. For example, All (nearly) UDs $U_n(n^s)$ with $s \leqslant n$ can be generated by the Latin square method, the *glp* method can not generate all these UDs $U_n(n^s)$ with $s > n/2$ and the extending orthogonal design method can produce only those (nearly) UDs $U_n(n^s)$ where $L_n(q^s)$ exists for some q. All these methods can generate only $U_n(q^s)$ for $q = n$. When $q < n$ we need to search UDs by some powerful optimization algorithms. Ma (1997c) proposed a method to construct uniform designs of form $U_n(q^s)$ where $n = q^2$. He combined an orthogonal design $L_n(q^s)$ and a uniform design $U_q(q^s)$ to generate a $U_n(n^s)$. Uniform design tables with large number n can thus be obtained.

5.3. *Searching uniform designs by optimization techniques*

From Definition 2 it is clear that searching a UD for given (n, s, q) is an optimization problem. As the domain $\mathcal{U}(n; q^s)$ is a finite set, all the classical optimization methods do not work. In the past twenty years many powerful optimization algorithms have been proposed. Among them simulated annealing, threshold accepting (TA) and genetic optimization are popular ones. Winker and Fang (1998) used the TA algorithm for searching UDs under the star discrepancy. Fang, Ma and Winker (2001) and Fang and Ma (2001a) applied the TA algorithm for finding UDs under the centered L_2-discrepancy and wrap-around L_2-discrepancy, respectively. This approach can also be applied for searching UDs with mixed levels. All the UDs in the UD-web are obtained by them. If the experimenter is urgent to use a UD that is not in the UD-web. It can be randomly generated by a number of times and then the experimenter can choose the one with the smallest CD-value.

5.4. *Construction of uniform designs by combinatorial designs*

There is a link between resolvable balanced incomplete block designs and U-type designs (Liu and Fang, 2000; Fang, Ge, Liu and Qin, 2003a, 2003b). By this link a lot of uniform designs $U_n(q^s)$, $q < n$ and $U_n(q_1^{s_1} \times q_2^{s_2})$ can be obtained from the theory of combinatorial designs.

6. Computer experiments

The uniform design was motivated by three projects of computer experiments in 1978. computer experiments. Illustrated by a case study, here we introduce the use of UD to computer experiments and modelling methods. The goal here is to seek a suitable approximate model

$$y = \hat{g}(x_1, \ldots, x_s) \tag{6.1}$$

which is close to the real one (2.3). For the modelling, many authors proposed a number of methods. When the function g is a periodic, a Fourier regression model is recommended. The spatial modelling technique of kriging (Koehler and Owen, 1996) is based on a stationary Gaussian stochastic process and the Bayesian approach (Sacks, Welch, Mitchell and Wynn, 1989; Morris, Mitchell and Ylvisaker, 1993) uses the prior information. Like most Bayesian methods, the user may have difficulty in finding an appropriate prior distribution. Fang and Wang (1994), on the other hand, prefer polynomial regression models.

EXAMPLE 4. In the study of the flow rate of water from an upper aquifer to a lower aquifer, the aquifers are separated by an impermeable rock layer but there is a borehole through that layer connecting them. The model formulation is based on assumption of no groundwater gradient, steady-state flow from the upper aquifer into the borehole and from the borehole into the lower aquifer, and laminar, isothermal flow through the borehole. The response variable y, the flow rate through the borehole in m^3/yr, is determined by

$$y = \frac{2\pi T_u[H_u - H_l]}{\ln\left(\frac{r}{r_w}\right)\left[1 + \frac{2LT_u}{\ln(r/r_w)r_w^2 K_w} + \frac{T_u}{T_l}\right]}, \tag{6.2}$$

where the 8 input variables are as follows:

$r_w(m)$: radius of borehole
$r(m)$: radius of influence
$T_u(m^3/yr)$: transmissivity of upper aquifer
$T_l(m^3/yr)$: transmissivity of lower aquifer
$H_u(m)$: potentiometric head of upper aquifer
$H_l(m)$: potentiometric head of lower aquifer
$L(m)$: length of borehole
$K_w(m/yr)$: hydraulic conductivity of borehole

and the domain $\mathcal{D}$ is given by

$$r_w \in [0.05, 0.15], \qquad r \in [100, 50000],$$
$$T_u \in [63070, 115600], \qquad T_l \in [63.1, 116],$$
$$H_u \in [990, 1110], \qquad H_l \in [700, 820],$$
$$L \in [1120, 1680], \qquad K_w \in [9855, 12045].$$

The input variables and the corresponding output are denoted by $\boldsymbol{x} = (x_1, \ldots, x_8)$ and $y(\boldsymbol{x})$, respectively. This example has been studied by Worley (1987), An and Owen (2001) and Morris, Mitchell and Ylvisaker (1993). The latter used the Latin hypercube design, maximin design, maximin Latin hypercube design and modified maximin design. For comparing different models they used the mean square error

(MSE) as the criterion, i.e.,

$$\text{MSE} = \frac{1}{N}\sum_{k=1}^{N}\big(y(\boldsymbol{x}_k) - \hat{y}(\boldsymbol{x}_k)\big)^2, \tag{6.3}$$

where $\boldsymbol{x}_k, i = 1, \ldots, N$, are randomly chosen from the domain $\mathcal{D}$ and $\hat{y}(\boldsymbol{x}_k)$ is its predicted value under the underlying model. The value of N is chosen to be greater than 1000.

6.1. *Design of experiment*

From the effect of each variable to the output y from (6.2), we sort 8 input variables into

$$r_w \geqslant L \geqslant H_u \geqslant H_l \geqslant k_w \geqslant T_l \geqslant T_u \geqslant r \tag{6.4}$$

and put them into three groups: $\{R_w\}$, $\{H_u, H_l, L, K_w\}$ and $\{T_l, T_u, r\}$. A justification of this grouping will be given in Section 6.3. The number of levels of each variable in these three groups is chosen as 16, 8, and 4, respectively. A uniform design table $U_{32}(32^8)$ can be found on the UD-web. By the pseudo-level technique a $U_{32}(16 \times 8^4 \times 4^3)$ table can be generated and is in fact used for the study. The design and related output are given in Table 8.

