

13. Uniform Design and Its Industrial Applications

Uniform design is a kind of space-filling design whose applications in industrial experiments, reliability testing and computer experiments is a novel endeavor. Uniform design is characterized by uniform scattering of the design points over the experimental domain, and hence is particularly suitable for experiments with an unknown underlying model and for experiments in which the entire experimental domain has to be adequately explored. An advantage of uniform design over traditional designs such as factorial design is that, even when the number of factors or the number of levels of the factors are large, the experiment can still be completed in a relatively small number of runs. In this chapter we shall introduce uniform design, the relevant underlying theories, and the methods of constructing uniform designs in the s -dimensional cube and in the $(q-1)$ -dimensional simplex for experiments with mixtures. We shall also give application examples of industrial experiments, accelerated stress testing and computer experiments.

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Human history shows that performing experiments systematically is a catalyst to speeding up the process of knowledge discovery. Since the 20th century, when design of experiments was first adopted in agriculture, technology has developed more quickly than ever before. In industry, design of experiments now has an important position in product design and process design. In recent decades, a large amount of theoretical work has been done on design of experiments, and many successful examples of industrial applications are available. For a comprehensive review of the different types of designs, readers may refer to *Ghosh and Rao* [13.1]. In this chapter, we shall focus on a type of design called the *uniform design*, whose concept was first introduced in 1978 [13.2] and has now gained popularity and proven to be very successful in industrial applications.

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A response in an industrial process may depend on a number of contributing factors. A major objective of an industrial experiment is to explore the relationship between the response and the various causes that may be contributing factors, and to find levels for the contributing factors that optimize the response. Examples of responses are the tensile strength of a material produced from different raw ingredients, the mean time to failure of an electrical component manufactured under different settings of the production equipment, or the yield of a product produced from a chemical process under different reaction conditions. To optimize the response, the relationship between the response and the contributing factors has to be established. If it is difficult to derive the theoretical relationship, experiments may be conducted and statistical methods may be used to establish empirical models or metamodels. When the

form of the model is unknown, one may wish to explore the entire design region by choosing a design whose design points are spread uniformly over the region. Such an objective may be achieved by using uniform design, which was formally introduced in Fang [13.3] and Wang and Fang [13.4]. Figure 2 shows some examples of uniform designs constructed in the two-dimensional square. There are many examples of successful applications of uniform designs in science, engineering and industries. A major multinational automobile manufacturer has recently adopted uniform designs as a standard procedure in product design and process design. A review of applications of uniform designs in chemistry and chemical engineering is given in Liang et al. [13.5]. An example of application in quality improvement in electronics manufacturing is given in Chan and Huang [13.6], Chan and Lo [13.7] and Li et al. [13.8]. Investigations have shown that uniform design performs better at estimating nonlinear problems than other designs, and is robust against model assumptions; see Zhang et al. [13.9] and Xu et al. [13.10].

Uniform design is different from traditional designs (such as orthogonal arrays and Latin square designs) in that it is not defined in terms of combinatorial structure but rather in terms of the spread of the design points over the entire design region. An advantage of uniform designs over traditional designs is that the former can be used for experiments in which the number of factors and the number of levels of the factor are not small, but a large number of runs is not available. In an experiment with 15 factors and 15 levels on each factor, for example, $225 = 15^2$ runs will be required if an orthogonal array is used, but if a uniform design is used it is possible to complete the experiment in 15 runs. In a Taguchi-type parameter design (Taguchi [13.11]), the number of runs required is smaller if uniform designs are used instead of orthogonal arrays. For example, if an $L_{36}(2^3 \times 3^{11})$ orthogonal array is used for the inner and outer arrays, a total of 36×36 runs are required, while if $U_{13}(13^8)$ and $U_{12}(12^{10})$ uniform designs are used instead, $13 \times 12 = 156$ runs will be sufficient [13.12]. Sometimes, to limit the number of runs in an experiment, one may choose designs with a small number of levels, say two- or three-level designs. However, when the behavior of the response is unknown, designs with small numbers of levels are generally unsatisfactory. In Fig. 13.1, all of the two-, three-, four- and five-level designs with equally spaced design points in $[-1, 1]$ (including the points ± 1) wrongly indicate that y decreases as x increases in $[-1, 1]$. Only designs with six or more levels

with equally spaced design points will disclose the peak of y .

A uniform design with n runs, q levels on each of the s factors is denoted by $U_n(q^s)$. Similar notation, for example $U_n(q_1^{s_1} \times q_2^{s_2})$, is used for mixed-level designs. Uniform design tables have been constructed and are available from the website www.math.hkbu.edu.hk/UniformDesign for convenient use. Plots of uniform designs constructed for $n = 2, 5, 8, 20$ are shown in Fig. 13.2. Uniform designs, whose design points are scattered uniformly over the design region, may be constructed by minimizing a discrepancy. Uniform designs can also be used as space-filling designs in numerical integration. In recent years, many theoretical results on uniform designs have been developed. Readers may refer to Fang and Wang [13.13], Fang and Hickernell [13.14], Hickernell [13.15], Fang and Mukerjee [13.16], Xie and Fang [13.17], Fang and Ma [13.18, 19], Fang et al. [13.20], Fang [13.21] and Hickernell and Liu [13.22].

In what follows, we will use “UD” as an abbreviation for “uniform design”. This chapter is organized as follows. Section 13.1 gives a general procedure for conducting an industrial experiment, and gives an example of an application of uniform design in a pharmaceutical experiment which has three contributing factors and where each factor has seven levels. No theoretical model is available for the relationship between these contributing factors and the response (the yield of the process). From the results of the experiment conducted according to a uniform design, several empirical models are proposed, and specific levels for the contributing factors are suggested to maximize the yield. Section 13.2 gives an example of the application of uniform design to accelerated stress testing for determining the

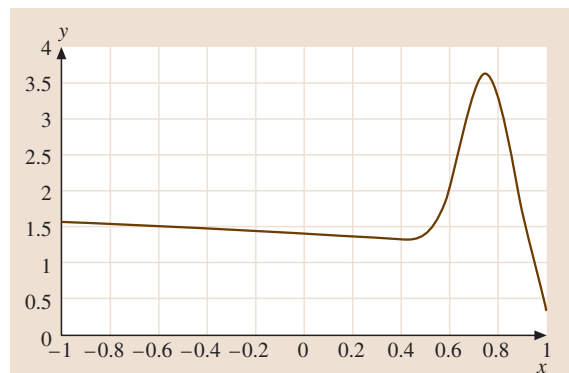


Fig. 13.1 An example of a response curve

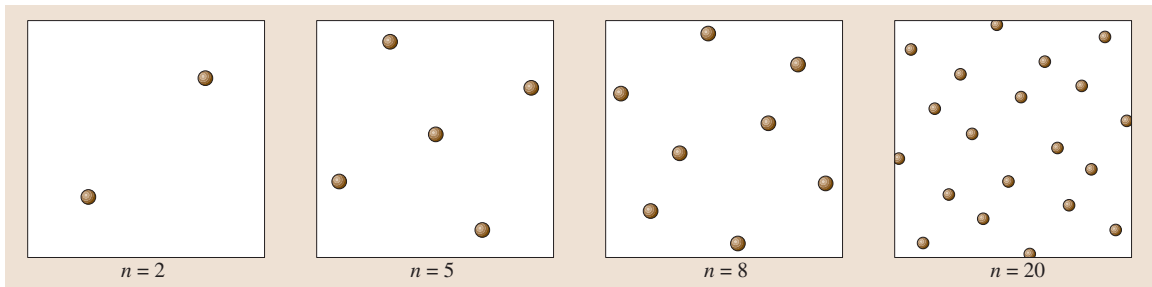


Fig. 13.2 Plots of uniform designs in S^2

median time to failure of an electronics device, with a known theoretical model. The values of the parameters in the theoretical model are determined from the results of accelerated stress testing conducting according to uniform design, and a predicted value for the median time to failure is obtained. Section 13.3 explains when computer experiments can be used for solving practical problems, and illustrates with a simple example on a robot arm how a computer experiment is conducted using uniform design to obtain an approximation of the true theoretical model of the robot arm position. Section 13.4 formally defines uniform design on the s -dimensional cube $[0, 1]^s$ in terms of minimization of the *discrepancy*, and introduces several different discrepancies and their computational formulas. The U -type design, which is used to define a discrete discrepancy, is also introduced. Section 13.5 states that the construction of uniform designs on the s -dimensional cube is an NP-hard problem even when high-power

computers are used, and explains how approximate uniform designs can be constructed more easily using U -type designs. Lower bounds for several discrepancies are given, and these lower bounds can be used to indicate how close (in terms of discrepancy) an approximate uniform design is to the theoretical uniform design. Some methods for construction of approximate uniform designs are given. Section 13.6 is devoted to uniform designs for experiments with mixtures in which the contributing factors are proportions of the ingredients in a mixture. It is explained with illustrations how uniform designs can be constructed on the simplex S^{q-1} , which is the complete design region, and on a subregion of it. Section 13.7 gives the relationships between uniform design and other designs or design criteria, including aberration, orthogonality, supersaturated design, isomorphic design, and equivalent Hadamard matrices. This chapter is concluded briefly in Section 13.8.

13.1 Performing Industrial Experiments with a UD

One purpose of performing industrial experiments is to acquire data to establish quantitative models, if such models cannot be built solely based on theoretical consideration or past experience. Such models can be used to quantify the process, verify a theory or optimize the process. The following steps may be taken as a standard procedure for performing industrial experiments.