6.2. *Quadratic regression model*

As previously mentioned, several methods for the modelling have been proposed. For this case study, Ho and Xu (2000) considered a centered quadratic model as follows. From the professional knowledge it is suggests the use of a *log* transformation of $\log(r)$ and $\log(r_w)$. With the model selection techniques, a suitable submodel is obtained. The residual plot of this submodel, however, indicates that some transformation for y is also needed. They used $log(y)$. By using the model selection techniques for the transformed variables, we obtain a submodel that involves 25 terms. The ANOVA table is given in Table 9. With 2000 random sampling in (6.3) we find its MSE = 0.293026 that is the same level with Morris, Mitchell and Ylvisaker (1993, p. 249), but they need the derivatives at each experimental point. This model involves too many terms. We thus delete the terms with minimum F-values. This is done by recalculating the ANOVA table, deleting the term with minimum F-value, and continue this process until all F-values are significantly large. The resulting model includes 9 terms whose MSE = 0.268626. The ANOVA table is given in Table 10. The effect of variable r to y is important to the Engineers (cf. Fig. 4), we thus add centerized $\log(r)$ term into the model and the final model becomes

$$\begin{aligned}\widehat{log(y)} = {} & 4.1560 + 1.9903\big(log(r_w) + 2.35443967732998\big) \\ & - 0.0007292 * (L - 1400) - 0.003554 * (H_l - 760) \\ & + 0.0035068 * (H_u - 1050) \\ & + 0.000090868 * (K_w - 10950)\end{aligned}$$

Table 8
Uniform design and related output

No.	r_w	r	T_u	T_l	H_u	H_l	L	K_w	y
1	0.05 (1)	33366.67(3)	63070(1)	116.00(4)	1110.00(8)	768.57(5)	1200(2)	11732.14(7)	26.18
2	0.05 (1)	100.00(1)	80580(2)	80.73(2)	1092.86(7)	802.86(7)	1600(7)	10167.86(2)	14.46
3	0.06 (2)	100.00(1)	98090(3)	80.73(2)	1058.57(5)	717.14(2)	1680(8)	11106.43(5)	22.75
4	0.06 (2)	33366.67(3)	98090(3)	98.37(3)	1110.00(8)	734.29(3)	1280(3)	10480.71(3)	30.98
5	0.06 (3)	100.00(1)	115600(4)	80.73(2)	1075.71(6)	751.43(4)	1600(7)	11106.43(5)	28.33
6	0.06 (3)	16733.33(2)	80580(2)	80.73(2)	1058.57(5)	785.71(6)	1680(8)	12045.00(8)	24.60
7	0.07 (4)	33366.67(3)	63070(1)	98.37(3)	1092.86(7)	768.57(5)	1200(2)	11732.14(7)	48.65
8	0.07 (4)	16733.33(2)	115600(4)	116.00(4)	990.00(1)	700.00(1)	1360(4)	10793.57(4)	35.36
9	0.08 (5)	100.00(1)	115600(4)	80.73(2)	1075.71(6)	751.43(4)	1520(6)	10793.57(4)	42.44
10	0.08 (5)	16733.33(2)	80580(2)	80.73(2)	1075.71(6)	802.86(7)	1120(1)	9855.00(1)	44.16
11	0.08 (6)	50000.00(4)	98090(3)	63.10(1)	1041.43(4)	717.14(2)	1600(7)	10793.57(4)	47.49
12	0.08 (6)	50000.00(4)	115600(4)	63.10(1)	1007.14(2)	768.57(5)	1440(5)	11419.29(6)	41.04
13	0.09 (7)	16733.33(2)	63070(1)	116.00(4)	1075.71(6)	751.43(4)	1120(1)	11419.29(6)	83.77
14	0.09 (7)	33366.67(3)	115600(4)	116.00(4)	1007.14(2)	717.14(2)	1360(4)	11106.43(5)	60.05
15	0.10 (8)	50000.00(4)	80580(2)	63.10(1)	1024.29(3)	820.00(8)	1360(4)	9855.00(1)	43.15
16	0.10 (8)	16733.33(2)	80580(2)	98.37(3)	1058.57(5)	700.00(1)	1120(1)	10480.71(3)	97.98
17	0.10 (9)	50000.00(4)	80580(2)	63.10(1)	1024.29(3)	700.00(1)	1520(6)	10480.71(3)	74.44
18	0.10 (9)	16733.33(2)	80580(2)	98.37(3)	1058.57(5)	820.00(8)	1120(1)	10167.86(2)	72.23
19	0.11(10)	50000.00(4)	98090(3)	63.10(1)	1024.29(3)	717.14(2)	1520(6)	10793.57(4)	82.18
20	0.11(10)	100.00(1)	63070(1)	98.37(3)	1041.43(4)	802.86(7)	1600(7)	12045.00(8)	68.06
21	0.12(11)	33366.67(3)	63070(1)	116.00(4)	990.00(1)	785.71(6)	1280(3)	12045.00(8)	81.63
22	0.12(11)	100.00(1)	98090(3)	98.37(3)	1092.86(7)	802.86(7)	1680(8)	9855.00(1)	72.54
23	0.12(12)	16733.33(2)	115600(4)	80.73(2)	1092.86(7)	734.29(3)	1200(2)	11419.29(6)	161.35
24	0.12(12)	16733.33(2)	63070(1)	63.10(1)	1041.43(4)	785.71(6)	1680(8)	12045.00(8)	86.73
25	0.13(13)	33366.67(3)	80580(2)	116.00(4)	1110.00(8)	768.57(5)	1280(3)	11732.14(7)	164.78
26	0.13(13)	100.00(1)	98090(3)	98.37(3)	1110.00(8)	820.00(8)	1280(3)	10167.86(2)	121.76
27	0.14(14)	50000.00(4)	98090(3)	63.10(1)	1007.14(2)	820.00(8)	1440(5)	10167.86(2)	76.51
28	0.14(14)	33366.67(3)	98090(3)	116.00(4)	1024.29(3)	700.00(1)	1200(2)	10480.71(3)	164.75
29	0.14(15)	50000.00(4)	63070(1)	116.00(4)	990.00(1)	785.71(6)	1440(5)	9855.00(1)	89.54
30	0.14(15)	50000.00(4)	115600(4)	63.10(1)	1007.14(2)	734.29(3)	1440(5)	11732.14(7)	141.09
31	0.15(16)	33366.67(3)	63070(1)	98.37(3)	990.00(1)	751.43(4)	1360(4)	11419.29(6)	139.94
32	0.15(16)	100.00(1)	115600(4)	80.73(2)	1041.43(4)	734.29(3)	1520(6)	11106.43(5)	157.59

Table 9
ANOVA table (SAS output)

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Stat	Prob > F
Model	25	13.1371	0.5255	33326205.8	0.0001
Error	6	9.461E-08	1.577E-08		
C Total	31	13.1371			

Type III Tests

Source	DF	Sum of Squares	Mean Square	F Stat	Prob > F
LOG_RW	1	1.4594	1.4594	92557449.3	0.0001
L	1	0.0455	0.0455	2885936.39	0.0001
HL	1	0.2962	0.2962	18783175.8	0.0001
HU	1	0.0490	0.0490	3107757.91	0.0001
KW	1	0.0177	0.0177	1120563.09	0.0001
HUHL	1	0.0015	0.0015	95459.3353	0.0001
L_2	1	0.0001	0.0001	9274.9263	0.0001
HL_2	1	0.0002	0.0002	12181.2757	0.0001
HU_2	1	0.0001	0.0001	6747.4395	0.0001
R	1	1.302E-05	1.302E-05	825.9765	0.0001
RWTU	1	2.212E-05	2.212E-05	1402.8296	0.0001
TUKW	1	3.719E-06	3.719E-06	235.8640	0.0001
TL	1	2.173E-05	2.173E-05	1377.8731	0.0001
TLHU	1	6.588E-06	6.588E-06	417.7864	0.0001
TL_2	1	5.225E-06	5.225E-06	331.3662	0.0001
RWR	1	5.726E-05	5.726E-05	3631.6044	0.0001
TLL	1	3.258E-06	3.258E-06	206.6327	0.0001
TULOG_R	1	1.041E-05	1.041E-05	660.4285	0.0001
TLHL	1	4.715E-06	4.715E-06	299.0113	0.0001
RWHL	1	2.862E-07	2.862E-07	18.1480	0.0053
TLKW	1	8.891E-07	8.891E-07	56.3840	0.0003
RW_2	1	6.352E-07	6.352E-07	40.2867	0.0007
TUHL	1	3.063E-07	3.063E-07	19.4263	0.0045
RWLOG_RW	1	3.997E-07	3.997E-07	25.3514	0.0024
TU_2	1	3.291E-07	3.291E-07	20.8691	0.0038

Table 10
ANOVA table (SAS output)

Analysis of Variance

Source	DF	Sum of Squares	Mean Square	F Stat	Prob > F
Model	9	13.1368	1.4596	108755.062	0.0001
Error	22	0.0003	1.342E-05		
C Total	31	13.1371			

Type III Tests

Source	DF	Sum of Squares	Mean Square	F Stat	Prob > F
LOG_RW	1	10.3539	10.3539	771441.372	0.0001
L	1	0.4083	0.4083	30420.3025	0.0001
HL	1	0.4714	0.4714	35124.6151	0.0001
HU	1	0.3239	0.3239	24134.5154	0.0001
KW	1	0.0732	0.0732	5457.3163	0.0001
HUHL	1	0.0085	0.0085	630.7976	0.0001
L_2	1	0.0008	0.0008	61.5301	0.0001
HL_2	1	0.0013	0.0013	96.0652	0.0001
HU_2	1	0.0013	0.0013	95.6290	0.0001

$$
\begin{aligned}
&+ 0.000015325 * (H_u - 1050) * (H_l - 760) \\
&+ 0.00000026487(L - 1400)^2 - 0.0000071759 * (H_l - 760)^2 \\
&- 0.0000068021 * (H_u - 1050)^2 \\
&- 0.00087286 * (log(r) - 8.8913547) \qquad (6.5)
\end{aligned}
$$

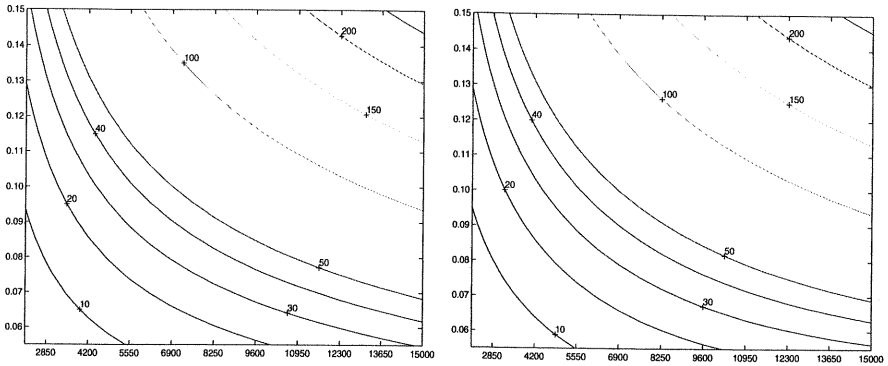

Fig. 4. Contours of $y = h(x_w, K_w)$.

Table 11
ANOVA table (SAS output)

Analysis of Variance					
Source	DF	Sum of Squares	Mean Square	F Stat	Prob > F
Model	10	13.1369	1.3137	126225.959	0.0001
Error	21	0.0002	1.041E-05		
C Total	31	13.1371			

Type III Tests					
Source	DF	Sum of Squares	Mean Square	F Stat	Prob > F
LOG_RW	1	10.2746	10.2746	987235.474	0.0001
L	1	0.3090	0.3090	29694.9581	0.0001
HL	1	0.4615	0.4615	44347.0990	0.0001
HU	1	0.2601	0.2601	24990.9369	0.0001
KW	1	0.0727	0.0727	6988.6817	0.0001
HUHL	1	0.0076	0.0076	725.7697	0.0001
L_2	1	0.0009	0.0009	81.9494	0.0001
HL_2	1	0.0013	0.0013	120.5167	0.0001
HU_2	1	0.0012	0.0012	111.9492	0.0001
LOG_R	1	7.671E-05	7.671E-05	7.3711	0.0130

whose ANOVA table is given in Table 11. This model has an MSE = 0.2578156. Ho and Xu (2000) recommended this model as the final one.

6.3. *B-spline function methods*

The polynomial regression models discussed in the previous subsection are simple and easy to learn. However, due to the multicollinearity among the variables, their squares and cross products, the process of variable selection is unstable and presents some difficulties to the user. The spline function has been well developed on modelling. Stone (1994) and Stone et al. (1997) gave a comprehensive study on the use of polynomial splines in multivariate function estimation. Following the idea, we introduce the B-spline function method for modelling.

Let $a = t_0 \leqslant t_1 \leqslant \cdots \leqslant t_k = b$ be a fixed knot points on $[a, b]$. A function $S(x)$ defined on $[a, b]$ is called a *spline function* of order m if $S(x)$ is a continuously $(m-1)$-differentiable function and is a polynomial of order m in each interval $[t_j, t_{j+1})$. The

B-spline basis on $[a, b]$ of order p is defined by

$$B_{i,0}(x) = \begin{cases} 1, & t_i \leqslant x < t_{i+1}, \\ 0, & \text{else}, \end{cases} \tag{6.6}$$

$$B_{i,p}(x) = \frac{x - t_i}{t_{i+p} - t_i} B_{i,p-1}(x) + \frac{t_{i+p+1} - x}{t_{i+p+1} - t_{i+1}} B_{i+1,p-1}(x), \quad p = 1, 2 \ldots. \tag{6.7}$$

The k-derivative of $B_{i,p}(x)$ can be iteratively calculated by

$$B_{i,p}^{(k)}(x) = p\left[\frac{B_{i,p-1}^{(k-1)}(x)}{t_{i+p} - t_i} - \frac{B_{i+1,p-1}^{(k-1)}(x)}{t_{i+p+1} - t_{i+1}}\right], \quad k = 1, 2, \ldots. \tag{6.8}$$

When $k = 0$ set $B_{i,p}^{(0)}(x) = B_{i,p}(x)$.