1. **Aim.** Specify the aim of the experiment (which may be maximizing the response, defining the operational windows of the contributing and noncontributing factors, etc.), and identify the process response to study.
2. **Factor and domain.** Specify possible contributing factors, and identify the domain of variation of

each factor according to experience and practical constraints.

3. **Numbers of levels and runs.** Choose a sufficiently large number of levels for each factor and the total number of runs according to experience, physical consideration and resources available.
4. **Design.** Specify the number of runs and choose a design for the first set of experiment. It is recommended to adopt a UD from the literature or from the website www.math.hkbu.edu.hk/UniformDesign that matches the requirements in Step 3.
5. **Implementation.** Conduct the experiment according to the design chosen in Step 4. Allocate the runs randomly.

6. **Modeling.** Analyze the results using appropriate statistical tools according to the nature of the data. Such tools may include regression methods, ANOVA, Kriging models, neural networks, wavelets, splines, etc. Establish models relating the response to the contributing factors.
7. **Diagnostics.** Make conclusions from the models established in Step 6 to fulfil the aim specified in Step 1.
8. **Further Experiments.** If applicable, perform additional runs of the experiment to verify the results obtained in Steps 6 and 7, or perform subsequent experiments in order to fulfil the aim in Step 1.

The following example illustrates a successful application of UD in an industrial experiment.

Example 13.1: The yield y of an intermediate product in pharmaceutical production depends on the percentages of three materials used: glucose (A), ammonia sulphate (B) and urea (C). The aim of the experiment is to identify the percentages of A, B and C, say x_1, x_2, x_3 , which will produce the highest yield. The region for the experiment was defined by the following possible ranges of variation of x_1, x_2, x_3 :

$$\begin{aligned} \text{A: } 8.0 \leq x_1 \leq 14.0(\%); \quad \text{B: } 2.0 \leq x_2 \leq 8.0(\%); \\ \text{C: } 0.0 \leq x_3 \leq 0.3(\%). \end{aligned} \quad (13.1)$$

It was planned to complete one experiment in not more than eight runs. The levels chosen for the factors are as follows:

$$\begin{aligned} x_1: (1)8.0, (2)9.0, (3)10.0, (4)11.0, (5)12.0, \\ (6)13.0, (7)14.0; \\ x_2: (1)2.0, (2)3.0, (3)4.0, (4)5.0, (5)6.0, (6)7.0, \\ (7)8.0; \\ x_3: (1)0.00, (2)0.05, (3)0.10, (4)0.15, (5)0.20, \\ (6)0.25, (7)0.30. \end{aligned}$$

Table 13.1 Experiment for the production yield y

No.	$U_7(7^3)$			x_1	x_2	x_3	y
1	1	2	3	8.0	3.0	0.10	7.33
2	2	4	6	9.0	5.0	0.25	5.96
3	3	6	2	10.0	7.0	0.05	6.15
4	4	1	5	11.0	2.0	0.20	9.59
5	5	3	1	12.0	4.0	0.00	8.91
6	6	5	4	13.0	6.0	0.15	6.47
7	7	7	7	14.0	8.0	0.30	4.82

A $U_7(7^3)$ UD was adopted. Table 13.1 shows the $U_7(7^3)$ UD adopted, the layout of the experiment, and the observed response y .

Fitting the data in Table 13.1 with a linear model in x_1, x_2, x_3 gives

$$\hat{y} = 8.1812 + 0.3192x_1 - 0.7780x_2 - 5.1273x_3, \quad (13.2)$$

with $R^2 = 0.9444$, $s^2 = 0.3202$, and an F probability of 0.022. The ANOVA is shown in Table 13.2. From (13.2), the maximum value of $\hat{y} = 11.094$ is attained at $x_1 = 14$, $x_2 = 2$ and $x_3 = 0$ within the ranges specified in (13.1).

Fitting the data with a second-degree polynomial by maximizing R^2 gives

$$\begin{aligned} \hat{y} = 7.0782 + 0.0542x_1^2 - 0.1629x_1x_2 \\ - 0.3914x_1x_3 + 0.1079x_3^2, \end{aligned} \quad (13.3)$$

with $R^2 = 0.9964$, $s^2 = 0.0309$, and an F probability of 0.007. The ANOVA table is shown in Table 13.3. From (13.3), the maximum value of $\hat{y} = 13.140$ is attained at $(x_1, x_2, x_3) = (14.0, 2.0, 0.0)$, within the ranges specified in (13.1).

On the other hand, fitting the data with a centered second-degree polynomial in the variables $(x_1 - \bar{x}_1)$, $(x_2 - \bar{x}_2)$ and $(x_3 - \bar{x}_3)$ by maximizing R^2 gives

$$\begin{aligned} \hat{y} = 8.2209 - 0.5652(x_2 - 5) - 4.5966(x_3 - 0.15) \\ - 0.4789(x_1 - 11)^2 + 0.3592(x_1 - 11)(x_2 - 5), \end{aligned} \quad (13.4)$$

with $R^2 = 0.9913$, indicating a good fit. The ANOVA table is shown in Table 13.4. From (13.4), the maximum value of $\hat{y} = 11.2212$ is attained at $(x_1, x_2, x_3) = (9.8708, 2.0, 0.0)$, within the ranges specified in (13.1).

The second-degree model (13.2) and the centered second-degree model (13.3) fit the data better than the linear model. The maximum predicted values of \hat{y} given by (13.2–13.4) are between 11.094 and 13.140 when x_1 is between 9.8708 and 14, $x_2 = 2$ and $x_3 = 0$ in the design region. These results show that the smaller x_2 and x_3 , the larger \hat{y} . Zero is the smallest possible value

Table 13.2 ANOVA for a linear model

Source	SS	df	MS	F	P
Regression	16.3341	3	5.4447	17.00	0.022
Error	0.9608	3	0.3203		
Total	17.2949	6			

Table 13.3 ANOVA for a second-degree model

Source	SS	df	MS	F	P
Regression	17.2331	4	4.3083	139.39	0.007
Error	0.0618	2	0.0309		
Total	17.2949	6			

of x_3 , but x_2 may be extended beyond its smallest value of 2, and x_1 can be extended beyond its largest value of 14 from the boundary of the design region. To explore whether any larger values of maximum y can be achieved

Table 13.4 ANOVA for a centered second-degree model

Source	SS	df	MS	F	P
Regression	17.1445	4	4.2861	56.99	0.0173
Error	0.1504	2	0.0752		
Total	17.2949	6			

outside the design region, further investigation can be carried out by fixing x_3 at 0 and performing two factor experiments with x_1 in the range [8, 16] and x_2 in the range [0, 3].

13.2 Application of UD in Accelerated Stress Testing

Accelerated stress testing is an important method in studying the lifetime of systems. As a result of advancement in technology the lifetime of products is increasing, and as new products emerge quickly product cycle is decreasing. Manufacturers need to determine the lifetime of new products quickly and launch them into the market before another new generation of products emerges. In many cases it is not viable to determine the lifetime of products by testing them under normal operating conditions. To estimate their lifetime under normal operating conditions, accelerated stress testing is commonly used, in which products are tested under high-stress physical conditions. The lifetime of the products are extrapolated from the data obtained using some lifetime models. Many different models, such as the Arrhenius model, the inverse-power-rule model, the proportional-hazards model, etc., have been proposed based on physical or statistical considerations. Readers may refer to *Elsayed* [13.23] for an introduction to accelerated stress testing. In this section we shall give an example to illustrate the application of UD to accelerated stress testing.

Example 13.2: The median time to failure t_0 of an electronics device under the normal operating conditions has to be determined under accelerated stress testing. Theoretical consideration shows that, for such a device, a model of the inverse response type should be appropriate. Under such a model, when the device is operating under voltage V (Volts), temperature T (Kelvin) and relative humidity H (%), its median time to failure t is given by

$$t = a V^{-b} e^{c/T} e^{-dH},$$

where a, b, c, d are constants to be determined. Under normal operating conditions, the device operates at $V = 1$, $T = 298$, $H = 60$. The ranges for V, T, H determined for this experiment were 2–5, 353–373, and 85–100, respectively. Logarithmic transformation on the above model gives

$$\ln t = \ln a - b \ln V + c/T - dH.$$

An experiment with eight runs and four equally spaced levels on each of $\ln V$, $1/T$ and H was planned. These

Table 13.5 The set up and the results of the accelerated stress test

No.	$U_8(4^3)$			$\ln V$	V	$1/T$	T	H	t
1	1	3	2	0.6931	2	0.0027821	359	90	296.5
2	1	1	3	0.6931	2	0.0026809	373	95	304.3
3	4	1	2	1.6094	5	0.0026809	373	90	95.0
4	4	3	3	1.6094	5	0.0027821	359	95	129.6
5	3	4	1	1.3040	3.68	0.0028328	353	85	278.6
6	3	2	4	1.3040	3.68	0.0027315	366	100	186.0
7	2	4	4	0.9985	2.71	0.0028328	353	100	155.4
8	2	2	1	0.9985	2.71	0.0027315	366	85	234.0

levels were as follows.

$\ln V$: (1)0.6931, (2)0.9985, (3)1.3040,
(4)1.6094 ;
 $1/T$: (1)0.0026809, (2)0.0027315, (3)0.0027821,
(4)0.0028328 ;
 H : (1)85, (2)90, (3)95, (4)100 .

The corresponding levels of V and T were

V : (1)2, (2)2.71, (3)3.68, (4)5 ;
 T : (1)373, (2)366, (3)359, (4)353 .

The test was performed according to a $U_8(3^4)$ UD. The layout of the experiment and the t values observed are shown in Table 13.5.

Table 13.6 ANOVA for an inverse responsive model

Source	SS	df	MS	F	P
Regression	1.14287	3	0.38096	11.70	0.019
Error	0.13024	4	0.03256		
Total	1.27311	7			

Regression analysis gives

$$\ln \hat{t} = 5.492 - 1.0365 \ln V + 1062/T - 0.02104H ,$$

or

$$\hat{t} = 240.327V^{-1.0365} e^{1062/T - 0.02104H} ,$$

with $R^2 = 0.898$ and $s^2 = 0.0325$. The ANOVA table in Table 13.6 shows a significance level of 0.019. The value of t at the normal operating condition $V = 1$, $T = 298$ and $H = 60$ is estimated to be $\hat{t}_0 = 2400.32$ (hours).

13.3 Application of UDs in Computer Experiments

Indeed, UDs were first used by mathematicians as a space-filling design for numerical integration, and application of UDs in experiments was motivated by the need for effective designs in *computer experiments* in the 1970s [13.2].

The computer can play its role as an artificial means for simulating a physical environment so that experiments can be implemented virtually, if such experiments are not performed physically for some reasons. For example, we do not wish to perform an experiment physically if the experiment may cause casualty. It is not practical to perform a hurricane experiment because we cannot generate and control a hurricane, but if a dynamical model can be established the experiment can be performed virtually on the computer. In such a situation, computer experiments, in which computation or simulation is carried out on the computer, may help study the relation between the contributing factors and the outcome. To perform a computer experiment, levels will have to be set for each of the contributing factors, and in order to have a wide coverage of the entire design region with a limited number of runs, a UD is a good recommendation.

Another use of computer experiments is to establish approximations of known theoretical models if such models are too complicated to handle in practice. From the theoretical model, if computation can be carried out using the computer in evaluating the numerical values of the response y at given values of the variants x_1, \dots, x_k , from the numerical results we can establish metamodels

that are good approximations to the theoretical model but yet simple enough for practical use. On the other hand, if the theoretical model is so complicated (for example, represented as a large system of partial differential equations) that it is not even practical to solve it using a computer but if it is possible to observe the values of the response y at different values of x_1, \dots, x_k , we can make use of the computer to establish mathematically tractable empirical models to replace the complicated theoretical model.

In computer experiments, UDs can be used for the selection of representative values of x_1, \dots, x_k that cover the design region uniformly in a limited number of runs. This is illustrated by an example on water flow in Fang and Lin [13.24]. Another example of the application of UDs in computer experiments is for real-time control of robotic systems in which the kinematics is described by a system of complicated equations containing various angles, lengths and speeds of movement. Control of robotic systems requires the solution of such a system of equations on a real-time basis at a sufficiently fast speed, which sometimes cannot be achieved because of the intensive computation required (which may involve inversion of high-order Jacobian determinants, etc.). For such a case, computer experiments may be employed, in which the system of equations is solved off-line and the results obtained are used to establish statistical models that are mathematically simple enough to be used for real-time computation. To achieve a sufficiently uniform coverage of the design region, UDs can be used. The fol-

lowing Example 3 is a simplified version of a robot arm in two dimensions which illustrates this application.

Example 13.3: A robot arm on the uv -plane consists of s segments. One end of the first segment is connected to the origin by a rotational joint, and the other end of the first segment is connected to one end of the second segment by a rotational joint. The other end of the second segment is connected to one end of the third segment by a rotational joint, and so on. Let L_j represent the length of the j^{th} segment, θ_1 represent the angle of the first segment with the u -axis, θ_j represent the angle between the $(j-1)^{\text{th}}$ and j^{th} segment, where $0 \leq \theta_j \leq 2\pi (j = 1, \dots, s)$. The length between the origin and the end point of the last segment of the robot arm is given by

$$y = f(L_1, \dots, L_s, \theta_1, \dots, \theta_s) = \sqrt{u^2 + v^2},$$

$$u = \sum_{j=1}^s L_j \cos \left(\sum_{i=1}^j \theta_i \right),$$

$$v = \sum_{j=1}^s L_j \sin \left(\sum_{i=1}^j \theta_i \right).$$

For simplicity, suppose that $s = 2$. We intend to represent y as a generalized linear function in the variables $L_1, L_2, \theta_1, \theta_2$. A computer experiment is performed with a $U_{28}(28^6)$ UD, in which the values of y were evaluated at different values of L_i and θ_i . The results of the computation is shown in the rightmost column of Table 13.7.

Fitting the data in Table 13.7 with a centered generalized linear regression model with variables $(L_i - 0.5)$, $(\theta_i - \pi)$ and $\cos(\theta_i - \pi)$ ($i = 1, 2, 3$) using

Table 13.7 Experiment for the robot arm example

No.	$U_{28}(28^6)$						L_1	L_2	L_3	θ_1	θ_2	θ_3	y
1	11	28	6	3	14	20	0.3704	1.0000	0.1852	0.4654	3.0252	4.4215	0.6196
2	17	2	23	27	20	21	0.5926	0.03704	0.8148	6.0505	4.4215	4.6542	0.3048
3	4	14	2	26	9	23	0.1111	0.4815	0.03704	5.8178	1.8617	5.1196	0.4851
4	13	10	4	24	27	13	0.4444	0.3333	0.1111	5.3523	6.0505	2.7925	0.6762
5	14	24	28	8	12	14	0.4815	0.8519	1.0000	1.6290	2.5598	3.0252	0.5636
6	12	5	25	20	4	8	0.4074	0.1482	0.8889	4.4215	0.6982	1.6290	0.7471
7	3	16	10	1	5	10	0.07407	0.5556	0.3333	0.0000	0.9308	2.0944	0.4901
8	21	9	14	7	2	22	0.7407	0.2963	0.4815	1.3963	0.2327	4.8869	1.2757
9	5	11	26	5	18	24	0.1482	0.3704	0.9259	0.9308	3.9561	5.3523	1.0384
10	9	4	12	17	11	27	0.2963	0.1111	0.4074	3.7234	2.3271	6.0505	0.4340
11	15	17	16	10	28	28	0.5185	0.5926	0.5556	2.0944	6.2832	6.2832	1.6667
12	23	19	1	6	19	9	0.8148	0.6667	0.0000	1.1636	4.1888	1.8617	0.7518
13	7	18	20	22	1	18	0.2222	0.6296	0.7037	4.8869	0.0000	3.9561	0.6310
14	18	12	21	4	10	2	0.6296	0.4074	0.7407	0.6981	2.0944	0.2327	0.8954
15	27	8	11	23	13	6	0.9630	0.2593	0.3704	5.1196	2.7925	1.1636	0.4991
16	24	27	17	25	8	12	0.8519	0.9630	0.5926	5.5851	1.6290	2.5598	0.6711
17	20	25	9	21	22	25	0.7037	0.8889	0.2963	4.6542	4.8869	5.5851	1.3362
18	25	6	19	2	24	17	0.8889	0.1852	0.6667	0.2327	5.3523	3.7234	0.3814
19	16	23	5	16	3	4	0.5556	0.8148	0.1482	3.4907	0.4654	0.6982	1.4331
20	8	3	8	9	23	3	0.2593	0.07407	0.2593	1.8617	5.1196	0.4654	0.5408
21	22	15	27	18	26	5	0.7778	0.5185	0.9630	3.9561	5.8178	0.9308	2.1111
22	2	22	13	19	25	16	0.03704	0.7778	0.4444	4.1888	5.5851	3.4907	0.4091
23	26	21	24	13	6	26	0.9259	0.7407	0.8619	2.7925	1.1636	5.8178	2.2386
24	28	13	7	15	17	19	1.0000	0.4444	0.2222	3.2579	3.7234	4.1888	0.6162
25	19	1	3	11	7	15	0.6667	0.0000	0.07407	2.3271	1.3963	3.2579	0.6665
26	6	26	22	12	21	7	0.1852	0.9259	0.7778	2.5598	4.6542	1.3963	1.4167
27	1	7	18	14	15	11	0.0000	0.2222	0.6296	3.0252	3.2579	2.2327	0.5038
28	10	20	15	28	16	1	0.3333	0.8037	0.5185	6.2832	3.4907	0.0000	0.9161

a stepwise procedure in the package SAS gives the model

$$\begin{aligned}\hat{y} = & 0.9088 + 0.1760(L_1 - 0.5) + 0.6681(L_2 - 0.5) \\ & + 0.3917(L_3 - 0.5) - 0.2197 \cos(\theta_2 - \pi) \\ & - 0.3296 \cos(\theta_3 - \pi) \\ & - 0.01919(\theta_1 - \pi)(\theta_2 - \pi) \\ & - 0.5258(L_2 - 0.5) \cos(\theta_3 - \pi)\end{aligned}$$

$$\begin{aligned}& - 0.0792L_3\theta_1 - 0.7622(L_3 - 0.5) \cos(\theta_3 - \pi) \\ & - 0.0114(\theta_1 - \pi)(\theta_3 - \pi) \\ & - 0.0274(\theta_2 - \pi)(\theta_3 - \pi) \\ & + 0.2894 \cos(\theta_2 - \pi) \cos(\theta_3 - \pi),\end{aligned}$$

with $R^2 = 0.9868$, $s^2 = 0.0063$, and an F of 0.0000. The ANOVA table is omitted here. Evaluation at different values of L_i and θ_i shows that \hat{y} is a good approximation of y .

13.4 Uniform Designs and Discrepancies

In this section, the formal definition of a UD will be introduced. A UD is, intuitively, a design whose points distribute *uniformly* over the design space. Such uniformity may be achieved by minimizing a discrepancy. There is more than one definition of discrepancy, and different discrepancies may produce different uniform designs.