Let $B_{i,p}$ be a B-spline basis. Then a B-spline function of order p is expressed as

$$c(x) = \sum_{i=-m}^{k-1} c_i B_{i,p}(x).$$

Any continuous function $f(x)$ on $[a, b]$ can be approximated by a $c(x)$ where c_i's are estimated via the following least squares regression:

$$\min \sum_{i=1}^{n} \left[f(x_i) - \sum_{i=-m}^{k-1} c_i B_{i,p}(x_i)\right]^2,$$

where $x_i, i = 1, \ldots, n$, are n points on $[a, b]$.

Let $f(x_1, \ldots, x_s)$ be a continuous function on $\mathcal{D}$. Without loss of generality, assume $\mathcal{D} = C^s = [0, 1]^s$. A simple B-spline basis on C^s is constructed by tensor products of $B_{i,p}$ as follows

$$B_{I,p}(x_1, \ldots, x_s) = \prod_{j=1}^{s} B_{i_j,p}(x_j),$$

where $I = \{i_1, \ldots, i_s\}$. The function $f(x_1, \ldots, x_s)$ can then be approximated by

$$\hat{f}(x_1, \ldots, x_s) = \sum_{I} C_I P_{I,p}(x_1, \ldots, x_s).$$

In this study, p is taken as 3 and knot points are chosen as $0, 0, 0, 1/m, 2/m, \ldots, (m-1)/m, 1, 1, 1$ where 0 and 1 are repeated $p = 3$ times and m is a positive integer.

Let $y_k = f(\boldsymbol{x}_k)$ and $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n$ are n points on C^s. The least squares estimate of C_I minimizes $\sum_{k=1}^{n}(\sum_I C_I P_{I,p}(\boldsymbol{x}_k) - y_k)^2$. However, such a solution is undesirable for most statistical applications (see Fan and Gijbels, 1996, Section 2.6.2). A smoothing spline solution is to minimize

$$Q = \omega \sum_{k=1}^{n} \Big(\sum_I C_I P_I(\boldsymbol{x}_k) - y_k \Big)^2 + (1-\omega) \sum_{i,j=1}^{s} \int_{[0,1]^s} \partial_{i,j}^2 \Big(\sum_I C_I P_I(\boldsymbol{x}) \Big)^2 \, \mathrm{d}\boldsymbol{x},$$

where ω is a weight, and $\partial_{i,j}^2$ denotes to take derivative with respect to x_i and x_j. The smallest ω and m are chosen such that $|f(\boldsymbol{x}_k) - \widehat{f(\boldsymbol{x}_k)}| < \varepsilon, k = 1, \ldots, n$, where ε is a pre-assigned accuracy.

Let $\hat{f}(x_1, \ldots, x_s)$ be a B-spline function approximation to the function $g(x_1, \ldots, x_s)$. For given $x_2, \ldots, x_s$, $\hat{f}$ can be considered as a function of x_1. Denote by $\hat{f}_{\max}(x_1|x_2, \ldots, x_s)$ and $\hat{f}_{\min}(x_1|x_2, \ldots, x_s)$ the largest and smallest value of $\hat{f}(x_1, \ldots, x_s)$ on $0 \leqslant x_1 \leqslant 1$, and set

$$G_1 = \int_{C^{s-1}} \big[\hat{f}_{\max}(x_1|x_2, \ldots, x_s) - \hat{f}_{\min}(x_1|x_2, \ldots, x_s) \big] \mathrm{d}x_2 \cdots \mathrm{d}x_s.$$

G_1 can be viewed as a measure of contribution of x_1 to the function g. Similarly, we can define $G_2, \ldots, G_s$. For the flow rate of water example, we find

$$G_{r_w} = 139.5162, \quad G_L = 32.9192, \quad G_{H_u} = 32.5932,$$
$$G_{H_l} = 31.5487, \quad G_{k_w} = 15.7172, \quad G_{T_l} = 0.0287,$$
$$G_{T_u} = 0.0004, \quad G_r = 0.0003$$

that gives a justification of variable grouping and level of each variable choosing. Following Morris, Mitchell and Ylvisaker's (1993) procedure, we study the function (6.2) as a function of r_w and K_w on $[0.05, 0.15] \times [1500, 15000]$, denoted by $y = h(r_w, K_w)$, and fix remaining inputs at their respective lowest values. Contours of y are shown in the left portion of Figure 4. Consider the function (6.2) with 8 input variables and the B-spline basis of order two for r_w and of order one for the rest of the variables. With iteration we find that $m = 1$ and $\omega = 0.99997$ and that the variables r, T_u and T_l can be deleted due to their less influence to y. The predictive mean square error MSE is 4.45.

6.4. *Comparisons among different design and models*

In this subsection we compare the performances of different designs: Latin hypercube design, maximin design, maximin Latin hypercube design, modified maximin design and uniform design, under different models. The first four designs are studied by Morris,

Mitchell and Ylvisaker (1993). The Bayesian approach used by Morris, Mitchell and Ylvisaker (1993) needs to calculate derivatives at each experimental points and to find maximum likelihood estimators of the parameters in the correlation functions of the model.

For comparing four different designs, Morris, Mitchell and Ylvisaker (1993) considered prediction errors at 400 random samples in $\mathcal{D}$ and at the 256 corner points of $\mathcal{D}$. They plot the prediction errors in two separate figures. Their plots are put on the left of Figures 5 and 6. Following their comparisons, plots of prediction errors for

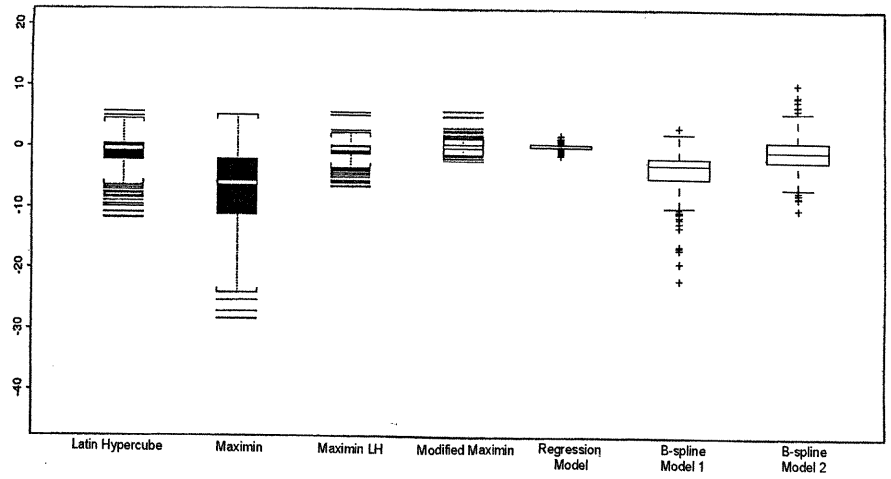

Fig. 5. Prediction errors at 400 random samples for seven design/models.