Without loss of generality, let the design space be the s -dimensional unit cube $C^s = [0, 1]^s$. We represent any point in C^s by $\mathbf{x}' = (x_1, \dots, x_s)$, where $x_1, \dots, x_s \in [0, 1]$, and the prime denotes the transpose of matrices. For a given positive integer n , a uniform design with n points is a collection of points $\mathcal{P}^* = \{\mathbf{x}_1^*, \dots, \mathbf{x}_n^*\} \subset C^s$ such that

$$M(\mathcal{P}^*) = \min M(\mathcal{P}),$$

where the minimization is carried out over all $\mathcal{P} = \{\mathbf{x}_1, \dots, \mathbf{x}_n\} \subset C^s$ with respect to some measure of uniformity, M . One choice for M is the classical L_p -discrepancy adopted in quasi-Monte-Carlo methods [13.25, 26],

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

where $[\mathbf{0}, \mathbf{x}]$ denotes the interval $[0, x_1] \times \dots \times [0, x_s]$, $N(\mathcal{P}, [\mathbf{0}, \mathbf{x}])$ denotes the number of points of \mathcal{P} falling in $[\mathbf{0}, \mathbf{x}]$, and $\text{Vol}[\mathbf{0}, \mathbf{x}]$ is the volume of the set $[\mathbf{0}, \mathbf{x}] \in C^s$, which is the distribution function of the uniform distribution on C^s .

The $D_\infty(\mathcal{P})$ discrepancy

$$\max_{\mathbf{x} \in C^s} \left| \frac{N(\mathcal{P}, [\mathbf{0}, \mathbf{x}])}{n} - \text{Vol}[\mathbf{0}, \mathbf{x}] \right|$$

is called the star discrepancy, which is the Kolmogorov-Smirnov statistic used for the goodness-of-fit test.

The L_p -discrepancy is a measure of uniformity of the distribution of points of \mathcal{P} in C^s . The smaller the value of $D_p(\mathcal{P})$, the more uniform the distribution of points of \mathcal{P} . The star discrepancy is not as sensitive as the L_p -discrepancy for finite values of p .

The quantity $D_p(\mathcal{P})$ is in general difficult to compute. Let $\mathbf{x}_k = (x_{k1}, \dots, x_{ks})'$ ($k = 1, \dots, n$). For $p = 2$, computation can be carried out more efficiently using the following closed-form analytic formula [13.27]:

$$\begin{aligned}D_2(\mathcal{P})^2 = & 3^{-s} - \frac{2^{1-s}}{n} \sum_{k=1}^n \prod_{l=1}^s (1 - x_{kl}^2) \\ & + \frac{1}{x^2} \sum_{k=1}^n \sum_{j=1}^n \prod_{i=1}^s [1 - \max(x_{ki}, x_{ji})].\end{aligned}$$

As pointed out by Fang et al. [13.20], the L_2 -discrepancy ignores the discrepancy of \mathcal{P} on lower-dimensional subspaces of C^s . To overcome this drawback, Hickernell [13.28] proposed the following modified L_2 -discrepancy, which includes L_2 -discrepancies of projections of \mathcal{P} in all lower dimensional subspaces of C^s

$$\begin{aligned}D_{2, \text{modified}}(\mathcal{P})^2 = & \sum_u \int_{C^u} \left| \frac{N(\mathcal{P}_u, J_{\mathbf{x}_u})}{n} - \text{Vol}(J_{\mathbf{x}_u}) \right|^p d\mathbf{x}_u, \quad (13.5)\end{aligned}$$

where u is a non-empty subset of the set of coordinate indices $S = \{1, \dots, s\}$, C^u is the $|u|$ -dimensional cube involving the coordinates in u , $|u|$ is the cardinality of u , \mathcal{P}_u is the projection of \mathcal{P} on C^u , \mathbf{x}_u is the projection of \mathbf{x} on C^u , and $J_{\mathbf{x}_u}$ is the projection of a rectangle $J_{\mathbf{x}}$ on C^u , which depends on \mathbf{x} and is defined based on some specific geometric consideration. Different choices of $J_{\mathbf{x}}$ produce discrepancies with different properties, the centered L_2 -discrepancy (CD)

(which contains all L_2 -discrepancies each calculated using one of the 2^s vertices of C^s as the origin), the wrap-around L_2 -discrepancy (WD) (which is calculated after wrapping around each one-dimensional subspace of C^s into a close loop), and others. Closed-form analytic formulas for CD and WD, the most commonly used discrepancies, are displayed below, and corresponding formulas for other discrepancies can be found in Fang et al. [13.20] and Hickernell [13.28, 29]

$$\begin{aligned} [\text{CD}(\mathcal{P})]^2 &= \left(\frac{13}{12}\right)^s - \frac{2}{n} \sum_{k=1}^n \prod_{j=1}^s \left(1 + \frac{1}{2}|x_{kj} - 0.5| \right. \\ &\quad \left. - \frac{1}{2}|x_{kj} - 0.5|^2\right) \\ &\quad + \frac{1}{n^s} \sum_{k=1}^n \sum_{j=1}^n \prod_{i=1}^s \left(1 + \frac{1}{2}|x_{ki} - 0.5| \right. \\ &\quad \left. + \frac{1}{2}|x_{ji} - 0.5| - \frac{1}{2}|x_{ki} - x_{ji}| \right), \quad (13.6) \\ [\text{WD}(\mathcal{P})]^2 &= \left(\frac{4}{3}\right)^s + \frac{1}{n^2} \sum_{k=1}^n \sum_{j=1}^n \prod_{i=1}^s \left[\frac{3}{2} - |x_{ki} - x_{ji}| \right. \\ &\quad \left. \times (1 - |x_{ki} - x_{ji}|) \right]. \quad (13.7) \end{aligned}$$

The CD is invariant under relabeling of coordinate axes. It is also invariant under reflection of points about any plane passing through the center and parallel to the faces of the unit cube C^s , that is, invariant when the i^{th} coordinate x_i is replaced by $1 - x_i$. It follows from the

Table 13.8 A design in $\mathcal{U}(6; 3^2 \times 2)$

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

definition that the CD takes into account the uniformity of \mathcal{P} over C^s and also over all projections of \mathcal{P} onto all subspaces of C^s . The uniform designs given in the website www.math.hkbu.edu.hk/UniformDesign are constructed using the CD [13.30].

Another useful discrepancy is called the *discrete discrepancy*, or *categorical discrepancy*. It is defined on the discrete space based on the following U -type designs, and can be used as a vehicle for construction of UD's via U -type designs.

Definition 13.1

A U -type design is an array of n rows and s columns with entries $1, \dots, q_j$ in the j -th column such that each entry in each column appears the same number of times ($j = 1, \dots, s$). The collection of all such designs is denoted by $\mathcal{U}(n; q_1 \times \dots \times q_s)$, which is the design space. When all q_j are the same, the design space will be denoted by $\mathcal{U}(n; q^s)$. Designs in $\mathcal{U}(n; q_1 \times \dots \times q_s)$ (where the q_j are distinct) are asymmetric, while designs in $\mathcal{U}(n; q^s)$ are symmetric.

Table 13.8 shows a U -type design in $\mathcal{U}(6; 3^2 \times 2)$. Obviously, in a U -type design in $\mathcal{U}(n; q_1 \times \dots \times q_s)$, n must be an integer multiple of q_j for all $j = 1, \dots, s$.

A discrete discrepancy is defined on $\mathcal{U}(n; q_1 \times \dots \times q_s)$ in terms of two positive numbers $a \neq b$, and is denoted by $D^2(U; a, b)$. The computational formula for $D^2(U; a, b)$ is

$$\begin{aligned} D^2(U; a, b) &= - \prod_{j=1}^s \left(\frac{a + (q_j - 1)b}{q_j} \right) \\ &\quad + \frac{1}{n^2} \sum_{k=1}^n \sum_{l=1}^n \prod_{j=1}^s \tilde{K}(u_{kj}, u_{lj}), \end{aligned} \quad (13.8)$$

where (u_{k1}, \dots, u_{ks}) represents the k -th point in U and

$$\tilde{K}(u_{kj}, u_{lj}) = \begin{cases} a & \text{if } u_{kj} = u_{lj}, \\ b & \text{if } u_{kj} \neq u_{lj}. \end{cases}$$

13.5 Construction of Uniform Designs in the Cube

In order to construct a uniform design on the continuum $C^s = [0, 1]^s$, we need to search for all possible sets of n points over C^s for a design with minimum discrepancy, which is an NP-hard problem for high-power computers even if n and s are not large. In general,

the coordinates of the points in a UD in C^s may be irrational. It can be proved that when $s = 1$, the set $\{\frac{1}{2n}, \frac{3}{2n}, \dots, \frac{2n-1}{2n}\}$ with equally spaced points is the n -point uniform design on $[0, 1]$ with $\text{CD} = 1/(\sqrt{12}n)$, which is the smallest possible value [13.30]. Since the

design points of a UD distribute *uniformly* over the design region, from the last result on $[0, 1]$ it is natural to expect that values of the coordinates of points in a UD in C^s are either equally spaced or nearly equally spaced on each one-dimensional subspace of C^s . Along this line of thought, while uniform designs defined for the continuum C^s are difficult to find, we can search over the discrete set of U -type designs to construct approximate uniform designs. Computation shows that this approach produces good results. The closeness between the UDs with exactly the minimum discrepancy constructed for C^2 and the approximate UDs constructed from U -type designs for $n = 2, \dots, 9$ is illustrated in Fig. 13.3 of Fang and Lin [13.24], and for larger values of n these two types of UDs are practically identical.

Tables of UDs in the website www.math.hkbu.edu.hk/UniformDesign are constructed from U -type designs. Figure 13.2 shows the plots of such designs constructed for $n = 2, 5, 8, 20$ for $s = 2$. An obvious advantage of using U -type designs for construction is that in the UD constructed values of each coordinate of the design are equally spaced. Such designs are much more convenient to use in practice than the exact UDs with irregular values of coordinates constructed for the continuum C^s .

If P is a design consisting of n points $\mathbf{x}_1 = (x_{11}, \dots, x_{1s})'$, \dots , $\mathbf{x}_n = (x_{n1}, \dots, x_{ns})'$, we shall use the following notations, on different occasions as

appropriate, to represent P : $P = \{\mathbf{x}_1, \dots, \mathbf{x}_n\}$, $P = \{x_{ij}\}_{i=1, \dots, n; j=1, \dots, s}$, $P = \{x_{ij}\}$, $P = \begin{pmatrix} x_{11} & \dots & x_{1s} \\ \vdots & \ddots & \vdots \\ x_{n1} & \dots & x_{ns} \end{pmatrix}$, $P = \begin{pmatrix} \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_n \end{pmatrix}$.

In the following Definition 13.2, we shall introduce uniform design defined on the discrete set $\mathcal{U}(n; q^s)$.

Definition 13.2

A design $U \in \mathcal{U}(n; q_1 \times \dots \times q_s)$ is called a uniform design under the measure of discrepancy M if

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

The collection of all such designs is denoted by $U_n(q_1 \times \dots \times q_s)$. When $q_1 = \dots = q_s$, U will be called a symmetric design, and $U_n(q_1 \times \dots \times q_s)$ will be denoted by $U_n(q^s)$.

If $U \in \mathcal{U}(n; q_1 \times \dots \times q_s)$ is a U -type design consisting of the n points $\mathbf{u}_1, \dots, \mathbf{u}_n$, where $\mathbf{u}_i = (u_{i1}, \dots, u_{is})'$ ($i = 1, \dots, n$), we define $x_{ij} = (u_{ij} - 0.5)/q_j$, so that $\mathcal{P} = \{\mathbf{x}_1, \dots, \mathbf{x}_n\} \in C^s$. If M is a discrepancy on C^s , we define $M(U) = M(\mathcal{P})$. Finding UDs in $U_n(q_1 \times \dots \times q_s)$ by minimizing discrepancies is still an NP-hard problem because of the amount of computation required, even though it is a more manageable task than finding UDs in the continuum C^s . To get around this difficulty, a variety of methods have been proposed by different authors.

For a given discrepancy, and given n and s , it can be seen from the definition that the discrepancy of all designs of n points has a positive lower bound. Thus, lower bounds of discrepancies are used as a benchmark in the construction of UDs or approximate UDs. A UD is a design whose discrepancy equals the lower bound, and a design whose discrepancy is close to the lower bound is a good design.

13.5.1 Lower Bounds of Categorical, Centered and Wrap-Around Discrepancies

(A) Lower Bounds of the Categorical Discrepancy

Let $c(kl)$ be the coincidence number of a pair of elements between rows k and l of a design. Clearly $c(kk) = s$,

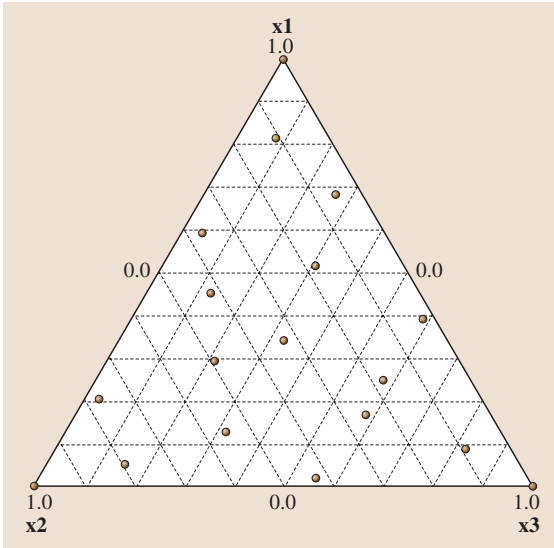


Fig. 13.3 A uniform design of 15 points in S^{3-1}

and $s - c(kl)$ is the Hamming distance between rows k and l .

Theorem 13.1

A lower bound of the categorical discrepancy in $\mathcal{U}(n; q_1 \times \cdots \times q_s)$ is given by

$$-\prod_{j=1}^s \left(\frac{a + (q_j - 1)b}{q_j} \right) + \frac{a^s}{n} + \frac{n-1}{n} b^s \left(\frac{a}{b} \right)^\psi, \quad (13.9)$$

where $\psi = (\sum_{j=1}^s n/q_j - s)/(n-1)$. This lower bound is attained if and only if ψ is an integer and all $c(kl)$ are equal to ψ . When the design space is $\mathcal{U}(n; q^s)$ the above lower bound becomes

$$-\left(\frac{a + (q-1)b}{q} \right)^s + \frac{a^s}{n} + \frac{n-1}{n} b^s \left(\frac{a}{b} \right)^\psi, \quad (13.10)$$

where $\psi = s(n/q - 1)/(n-1)$.

The above lower bounds can be used in searching for UD in $\mathcal{U}(n; q_1 \times \cdots \times q_s)$.

It is known that block designs have a very good balance structure. Balanced incomplete block (BIB) designs have appeared in many textbooks. Liu and Fang [13.31] and Lu and Sun [13.32] found that there is a link between UD and resolvable BIB designs, a subclass of BIB. Through this link, many UD can be generated from the large amount of resolvable BIB designs available in the literature. Reader may refer to Fang et al. [13.33], Fang et al. [13.34] and Qin [13.35] for the details.

(B) Lower Bounds of the Wrap-Around L_2 -Discrepancy

Values of the wrap-around discrepancy of a design in $\mathcal{U}(n; q^s)$ can be calculated by (13.7). Let $\alpha_{ij}^k \equiv |x_{ik} - x_{jk}|(1 - |x_{ik} - x_{jk}|)$ ($i, j = 1, \dots, n, i \neq j$ and $k = 1, \dots, s$). For any two rows of a design denote the distribution of values of α_{ij}^k by F_{ij}^α . Fang et al. [13.36] obtained lower bounds for $q = 2, 3$. Recently, Fang et al. [13.37] gave lower bounds of the wrap-around discrepancy for any number of levels q as follows:

Theorem 13.2

Lower bounds of the wrap-around L_2 -discrepancy on $\mathcal{U}(n; q^s)$ for even and odd q are given by

$$\begin{aligned} \text{LB}_{\text{even}} &= \Delta + \frac{n-1}{n} \left(\frac{3}{2} \right)^{\frac{s(n-q)}{q(n-1)}} \left(\frac{5}{4} \right)^{\frac{sn}{q(n-1)}} \\ &\quad \times \left(\frac{3}{2} - \frac{2(2q-2)}{4q^2} \right)^{\frac{2sn}{q(n-1)}} \cdots \\ &\quad \times \left(\frac{3}{2} - \frac{(q-2)(q+2)}{4q^2} \right)^{\frac{2sn}{q(n-1)}}, \\ \text{LB}_{\text{odd}} &= \Delta + \frac{n-1}{n} \left(\frac{3}{2} \right)^{\frac{s(n-q)}{q(n-1)}} \\ &\quad \times \left(\frac{3}{2} - \frac{2(2q-2)}{4q^2} \right)^{\frac{2sn}{q(n-1)}} \cdots \\ &\quad \times \left(\frac{3}{2} - \frac{(q-1)(q+1)}{4q^2} \right)^{\frac{2sn}{q(n-1)}}, \end{aligned}$$

respectively, where $\Delta = -\left(\frac{4}{3}\right)^s + \frac{1}{n}\left(\frac{3}{2}\right)^s$. A U -type design in $\mathcal{U}(n; q^s)$ is a uniform design under the wrap-around L_2 -discrepancy if all its F_{ij}^α distributions, for $i \neq j$, are the same. In this case, the WD_2 value of this design achieves the above lower bound.

Fang et al. [13.37] also proposed a powerful algorithm based on Theorem 13.2 and obtained many new UD.

(C) Lower Bounds of the Centered L_2 -Discrepancy

A tight lower bound for the centered L_2 -discrepancy is rather difficult to find. Fang and Mukerjee [13.16] gave a lower bound for the centered L_2 -discrepancy on $\mathcal{U}(n; 2^s)$. Fang et al. [13.36] gave some improvement of Fang and Mukerjee's results. Recently, Fang et al. [13.38] provided a tight lower bound for the centered L_2 -discrepancy for $q = 3, 4$. They also proposed an efficient algorithm for searching for UD.