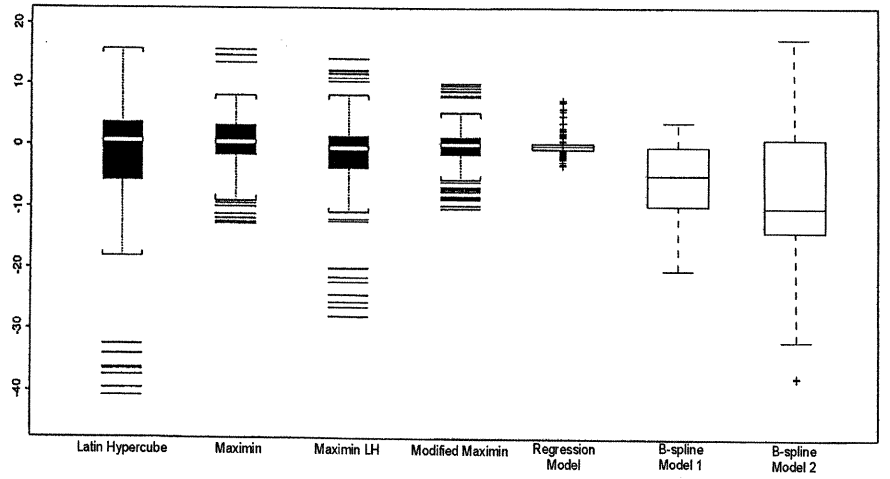

Fig. 6. Prediction errors at 256 corner points for seven design/models.

uniform design with quadratic model (6.5) and B-spline model discussed in the previous subsection are placed at the fifth and seventh items of Figures 5 and 6. Obviously, the B-spline model has large errors for the 256 corner points. This bias may be resulted from small number of levels for some input variables. Ho and Xu (2000) employed the table $U_{30}(30^8)$ to design 30 level-combinations with the B-spline model mentioned above for modelling. The corresponding prediction errors for two sets of points are plot on the sixth and seventh items of Figures 5 and 6.

From the above discussion along with Figures 5 and 6, we conclude that

(1) The modelling methods based on polynomial regression or B-spline models do not require derivatives of the underlying function. Therefore, these methods can apply to the experiment where the underlying model is unknown. This is very common in most industrial experiments.
(2) From Figures 5 and 6, the quadratic regression model (6.5) is the best and the modified maximin design is the second. The latter needs to calculate derivatives of the underlying function at experimental points, however.
(3) The B-spline model based on the $U_{30}(30^8)$ design is better than the B-spline model based on the $U_{32}(16 \times 8^4 \times 4^3)$ design. It shows that the B-spline modelling method needs more levels of the input variables.
(4) Considering the squared MSE value, the three designs used by Worley (1987) have MSE $= 1.89^2 = 3.5721$, $2.45^2 = 6.0025$, and $2.37^2 = 5.6169$, respectively. Morris, Mitchell and Ylvisaker (1993) reported that their modelling method applied to Worley's design resulted in MSE $= 0.61^2 = 0.3721$. Unfortunately, the MSE values for their four designs were not reported. The quadratic regression model (4.5) has MSE $= 0.2578$ while the B-spline model based on $U_{32}(16 \times 8^4 \times 4^3)$ design has MSE $= 4.45$ and the B-spline model based on $U_{30}(30^8)$ design has MSE $= 4.27$.

Besides the designs mentioned before, combining the uniform design and the Latin hypercube sampling can produce other designs for computer experiments. Zhang and Wang (1996) and Ma (1999) proposed such designs.

7. The connections between uniformity and other designs

Most experimental designs, such as simple random design, random block design, Latin square design, fractional factorial design, optimal design and robust design are concerned with *randomness, balance between factors and levels of each factor, orthogonality, efficiency and robustness*. From the previous sections, we see that the uniformity has played a key role in computer experiments. In this section we shall show that uniformity is also a useful criterion in many classical designs.

7.1. Uniformity and isomorphism

Let $d(n, q, s)$ be a factorial design of n run and s factors each having q levels. The orthogonal designs $L_n(q^s)$ defined in Section 3.2 are special cases of factorial designs. Two factorial designs are called *isomorphic* if one can be obtained from

the other by relabeling the factors, reordering the runs, or switching the levels of factors. Two isomorphic designs are considered to be equivalent because they share the same statistical properties as a classical ANOVA model. Therefore, it is important to identify design-isomorphism. For identifying two $d(n, q, s)$ designs, a complete search compares $n!(q!)^s s!$ designs from the definition of isomorphism. For example, to see if two factorial $d(12, 2, 11)$ designs are isomorphic requires $12!11!2^{11} \approx 3.9158 \times 10^{19}$ comparisons. Several methods have been proposed to reduce the complexity of the computation. This includes Draper and Mitchell (1968, 1970), Chen and Lin (1991) and Clark and Dean (2001). Unfortunately, those methods are either insufficient or computational infeasible. Therefore, Ma, Fang and Lin (2001) employed the uniformity to detect non-isomorphic designs.

A factorial design $d(n, q, s)$ corresponds to an $n \times s$ matrix where the (i, j)-element, d_{ij}, corresponds to the level of the jth factor in the ith trial. Let $P_d = (p_{ij})$ where $p_{ij} = (d_{ij} - 0.5)/q$ and M be a measure of uniformity. We define $M(d(n, q, s)) = M(P_d)$. In particular, if we choose CD or WD (see (5.7) and (5.8)) we can easily calculate CD$(d(n, q, s))$ and WD$(d(n, q, s))$. For simplicity, we use the CD as the measure of uniformity.

For a given factorial design $D = d(n, q, s)$ and k $(1 \leqslant k \leqslant s)$, there are $\binom{s}{k}$ $d(n, q, k)$ subdesigns. The CD-values of these subdesigns form a distribution, denoted by $F_k(D)$, that is called the *k-marginal CD-value distribution of D*. Ma, Fang and Lin (2001) pointed out that two isomorphic $d(n, 2, s)$ designs have the same CD-value as well as the same F_k distribution for $1 \leqslant k \leqslant s$. Based on this, they proposed the following algorithm, called *NIU algorithm*, for detecting non-isomorphic $d(n, 2, s)$ designs. Let D_1 and D_2 be two $d(n, 2, s)$ designs.

NIU ALGORITHM

Step 1. Compare CD(D_1) and CD(D_2), if CD$(D_1) \neq$ CD(D_2) we conclude D_1 and D_2 are not isomorphic and terminate the process, otherwise go to Step 2.

Step 2. For $k = 1, s-1, 2, s-2, \ldots, [s/2], s-[s/2]$ where $[x]$ denotes the largest integer that is smaller than x, compare $F_k(D_1)$ and $F_k(D_2)$, if $F_k(D_1) \neq F_k(D_2)$ we conclude D_1 and D_2 are not isomorphic and terminate the process, otherwise go to the next k-value of this step.

For example, we apply this algorithm to two $L_{32768}(2^{31})$ designs studied by Chen and Lin (1991). The process indicates: two designs have the same CD $= 4.279$; all the k-dimensional subdesigns have the same CD-value for $k = 1, 30, 2, 29$; but $F_{28}(D_1) \neq F_{28}(D_2)$. It turns out that two designs are not isomorphic by implementing only a few steps of the algorithm. It shows that the NIU algorithm is powerful in detecting nonisomorphic designs. The above idea and algorithm can be extended to detect factorial designs with higher levels (see Ma, Fang and Lin, 2001) and to investigate the design projection properties (see Lin and Draper, 1992).

There is a close relationship between Hadamard matrices and orthogonal designs with 2-levels. A Hadamard matrix, $\boldsymbol{H}$, of order n is an $n \times n$ matrix with elements 1 or -1, which satisfies $\boldsymbol{H}'\boldsymbol{H} = n\boldsymbol{I}$. Two Hadamard matrices are called *equivalent* if one

can be obtained from the other by some sequence of row and column permutations and negations. To identify two Hadamard matrices to be equivalent is a NP hard problem when n increases. The profile method (cf. Lin, Wallis and Zhu, 1993) has been used for detecting inequivalent Hadamard matrices. This method is not sensitive enough. However, a Hadamard matrix of order n can be regarded n points in $\{-1, 1\}^n$. Recently, Fang and Ge (2003) proposed an algorithm to detect inequivalent Hadamard matrices based on so-called symmetric Hamming distances. The criterion used there is more sensitive than the profile and has a close relation with several measures of uniformity. As an application we apply the new algorithm to verify the inequivalence of the known 60 inequivalent Hadamard matrices of order 24 and to show that there are at least 382 pairwise inequivalent Hadamard matrices of order 36. The latter is a new discovery.

7.2. *Uniformity and aberration*

Fractional factorial designs are probably the most popular experimental designs. A q^{s-p} fractional factorial design D, which has s factors of q levels and $n = q^{s-p}$ runs, is uniquely determined by p independent defining words. There are many useful criteria for comparing fractional factorial designs, such as resolution (Box, Hunter and Hunter, 1978), minimum aberration (Fries and Hunter, 1980) and estimation capacity (Cheng and Mukerjee, 1998). See Dey and Mukerjee (1999) for a comprehensive review. In this subsection we discuss connections between the uniformity and the aberration.

A *word* consists of letters which are names of factors denoted by $F_1, \ldots, F_s$. The number of letters in a word is called the *word-length* and the group formed by the p defining words is the defining contrast subgroup. The vector $W = (A_1(D), \ldots, A_s(D))$ is called the *word-length pattern*, where $A_i(D)$ denotes the number of words of length i in the defining contrast subgroup of D. The *resolution* of D is the smallest t with positive $A_t(D)$ in its word length pattern. A resolution III design is a design in which no main effects are aliased with any other main effect, but main effects are aliased with 2-factor interactions and 2-factor interactions may be aliased with each other. A resolution IV design is a design in which no main effect is aliased with any other main effect or with any 2-factor interaction, but 2-factor interactions are aliased with each other. For example, a 2^{3-1} design with defining relation $I = ABC$ is of resolution III; a 2^{4-1} design with defining relation $I = ABCD$ is of resolution IV; and a 2^{5-1} design with defining relation $I = ABCDE$ is of resolution V. Obviously, designs with high level resolution have better estimation ability.

Two designs with the same resolution may have different performance in estimation. The word-length pattern can still distinguish designs that have the same level of resolution. Given two regular fractions of a q^{s-p} factorial, D_1 and D_2, we say that D_1 has less aberration than D_2 if there exists an integer k $(1 \leqslant k \leqslant s)$ such that

$$A_1(D_1) = A_1(D_2), \quad \ldots, \quad A_{k-1}(D_1) = A_{k-1}(D_2), \quad A_k(D_1) < A_k(D_2).$$

A design has *minimum aberration* if there is no other design that has smaller aberration than this design. For given q, s, p one searches for the minimum aberration q^{s-p} design. The minimum aberration has been considered as a popular criterion for comparing fractional factorial designs.

Recently, Fang and Mukerjee (2000) found a connection between the two apparently unrelated areas, the uniformity and the aberration, in regular fractions of two-level factorials. They proved the following

THEOREM 2.

$$[\mathrm{CD}(D)]^2 = \left(\frac{13}{12}\right)^s - 2\left(\frac{35}{32}\right)^s + \left(\frac{8}{9}\right)^s \left\{1 + \sum_{i=1}^{s} \frac{A_i(D)}{9^i}\right\},$$

where D is a regular fraction of a 2^s factorial involving $n = 2^{s-p}$ runs.

From this relation we can see that the minimum aberration and the CD are almost equivalent for regular factorial 2^{s-p}, but it is true that the CD criterion can still distinguish minimum aberration designs. Fang and Ma (2002) extended this connection to regular fraction 3^{s-1} designs and found that there exists essential difficulties to find more general results under the CD. Alternatively, Fang, Ma and Mukerjee (2002) employed the wrap-around L_2-discrepancy as the measure of uniformity. They gave analytic connection between the WD and the aberration for any regular factorials 2^{s-p} and 3^{s-p} as follow.

THEOREM 3. *Let D be a regular fractional factorial design q^{s-k} ($q = 2$ or 3). Its square* WD*-value can be expressed in terms of the word length pattern*

$$\big(\mathrm{WD}(D)\big)^2 = \begin{cases} \left(\frac{11}{8}\right)^s \sum_{r=1}^{s} \frac{A_r(D)}{11^r} + \left(\frac{11}{8}\right)^s - \left(\frac{4}{3}\right)^s, & \text{if } q = 2, \\ \left(\frac{73}{54}\right)^s \left[1 + 2\sum_{j=1}^{s} \left(\frac{4}{73}\right)^j A_j(D)\right] - \left(\frac{4}{3}\right)^s, & \text{if } q = 3. \end{cases}$$

Such a connection provides a way for searching minimum aberration designs by uniformity that can significantly reduce complexity of the computation.