13.5.2 Some Methods for Construction

The design space $\mathcal{U}(n; q^s)$ contains many poor designs with large values of discrepancy. Confining our search to subspaces in $\mathcal{U}(n; q^s)$ with good designs will significantly reduce the amount of computation. Methods developed along this direction are the *good lattice point method* (see Sect. 1.3 of Fang and Wang [13.13]), the *Latin square method* and the *extending orthogonal design method* (see Fang and Hickernell [13.14]). Ma and Fang [13.39] proposed the *cutting method* that con-

constructs a subdesign from a large uniform design. Fang and Qin [13.40] suggested merging two uniform designs to generate a larger design. Let $U = \{u_{ij}\}$ be a U -type design in $\mathcal{U}(n; q_1 \times \cdots \times q_s)$ and $V = \{v_{kl}\}$ be one in $\mathcal{U}(m; m')$. We can construct a new U -type design $D_{U,V}$ by collapsing U and V as follows:

$$D_{U,V} = (\mathbf{1}_m \otimes U; V \otimes \mathbf{1}_n),$$

where $\mathbf{1}_n$ is the column vector of ones and $A \otimes B$ is the Kronecker product of $A = (a_{ij})$ and $B = (b_{kl})$ defining by $A \otimes B = (a_{ij} b_{kl})$. For example, if

$$A = \begin{pmatrix} 1 & 2 & 4 \\ 2 & 1 & 3 \\ 3 & 4 & 2 \\ 4 & 3 & 1 \end{pmatrix}, \quad \text{and} \quad B = \begin{pmatrix} 1 & 2 \\ 2 & 1 \end{pmatrix},$$

then

$$A \otimes B = \begin{pmatrix} 1 & 2 & 2 & 4 & 4 & 8 \\ 2 & 1 & 4 & 2 & 8 & 4 \\ 2 & 4 & 1 & 2 & 3 & 6 \\ 4 & 2 & 2 & 1 & 6 & 3 \\ 3 & 6 & 4 & 8 & 2 & 4 \\ 6 & 3 & 8 & 4 & 4 & 2 \\ 4 & 8 & 3 & 6 & 1 & 2 \\ 8 & 4 & 6 & 3 & 2 & 1 \end{pmatrix}.$$

If both U and V are uniform designs, Fang and Qin [13.40] proved that the new design $D_{U,V}$ has the lowest discrepancy in a subclass of $\mathcal{U}(nm; q_1, \times \cdots \times q_s \times m')$.

13.6 Construction of UD for Experiments with Mixtures

Experiments with mixtures are experiments in which the variants are proportions of ingredients in a mixture. An example is an experiment for determining the proportion of ingredients in a polymer mixture that will produce plastics products with the highest tensile strength. Similar experiments are very commonly encountered in industries. A mixture can be represented as $\mathbf{x} = (x_1, \dots, x_q)' \in \{(x_1, \dots, x_q)' : x_1 + \cdots + x_q = 1; x_1, \dots, x_q \geq 0\} = S^{q-1}$, where $q \geq 2$ is the number of ingredients in the mixture. The set S^{q-1} is called the $(q-1)$ -dimensional simplex. Readers may refer to the monograph by Cornell [13.41] and the survey article by Chan [13.42] for details of design and modeling in experiments with mixtures. Among the designs for experiments with mixtures, simplex lattice designs have the longest history, followed by simplex centroid designs and axial designs. UD on S^{q-1} , however, provide a more uniform coverage of the design region than these designs. In this section, we shall explain how UD on S^{q-1} can be constructed using UD constructed for C^s .

Suppose that $U = (u_{ki})_{k=1, \dots, n; i=1, \dots, q-1}$ is a $U_n(n^{q-1})$ selected from the website. Let $c_{ki} = (u_{ki} - 0.5)/n$ ($k = 1, \dots, n; i = 1, \dots, q-1$), and let $\mathbf{c}'_k = (c_{k1}, \dots, c_{k,q-1})$. Then

$$C = \begin{pmatrix} \mathbf{c}'_1 \\ \mathbf{c}'_2 \\ \vdots \\ \mathbf{c}'_n \end{pmatrix}$$

is a UD on $[0, 1]^{q-1}$ from which a UD on S^{q-1} can be constructed. In the construction, special consideration is required because $(x_1, \dots, x_q)'$ in S^{q-1} is under the constant-sum constraint $x_1 + \cdots + x_q = 1$.

(A) When the Design Region is S^{q-1}

When the design region is the entire simplex S^{q-1} , the variables x_1, \dots, x_q can take any value in $[0, 1]$ as far as $x_1 + \cdots + x_q = 1$. The following method of constructing UD on S^{q-1} is due to Wang and Fang [13.43, 44] which is also contained in Fang and Wang [13.13]. For each \mathbf{c}'_k ($k = 1, \dots, n$) in the above uniform design C , let

$$\begin{aligned} x_{k1} &= 1 - c_{k1}^{1/(q-1)}, \\ x_{k2} &= (1 - c_{k2}^{1/(q-2)}) c_{k1}^{1/(q-1)}, \\ x_{k3} &= (1 - c_{k3}^{1/(q-3)}) c_{k1}^{1/(q-1)} c_{k2}^{1/(q-2)}, \\ &\vdots \\ x_{k,q-1} &= (1 - c_{k,s-1}^{1/1}) c_{k1}^{1/(q-1)} c_{k2}^{1/(q-2)} \cdots c_{k,q-2}^{1/2}, \\ x_{kq} &= c_{k1}^{1/(q-1)} c_{k2}^{1/(q-2)} \cdots c_{k,q-2}^{1/2} c_{k,q-1}^{1/1}. \end{aligned}$$

Let $\mathbf{x}'_k = (x_{k1}, \dots, x_{k,q})$ ($k = 1, \dots, n$). Then $\begin{pmatrix} \mathbf{x}'_1 \\ \mathbf{x}'_2 \\ \vdots \\ \mathbf{x}'_n \end{pmatrix}$ is

a UD on S^{q-1} . This method of construction is based on the following theory of transformation.

Let $\mathbf{x} = (X_1, \dots, X_s)$ be uniformly distributed on S^{s-1} . Let

$$X_i = C_i^2 \prod_{j=1}^{i-1} S_j^2 (i = 1, \dots, s-1),$$

$$X_s = \prod_{j=1}^{s-1} S_j^2$$

where

$$S_j = \sin(\pi\phi_j/2),$$

$$C_j = \cos(\pi\phi_j/2)$$

$$(j = 1, \dots, s-1),$$

$$(\phi_1, \dots, \phi_{s-1}) \in C^{s-1}.$$

Then, we have

(a) $\phi_1, \dots, \phi_{s-1}$ are mutually independent;

(b) the cumulative distribution function of ϕ_j is

$$F_j(\phi) = \sin^{2(s-j)}(\pi\phi/2),$$

$$(j = 1, \dots, s-1).$$

With the inverse transformation, the above formulas for x_{k1}, \dots, x_{ks} follow.

When $q = 3$, this construction is expressed as

$$x_{k1} = 1 - c_{k1}^{1/2},$$

$$x_{k2} = (1 - c_{k2})c_{k1}^{1/2},$$

$$x_{k3} = c_{k1}^{1/2} c_{k2},$$

and under this transformation a rectangle in S^2 is transformed into a trapezium in S^{3-1} . Figure 13.3 shows a plot of a UD of 15 points on S^{3-1} constructed from the $U_{15}(15^2)$ design

$$\begin{pmatrix} 10 & 15 & 14 & 9 & 6 & 2 & 12 & 13 & 11 & 5 & 1 & 8 & 3 & 4 & 7 \\ 1 & 9 & 3 & 12 & 15 & 13 & 6 & 14 & 17 & 4 & 7 & 5 & 2 & 10 & 8 \end{pmatrix}^T.$$

(B) When There are Restrictions on the Mixture Components

In many cases, lower and upper bounds are imposed on the components in a mixture. For example, in a concrete mixture, the amount of water cannot be less than 10% nor more than 90%. Let $a_i, b_i \in [0, 1]$ ($i = 1, \dots, q$), $\mathbf{a} = (a_1, \dots, a_q)'$, $\mathbf{b} = (b_1, \dots, b_q)'$, and let $a = a_1 + \dots + a_q$ and $b = b_1 + \dots + b_q$. Define $S_{a,b}^{q-1} = \{\mathbf{x}' = (x_1, \dots, x_q) \in S^{q-1} : a_i \leq x_i \leq b_i (i = 1, \dots, q)\}$. From $x_1 + \dots + x_q = 1$ it is not difficult to see that $S_{a,b}^{q-1}$ is non-empty if and only if $a \leq 1 \leq b$, and $S_{a,b}^{q-1}$ contains

more than one point if and only if $a < 1 < b$. Fang and Yang [13.45] proposed a method for construction of n -point UD on $S_{a,b}^{q-1}$ using a conditional distribution and the Monte Carlo method. It is more complicated than the method due to Wang and Fang [13.44], but produces designs with better uniformity. To use this method, the following steps may be followed.

1. Check whether the condition $a < 1 < b$ is satisfied. If this condition is not satisfied, the set $S_{a,b}^{q-1}$ is either empty or contains only one point, and in both cases there is no need to construct UD on $S_{a,b}^{q-1}$.
2. Suppose that $a < 1 < b$. Some of the restrictions $a_1 \leq x_i \leq b_i$ ($i = 1, \dots, q$) may be redundant. To remove redundant restrictions, define

$$a_i^0 = \max(a_i, b_i + 1 - b),$$

$$b_i^0 = \min(b_i, a_i + 1 - a) (i = 1, \dots, q).$$

The restrictions $a_1^0 \leq x_i \leq b_i^0$ ($i = 1, \dots, q$) do not contain redundant ones, and $a_1 \leq x_i \leq b_i$ is equivalent to $a_1^0 \leq x_i \leq b_i^0$ ($i = 1, \dots, q$).