7.3. *Uniformity and orthogonality*

The orthogonal design requires a good balance between levels of each factor and between level-combinations of any two factors, in other words, it requires one and two dimensional projection uniformity. The uniform design concerns with one dimension projection and s-dimensional uniformity. These two kinds of designs should have some relationships, some of which have been mentioned in Section 3.2.

Fang and Winker (1998) found that many uniform designs with a small number of runs, such as $U_4(2^3)$, $U_8(2^7)$, $U_{12}(2^{11})$, $U_{16}(2^{15})$, $U_9(3^4)$, $U_{12}(3 \times 2^3)$, $U_{16}(4^5)$, $U_{16}(4 \times 2^{12})$, $U_{18}(2 \times 3^7)$ and $U_{25}(5^6)$, are also orthogonal designs. This fact shows that many existing orthogonal designs are also uniform designs under the centered L_2-discrepancy and can be founded by a computer search. They conjectured that any orthogonal design is a uniform design under a certain discrepancy. Ma, Fang and Lin (2003) proved that the conjecture is true for complete designs and for 2^{s-1} factorials if the centered L_2-discrepancy is chosen as the measure of uniformity. A design is

called complete (or full) if all the level-combinations of the factors appear equally often. Recently, Fang and Ma (2001a, 2001b) proved that the conjecture is true for complete designs if the wrap-around L_2-discrepancy (5.8) is used as the measure of uniformity.

7.4. *Uniformity and confounding*

Two isomorphic factorial designs have been considered to be equivalent in the sense that they have the same statistical performance in ANOVA model. However, two isomorphic designs may have different uniformity. For example, two $L_9(3^4)$ in Table 12, denoted by D_1 and D_2, are isomorphic to each other, but their CD-values are 0.050059 and 0.0493645, respectively. Suppose that there are three factors A, B, and C each having three levels in an experiment. We can choose any 3 columns of D_1/D_2 for the factors. Denote by d_1 and d_2 be designs formed by the first three columns of D_1 and D_2, respectively. Denote the linear and quadratic main effects of A by A_l and A_q, respectively (similarly, for the notations B_l, B_q, C_l, and C_q). The interaction $A \times B$ between A and B, if it exists, can be split into 4 terms A_lB_l, A_lB_q, A_qB_l, and A_qB_q (Box and Draper, 1987, pp. 236–239). When there are interactions $A \times B$, $A \times C$ and $B \times C$ in the experiment, it is impossible to separate the true interactions from the main effects. For the use of d_2, the confounded situations are given by the alias statements:

$$
\begin{aligned}
A_l &= 0.5B_lC_q + 0.5B_qC_l,\\
A_q &= 1.5B_lC_l - 0.5B_qC_q,\\
B_l &= 0.5A_lC_q + 0.5A_qC_l,\\
B_q &= 1.5A_lC_l - 0.5A_qC_q,\\
C_l &= 0.5A_lB_q + 0.5A_qB_l,\\
C_q &= 1.5A_lB_l - 0.5A_qB_q.
\end{aligned}
$$

On the other hand, with the use of d_1, the alias statements are

$$
\begin{aligned}
A_l &= -0.75B_lC_l - 0.25B_lC_q + 0.25B_qC_l - 0.25B_qC_q,\\
A_q &= 0.75B_lC_l - 0.75B_lC_q + 0.75B_qC_l + 0.25B_qC_q,\\
B_l &= -0.75A_lC_l - 0.25A_lC_q + 0.25A_qC_l - 0.25A_qC_q,\\
B_q &= 0.75A_lC_l - 0.75A_lC_q + 0.75A_qC_l + 0.25A_qC_q,\\
C_l &= -0.75A_lB_l + 0.25A_lB_q + 0.25A_qB_l + 0.25A_qB_q,\\
C_q &= -0.75A_lB_l - 0.75A_lB_q - 0.75A_qB_l + 0.25A_qB_q.
\end{aligned}
$$

Table 12
Two $L_9(3^4)$ tables

No.	D_1				D_2			
1	1	1	1	1	1	1	1	2
2	1	2	2	2	1	2	3	1
3	1	3	3	3	1	3	2	3
4	2	1	2	3	2	1	3	3
5	2	2	3	1	2	2	2	2
6	2	3	1	2	2	3	1	1
7	3	1	3	2	3	1	2	1
8	3	2	1	3	3	2	1	3
9	3	3	2	1	3	3	3	2

If the higher-order interactions $A_lB_q, A_qB_l, A_qB_q, \ldots, B_qC_q$ can be ignored, the alias statements for d_2 become

$$
d_2\colon \begin{cases} A_q = 1.5B_lC_l, \\ B_q = 1.5A_lC_l, \\ C_q = 1.5A_lB_l. \end{cases}
$$

In this case we can estimate all the linear effects A_l, B_l and C_l without any confounding. Now, the alias formulas for d_1 become

$$
d_1\colon \begin{cases} A_l = -0.75B_lC_l, & A_q = 0.75B_lC_l, \\ B_l = -0.75A_lC_l, & B_q = 0.75A_lC_l, \\ C_l = -0.75A_lB_l, & C_q = -0.75A_lB_l. \end{cases}
$$

In this case the main effects are confounded with the interactions. Obviously, the design d_2 is better than d_1 in the sense of confounding. In fact, the design D_2 was obtained by Fang, Lin, Winker and Zhang (2000) as a uniform design $U_9(3^4)$. There are four choices of choosing three columns from D_1/D_2. We can show that there is only one choice from D_1 that has the same confounding situation to d_2 and the rest three choices have the same confounding situation to d_1. On the other hand, all the four choices from D_2 have the same confounding situation to d_2. We thus conclude that D_2 is better than D_1 in the sense of confounding. From this example, we propose the following concept.

DEFINITION 5. For given (n, q, s) an OD $L_n(q^s)$ is called an *uniformly orthogonal design* and is denoted by $UL_n(q^s)$ if it has the smallest CD-value over all such OD's.

Obviously, one might choose other measures of uniformity to replace the CD in Definition 5. Several uniformly orthogonal designs for $q_i > 2$ are obtained in Fang and Winker (1998). Properties of these designs are yet to be studied. Hickernell and Liu (2002) used the reproducing kernel approach to define a new discrepancy, called the discrete discrepancy (DD for short). They show that the uniform designs limit aliasing.

The DD played an important role for construction uniform designs via combinatorial designs (Fang, Ge, Liu and Qin, 2003b).

7.5. Uniformity in supersaturated designs

Supersaturated designs are fractional factorials in which the number of estimated (main or interaction) effects is greater than the number of runs. In industrial and 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 expensive costs. However, in many situations only a few factors are believed to have significant effects. Under this assumption of *effect sparsity*, supersaturated designs can be effectively used to identify the dominant factors. Most studies have focused on 2-level supersaturated designs, including Lin (1993, 1995), Wu (1993), Nguyen (1996), Li and Wu (1997), Chen and Lin (1998), Cheng (1997), Yamada and Lin (1997), Deng, Lin and Wang (1999), Liu and Zhang (2000), Liu and Hickernell (2002). For multi-level supersaturated designs, see, Yamada and Lin (1999) and Yamada et al. (1999) on 3-level designs.

It is clear that all supersaturated designs can not be completely orthogonal among columns of the design. The block orthogonality (meaning that columns of the design are grouped as blocks and columns in each block are orthogonal) has been considered by many authors. Fang, Lin and Ma (2003b) proposed a way that collapses a uniform design to an orthogonal array for construction of multi-level supersaturated designs.

There are many criteria, such as Ave(s^2) or $E(s^2)$, Ave$(|s|)$, $s_{\max}$, and ave(χ^2) for construction of supersaturated designs in the literature. These criteria are based on correlations among the design columns. Ma, Fang and Liski (2000) defined a criterion, called the (ϕ, θ) criterion, where ϕ and θ are two kinds of functions with some given properties. An important (ϕ, θ) criterion is the $D_{\phi,\theta}$ criterion there. It is defined as

$$D_{\phi,\theta} = \sum_{1 \leqslant i < j \leqslant m} f_{\phi}^{ij} \Big/ \binom{m}{2}, \tag{7.1}$$

where

$$f_{\phi}^{ij} = \sum_{u=1}^{q_i} \sum_{v=1}^{q_j} \left(n_{uv}^{(ij)} - \frac{n}{q_i q_j} \right)^2, \tag{7.2}$$

and $n_{uv}^{(ij)}$ is the number of (u, v)-pairs in $(\boldsymbol{x}^i, \boldsymbol{x}^j)$, and $n/(q_i q_j)$ is the average frequency of level-combinations in each pair of columns i and j. It is obvious that $D_{\phi,\theta} = 0$ for an orthogonal array. Fang, Lin and Liu (2003) proved that the $E(s^2)$ and aveχ^2 criteria are in fact special cases of the $D_{\phi,\theta}$ criterion, and they showed the equivalence between $D_{\phi,\theta}$ optimality and uniformity of any supersaturated design. They also proposed a way for construction of supersaturated designs with mixed levels. More supersaturated designs were obtained by the combinatorial approach (see Fang, Ge and Liu, 2003, Fang, Ge, Liu and Qin, 2003b).

7.6. Uniform design in quality engineering

Quality engineering has received a great deal of attention in the last two decades. Taguchi's method has been widely used in design of quality engineering (see Taguchi, 1986). The parameter design plays an important role in modern quality engineering. The orthogonal design tables are commonly used there. The parameters (experimental variables) are arranged in the inner (array) table, while the noise variables are accommodated in the outer (array) table. Since the roles of inner and outer arrays are very different, Wang, Lin and Fang (1995) has proposed the use of uniform design for the outer array.

Denote inner and outer tables by $L_n(q^s)$ and $L_m(p^t)$, respectively. Then the total number of runs is $N = nm$. Even when both n and m are moderate, the number of runs becomes too many for the experimenter. Lo, Zhang and Han (2000) suggested to use two uniform design tables replacing two orthogonal design tables for the inner and outer tables. They gave three case studies, among which the Wheatstone Bridge is a good representative example. Both inner and outer tables were chosen to be $L_{36}(2^3 \times 3^{11})$. As a result the total number of runs is $36 \times 36 = 1269$. Lo, Zhang and Han (2000) used $U_{13}(13^8)$ and $U_{12}(12^{10})$ for the inner and outer tables with a total number of runs $12 \times 13 = 156$, by which they found a result more efficient than the results by 1269 runs. This indicates that there is a great potential of applications of uniform designs to quality engineering.

7.7. Uniform design in chemistry and chemical engineering

There are high potentials for the applications of the uniform design in chemistry and chemical engineering, because chemistry is a field of science which heavily depends on experiments. Lee et al. (1997) applied the uniform design to capillary electrophoresis. The capillary electrophoresis is an useful analytical instrument in chemistry, biochemistry and medicine, because of its high resolution, short analysis time and little necessary sample amount. The artificial neural networks (ANN) are useful for dealing with non-linear problems. Zhang et al. (1998) studied nonlinear systems in chemistry and chemical engineering. and have applied the UD to ANN. They found that the UD provides better estimates than other designs and are robust against model assumptions. Atkinson et al. (1998) discussed the possibility of the use of D-optimal designs to the kinetics of reversible chemical reaction. Xu, Liang and Fang (2000) gave comparisons among D-optimal, orthogonal, and uniform designs for this chemical reaction and found that the uniform design is the robust. Comparisons on UD with other types of designs can also be found in Simpson, Lin and Chen (2001). Ling, Fang and Xu (2001) gave a comprehensive review on applications of UD in chemistry and chemical engineering.

8. Summary and discussion

The uniform experimental design is one kind of space filling designs. It seeks its design points to be uniformly scattered on the experimental domain. In this chapter,

we have introduced the fundamental idea of the uniform design and have tabulated most uniform design tables on the website at `http://www.math.hkbu.edu.hk/UniformDesign` for the practitioners. Some industrial applications of uniform design are given. In particular, the applications to computer experiments are discussed in details. Note that uniform design requires all design points distributed uniformly in all dimensions, while the popular Latin hypercube sampling requires all design points uniformly distributed in each dimension.

The theoretical aspects of the uniform design were also given: from the measures of uniformity to the theoretical properties and construction methods of uniform design. Furthermore, it is shown at the end of the chapter that the uniformity criteria is intimately connected with many other design criteria, such as orthogonality, aberration, design isomorphism, estimation capacity, model robustness, and supersaturated design. Thus, minimizing uniformity will automatically optimize other design criteria in many situations. This clearly demonstrates the superiority of uniform design. Due to limited space we do not introduce statistical models for uniform designs. The interesting reader can refer to Hickernell (1999), Xie and Fang (2000) and Hickernell and Liu (2002). They show that the uniform design is the best in a certain sense.

The uniform design can be utilized as

- a factorial design with model unknown,
- a space filling design for computer experiments,
- a robust design against the model specification, and
- a design of experiments with mixtures.

Advantages of uniform designs include

- more choices for the users,
- many designs tables to be provided,
- both factorial and computer experiments can be applied, and
- less information of the underlying model is required.

The use of UD is considered to be relatively novel endeavor. We hope that this chapter will provide the practitioners and researchers a new class of design useful for their work. As previously mentioned, there are many interesting theoretical research problems in this area, we welcome more people to join us for the future study.

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