3. Reduce the lower bounds to 0 by defining $y_i = (x_i - a_i^0) / [1 - (a_1^0 + \dots + a_q^0)]$ and $b_i^* = (b_i^0 - a_i^0) / [1 - (a_1^0 + \dots + a_q^0)]$ ($i = 1, \dots, q$). Then $a_i^0 \leq x_i \leq b_i^0$ is equivalent to $0 \leq y_i \leq b_i^*$ ($i = 1, \dots, q$).
4. Define the function $G(c, d, \phi, \Delta, \ell) = \Delta(1 - [c(1 - \phi)^\ell + (1 - c)(1 - d)^\ell]^{1/\ell})$, and follow the steps below to make use the uniform design C on $[0, 1]^{q-1}$ selected above to construct a UD design on the set $S_{0,b^*}^{q-1} = \{(y_1, \dots, y_q) : 0 \leq y_i \leq b_i^* (i = 1, \dots, q)\}$, where $\mathbf{b}^* = (b_1^*, \dots, b_q^*)'$. Recall that $\mathbf{c}'_k = (c_{k1}, \dots, c_{k,q-1})$ ($k = 1, \dots, q-1$).

Step 1. Let $\Delta_q = 1$,

$$d_q = \max[0, 1 - (b_1^* + \dots + b_{q-1}^*) / \Delta_q]$$

$$\phi_q = \min(1, b_q^* / \Delta_q).$$

$$\text{Let } y_q = G(c_{1,1}, d_q, \phi_q, \Delta_q, q-1).$$

Step 2. Let $\Delta_{q-1} = \Delta_q - y_q$

$$d_{q-1} = \max[0, 1 - (b_1^* + \dots + b_{q-2}^*) / \Delta_{q-1}]$$

$$\phi_{q-1} = \min(1, b_{q-1}^* / \Delta_{q-1}).$$

$$\text{Let } y_{q-1} = G(c_{1,2}, d_{q-1}, \phi_{q-1}, \Delta_{q-1}, q-2).$$

\vdots

Step (q-2). Let $\Delta_3 = \Delta_4 - y_4$,

$$d_3 = \max[0, 1 - (b_1^* + b_2^*) / \Delta_3],$$

$$\phi_3 = \min(1, b_3^* / \Delta_3).$$

$$\text{Let } y_3 = G(c_{1,q-2}, d_3, \phi_3, \Delta_4, 2).$$

Table 13.9 Construction of UD in $S_{a,b}^{3-1}$

$$c'_1 = (0.625, 0.125)$$

(1) $^\circ$	$\Delta_3 = 1$	$d_3 = 0$	$\phi_3 = 1$	$c_{1,1} = 0.062500$	$y_3 = 0.387628$
(2) $^\circ$	$\Delta_2 = 0.612372$	$d_2 = 0$	$\phi_2 = 0.816497$	$c_{1,2} = 0.125$	$y_2 = 0.0625$
(3) $^\circ$	nil	nil	nil	nil	$y_1 = 0.549872$

$$(x_1, x_2, x_3) = (0.432577, 0.137500, 0.429923).$$

$$c'_2 = (0.125, 0.375)$$

(1) $^\circ$	$\Delta_3 = 1$	$d_3 = 0$	$\phi_3 = 1$	$c_{2,1} = 0.125$	$y_3 = 0.064586$
(2) $^\circ$	$\Delta_2 = 0.935414$	$d_2 = 0.109129$	$\phi_2 = 0.534522$	$c_{2,2} = 0.375$	$y_2 = 0.25130$
(3) $^\circ$	nil	nil	nil	nil	$y_1 = 0.684113$

$$(x_1, x_2, x_3) = (0.238751, 0.250781, 0.510468).$$

$$c'_3 = (0.875, 0.625)$$

(1) $^\circ$	$\Delta_3 = 1$	$d_3 = 0$	$\phi_3 = 1$	$c_{3,1} = 0.875$	$y_3 = 0.646447$
(2) $^\circ$	$\Delta_2 = 0.853553$	$d_2 = 0$	$\phi_2 = 1$	$c_{3,2} = 0.625$	$y_2 = 0.220971$
(3) $^\circ$	nil	nil	nil	nil	$y_1 = 0.132583$

$$(x_1, x_2, x_3) = (0.587868, 0.232583, 0.179550).$$

$$c'_4 = (0.375, 0.875)$$

(1) $^\circ$	$\Delta_3 = 1$	$d_3 = 0$	$\phi_3 = 1$	$c_{4,1} = 0.375$	$y_3 = 0.209431$
(2) $^\circ$	$\Delta_2 = 0.790569$	$d_2 = 0$	$\phi_2 = 0.632456$	$c_{4,2} = 0.875$	$y_2 = 0.437500$
(3) $^\circ$	nil	nil	nil	nil	$y_1 = 0.353069$

$$(x_1, x_2, x_3) = (0.325659, 0.362500, 0.311841).$$

Step (q-1). Let $\Delta_2 = \Delta_3 - y_3$,
 $d_2 = \max(0, 1 - b_1^*/\Delta_2)$,

$\phi_2 = \min(1, b_2^*/\Delta_2)$.
 Let $y_2 = G(c_{1,q-1}, d_2, \phi_2, \Delta_2, 1)$.

Step q. Let $y_1 = 1 - (y_q + \cdots + y_2)$.

The point $y'_1 = (y_1, \cdots, y_q)$ is a point for a UD in S_{0,b^*}^{q-1} . Let

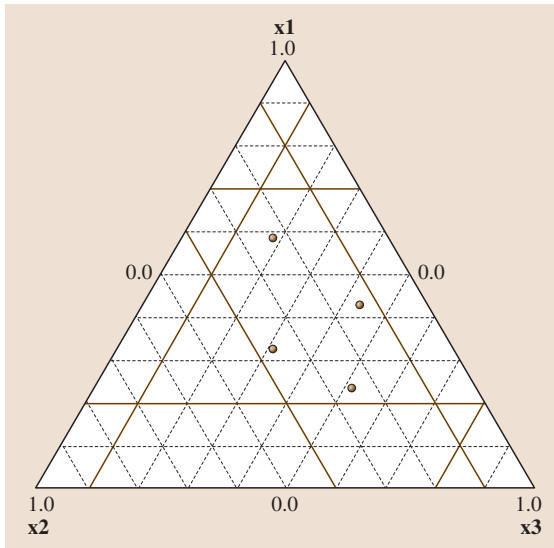
$$x_1 = \left[1 - (a_1^0 + \cdots + a_q^0)\right] y_1 + a_1^0,$$

$$\vdots$$

$$x_q = \left[1 - (a_1^0 + \cdots + a_q^0)\right] y_q + a_q^0.$$

The point $x'_1 = (x_1, \cdots, x_q)$ is a point for a UD in $S_{a,b}^{q-1}$. Repeat the above with each of c_2, \cdots, c_{q-1} to obtain another $(n-1)$ points y'_2, \cdots, y'_n , and thus another $(n-1)$ points x'_2, \cdots, x'_n . Let

$$Y = \begin{pmatrix} y'_1 \\ y'_2 \\ \vdots \\ y'_n \end{pmatrix},$$

**Fig. 13.4** An example of a uniform design with constraints

and let

$$X = \begin{pmatrix} x'_1 \\ x'_2 \\ \vdots \\ x'_n \end{pmatrix}.$$

Then Y is a UD on S_{0,b^*}^{q-1} , and X is a UD on $S_{a,b}^{q-1}$.

The following example illustrates construction of a UD of $n = 4$ points on S^{3-1} when there are restrictions on x_1, x_2, x_3 .

Example 13.4: Let x_i be subject to the restriction $a_i \leq x_i \leq b_i$ ($i = 1, 2, 3$), where $(a_1, a_2, a_3) = (0.2, 0.1, 0.1) = \mathbf{a}'$, $(b_1, b_2, b_3) = (0.7, 0.4, 0.8) = \mathbf{b}'$. Suppose that we want to find a UD with four points on S^{3-1} . We choose the following $U_4(4^{3-1})$ uniform design U from the website, and from U we construct the following UD, C , on $[0, 1]^{3-1}$ by defining $c_{ki} = (u_{ki} - 0.5)/4$:

$$U = \begin{pmatrix} 3 & 1 \\ 1 & 2 \\ 4 & 3 \\ 2 & 4 \end{pmatrix}, \quad C = \begin{pmatrix} 0.625 & 0.125 \\ 0.125 & 0.375 \\ 0.875 & 0.625 \\ 0.375 & 0.875 \end{pmatrix}.$$

1. We have $a = 0.2 + 0.1 + 0.1 = 0.4$ and $b_1 + b_2 + b_3 = 1.9$. Since the condition $a < 1 < b$ is satisfied, the set $S_{a,b}^{3-1}$ contains more than one point and the construction of the UD proceeds.
2. We have

$$a_1^0 = \max(0.2, 0.7 + 1 - 1.9) = 0.2,$$

$$b_1^0 = \min(0.7, 0.2 + 1 - 0.4) = 0.7,$$

$$a_2^0 = \max(0.1, 0.4 + 1 - 1.9) = 0.1,$$

$$b_1^0 = \min(0.4, 0.1 + 1 - 1.9) = 0.4,$$

$$a_3^0 = \max(0.1, 0.8 + 1 - 1.9) = 0.1,$$

$$b_1^0 = \min(0.8, 0.1 + 1 - 0.4) = 0.7.$$

3. Define

$$y_1 = (x_1 - 0.2)/0.6,$$

$$b_1^* = (0.7 - 0.2)/0.6 = 5/6,$$

$$y_2 = (x_2 - 0.1)/0.6,$$

$$b_2^* = (0.4 - 0.1)/0.6 = 1/2,$$

$$y_3 = (x_3 - 0.1)/0.6,$$

$$b_3^* = (0.7 - 0.1)/0.6 = 1.$$

Then $0.2 \leq x_1 \leq 0.7$, $0.1 \leq x_2 \leq 0.4$ and $0.1 \leq x_3 \leq 0.7$ are equivalent to $0 \leq y_1 \leq 5/6$, $0 \leq y_2 \leq 1/2$, $0 \leq y_3 \leq 1$.

4. Table 13.9 displays the values of Δ_k , d_k , ϕ_k and y_k ($k = 1, 2, 3, 4$) calculated from the rows c'_1, c'_2, c'_3, c'_4 of C .

Hence

$$Y = \begin{pmatrix} 0.387628 & 0.062500 & 0.549872 \\ 0.064586 & 0.251301 & 0.684113 \\ 0.646447 & 0.229071 & 0.132582 \\ 0.209431 & 0.437500 & 0.353069 \end{pmatrix},$$

$$X = \begin{pmatrix} 0.432577 & 0.137500 & 0.429923 \\ 0.238751 & 0.250781 & 0.510468 \\ 0.587868 & 0.232583 & 0.179550 \\ 0.325659 & 0.362500 & 0.311841 \end{pmatrix},$$

Y is a UD on S_{0,b^*}^{3-1} , and X is a UD on $S_{a,b}^{q-1}$. The plot of the points of X is shown in Fig. 13.4.

13.7 Relationships Between Uniform Design and Other Designs

13.7.1 Uniformity and Aberration

A q^{s-p} factorial design D is uniquely determined by p defining words. A word consists of letters that represent the factors, and the number of letters in a word is called the word-length. The group formed by the p defining words is the defining contrast subgroup of D . Let $A_i(D)$ be the number of words of word-length i in the defining contrast subgroup. If D_1 and D_2 are two

regular fractions of a q^{s-p} factorial, and there exists an integer k ($1 \leq k \leq s$) such that

$$\begin{aligned} A_1(D_1) &= A_1(D_2), \dots, A_{k-1}(D_1) \\ &= A_{k-1}(D_2), A_k(D_1) < A_k(D_2), \end{aligned}$$

then D_1 is said to have less aberration than D_2 . Aberration is a criterion for comparing designs in terms of confounding. The smaller the aberration, the less

confounding the design has, and hence designs with small aberration are preferred. Minimum aberration, as well as maximum resolution, which is also a criterion defined in terms of confounding for comparing designs, are two such commonly used criteria in the literature.

Fang and Mukerjee [13.16] proved the following relationship, which connects two seemingly unrelated criteria, CD and aberration, for two-level designs:

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

This relationship shows that minimum CD is essential equivalent to minimum aberration. Fang and Ma [13.46] extended this result to regular fraction 3^{s-1} designs, and proved the following relationships concerning WD for a regular fractional factorial design q^{s-k} ($q = 2, 3$):

$$\begin{aligned} [\text{WD}(D)]^2 &= \left(\frac{11}{8}\right)^s - \left(\frac{4}{3}\right)^s + \left(\frac{11}{8}\right) + \sum_{i=1}^s \frac{A_i(D)}{11^i} \quad (q = 2), \\ [\text{WD}(D)]^2 &= -\left(\frac{4}{3}\right)^s + \left(\frac{73}{54}\right)^s \times \left[1 + \sum_{i=1}^s \left(\frac{4}{73}\right)^i A_i(D)\right] \quad (q = 3). \end{aligned}$$

The last two relationships show that minimum WD and minimum aberration are essentially equivalent.

13.7.2 Uniformity and Orthogonality

An orthogonal array has a balanced structure. In any r columns in an orthogonal array of strength r , combinations of different of $1 \times r$ vectors occur the same number of times. Because of the balanced structure of orthogonal arrays, it is not surprising that an orthogonal array has a small discrepancy and is a uniform design. Fang and Winker [13.47] showed that many UD's are also orthogonal arrays of strength 2, for example, $U_4(2^3)$, $U_8(2^7)$, $U_{12}(2^{11})$, $U_{12}(2^{11})$, $U_{16}(2^{15})$, $U_9(3^4)$, $U_{12}(3 \times 2^3)$, $U_{16}(4^5)$, $U_{16}(4 \times 2^{12})$, $U_{18}(2 \times 3^7)$ and $U_{25}(25^6)$, and they conjectured that an orthogonal array is a uniform design under a certain discrepancy. Ma et al. [13.48] proved this conjecture for complete designs (designs in which all

level combinations of the factors appear equally often) and for 2^{s-1} factorials, under L_2 -discrepancy.

13.7.3 Uniformity of Supersaturated Designs

A design whose number of runs is equal to the number of effects to estimate is called a *saturated design*. A *supersaturated design* is a design in which the number of runs is less than the number of effects to estimate. In an industrial or scientific experiment, sometimes a large number of possible contributing factors are present, but it is believed that only a few of these factor contribute significantly to the outcome. In this situation of *effect scarcity*, one may use supersaturated designs to identify the major contributing factors. Studies on two- and three-level supersaturated designs are available in the literature [13.49–54].

A supersaturated design can be formed by adding columns to an orthogonal array. Since the number of rows in a supersaturated design is less than the number of columns, a supersaturated design cannot be an orthogonal array. Many criteria have been defined for construction of supersaturated designs that are as close to being orthogonal as possible; they are $\text{Ave}(s^2)$, $E(s^2)$, $\text{ave}(\chi^2)$, and others. Ma et al. [13.55] defined a more general criterion, the $D_{\phi, \theta}$ criterion

$$D_{\phi, \theta} = \sum_{1 \leq j \leq m} \theta \left(\sum_{u=1}^{q_i} \sum_{v=1}^{q_j} \phi \left| n_{uv}^{(ij)} - \frac{n}{q_i q_j} \right| \right),$$

where $\phi(\cdot)$ and $\theta(\cdot)$ are monotonic increasing functions on $[0, \infty)$, $\phi(0) = \theta(0) = 0$, $n_{uv}^{(ij)}$ is the number of occurrences of the pair (u, v) in the two-column matrix formed by column i and column j of the matrix design. The smaller the value of $D_{\phi, \theta}$, the closer the supersaturated design is to an orthogonal design. Since $n/(q_i q_j)$ is the average number of occurrence of level combinations of the pair (u, v) , it is clear that $D_{\phi, \theta} = 0$ for an orthogonal array. Fang et al. [13.56] considered a special case of $D_{\phi, \theta}$, denoted by $E(f_{\text{NOD}})$, from which they proposed a way of construction of supersaturated designs. Fang et al. [13.56] also proposed a way for constructing supersaturated design with mixed levels. Fang et al. [13.57] proposed a way that collapses a uniform design to an orthogonal array for construction of multi-level supersaturated designs. Fang et al. [13.33] and Fang et al. [13.58] proposed construction of supersaturated designs by a combinatorial approach.

13.7.4 Isomorphic Designs, and Equivalent Hadamard Matrices

Two factorial designs are said to be isomorphic if one can be obtained from the other by exchanging rows and columns and permutating levels of one or more factors. Two isomorphic designs are equivalent in the sense that they produce the same result under the ANOVA model. In the study of factorial designs, a task is to determine whether two designs are isomorphic. To identify two isomorphic designs $d(n, q, s)$ of n runs and s factors each having q levels requires a search over $n!(q!)^s s!$ designs, which is an NP-hard problem even if the values of (n, s, q) are of moderate magnitudes. Some methods have been suggested for reducing the computation load, but such methods are not very satisfactory. The following method using discrepancy suggested by Ma et al. [13.59] is a much more efficient alternative.

Given a factorial design $D = d(n, q, s)$ and k ($1 \leq k \leq s$), there are $[s!/(k!(s-k)!)]$ $d(n, q, s)$ sub-

designs. The values of CD of these subdesigns form a distribution $F_k(D)$. It is known that two isomorphic designs $d(n, q, s)$ have the same value of CD and the same distribution $F_k(D)$ for all k , ($1 \leq k \leq s$). Based on this, Ma et al. [13.59] proposed an algorithm for detecting non-isomorphic designs.

Two Hadamard matrices are said to be equivalent if one can be obtained from the other by some sequence of row and column permutation and negations. To identify whether two Hadamard matrices are equivalent is also an NP-hard problem. A method called the profile method suggested by Lin et al. [13.60] can be used, but this method is still not satisfactory. Recently, Fang and Ge [13.61] proposed a much more efficient algorithm using a symmetric Humming distance and a criterion which has a close relationship with several measures of uniformity. Applying this algorithm, they verified the equivalence of 60 known Hadamard matrices of order 24 and discovered that there are at least 382 pairwise-equivalent Hadamard matrices of order 36.

13.8 Conclusion

In this chapter, we have introduced the *uniform design* (UD) which is a space-filling design characterized by uniform distribution of its design points over the entire experimental domain. Abundant theoretical results on UD and the relationships between UD and other well-established design criteria are now available in the literature, as are many successful examples of application of UD in industry.

Theoretical studies show that UD is superior, in the sense that establishing uniformity of design by minimizing discrepancies will automatically optimize many other design criteria. An advantage of using UD in experiments is that, even when the number of factors and the levels of factors are large, the experiment can be conducted in a much smaller number of runs than many other commonly used designs such as factorial designs.

UDs can be used in industrial experiments. Since their design points uniformly cover the design region,

UDs are suitable for experiments in which the underlying model is unknown. The UD can be used as a space-filling design for numerical integration and computer experiments, and as a robust design against model specification. For users' convenience, many tables for UD are documented in the website www.math.hkbu.edu.hk/UniformDesign.

Research in the UD is a new area of study compared with classical areas in experimental designs. Some existing theoretical problems have not yet been solved, and many other problems can be posed. Many successful industrial applications have been recorded, but widespread application of UD in industries still needs further promotion. We hope that this short chapter can serve as an introduction to the UD, and in the future more researchers and industrial practitioners will join us in studying and applying the UD.

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