Uniform Design in Computer and Physical Experiments*

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Summary. Computer experiments have been widely used in various fields of industry, system engineering, and others because many physical phenomena are difficult or even impossible to study by conventional experimental methods. Design and modeling of computer experiments have become a hot topic since late Seventies of the Twentieth Century. Almost in the same time two different approaches are proposed for design of computer experiments: Latin hypercube sampling (LHS) and uniform design (UD). The former is a stochastic approach and the latter is a deterministic one. A uniform design is a low-discrepancy set in the sense of the discrepancy, the latter is a measure of uniformity. The uniform design can be used for computer experiments and also for physical experiments when the underlying model is unknown. In this paper we review some developments of the uniform design in the past years. More precisely, review and discuss relationships of fractional factorial designs including orthogonal arrays, supersaturated designs and uniform designs. Some basic knowledge of the uniform design with a demonstration example will be given.

Key words: Computer Experiments, experimental design, factorial design, supersaturated design, uniform design

1 Motivation

Computer experiments and/or computer simulations have been widely used for studying physical phenomena in various fields of industry, system engineering, and others because many physical processes/phenomena are difficult or even impossible to study by conventional experimental methods. We describe the physical process by a mathematical model, implemented with code

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on a computer. Design and modeling of computer experiments have become a hot topic since late Seventies of the Twentieth Century. Motivated by three big projects in system engineering in 1978 Prof. Y. Wang and myself in [4, 36] proposed the so-called the uniform experimental design or uniform design (UD) for short. There were six or more input variables in one of the three projects and the output y can be obtained by solving a system of differential equations. It costed one day calculation from an input to the corresponding output. Clearly, the relationship between the input and output has no analytic formula and is very complicated. The true model can be expressed as

$$y = f(x_1, \ldots, x_s) \equiv f(\boldsymbol{x}), \qquad \boldsymbol{x} \in T, \tag{1.1}$$

where $\boldsymbol{x} = (x_1, \ldots, x_s)$ is the input, y the output, T the experimental domain and function f is known and has no analytic expression. The engineers wanted to find a simple and approximate model or called as a metamodel

$$y = g(x_1, \ldots, x_s) = g(\boldsymbol{x}) \tag{1.2}$$

such that the difference of $|f(\boldsymbol{x}) - g(\boldsymbol{x})|$ is small over the domain T in a certain sense. The metamodel g should be much easy to compute, i.e., the computation complexity for $g(\boldsymbol{x})$ is much less than one for $f(\boldsymbol{x})$. For searching a good metamodel it is suggested to choose a set of points, $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n$ in T and calculate their corresponding outputs to form a data set $\{(\boldsymbol{x}_i, y_i),\ i = 1, \ldots, n\}$. Then applying some useful modeling techniques to find a good model to fit the data. If the chosen model can predict the output at any point in T well, this model can be regarded as a metamodel. This created a new concept: *design and modeling for computer experiments* (DMCE) (or DACE, design and analysis for computer experiments) in that era. Figure 1 shows the idea of computer experiments.

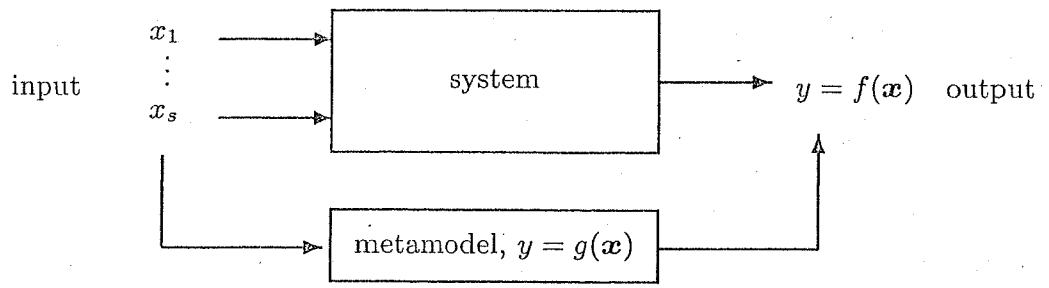

Fig. 1. Computer Experiments

We may have several goals in computer experiments, such as a) to explore the relationships between the input and the output; b) To find maximum/minimum value of y and the corresponding input-combination; c) to quantify the leverage of each input variable to the output; d) to determinate variables for which the values are optimized to minimize the variability of response variable, y.

Almost in the same time the author met many industrial experiments, the related engineer did not know the underlying model well. We can express the model for these experiments by

$$y = f(x_1, \ldots, x_s) + \varepsilon \equiv f(\boldsymbol{x}) + \varepsilon, \qquad \boldsymbol{x} \in T, \tag{1.3}$$

where $f(\boldsymbol{x})$ is unknown, maybe nonlinear, the domain T may be large, and ε is the random error. The experimenter wants to find a model

$$y = g(\boldsymbol{x}) + \varepsilon \tag{1.4}$$

for estimation of the true model by an experimental data such that $g(\boldsymbol{x})$ is very close to $f(\boldsymbol{x})$ in a certain sense. Both of computer experiments and physical experiments with model unknown meet the same aspects:

A. Experimental Design: Note that the true model in many studies may have the following complexities: 1) multi-factor: the number of factors may be high; 2) non-linearity: the function $f(\boldsymbol{x})$ is a non-linear function in $\boldsymbol{x}$; and 3) large domain: the experimental domain is large so that $f(\boldsymbol{x})$ may have more than one local minimum/maximum point. Due to the above complexities we want to choose experimental points uniformly scattered in the domain so that we can have a good estimation for the true model. This leads to the terminology "uniform design", or "space-filling design".

B. Modeling: We wish to find a high quality metamodel that approximates the true model well over the domain. A good metamodel should have less computation complexity and easy to explore relationship between the input variables and the output.

Computer experiments have no random errors while physical experiments have measurement errors, environment effects and so on. This fact leads to much different between computer experiments and physical experiments with model unknown. For example, three well-known principles for physical experiments: *replication, randomization* and *blocking* are meaningless for computer experiments. Various statistical methods can't be directly used for analyzing data from computer experiments. However, the idea of many statistical methods can still be applied for modeling computer experiments. We shall discuss this issue late.

There are many approaches to computer experiments. In this paper I focus only on the uniform design for its theory, method and recent development. In Section 2 an introduction to theory and methodology of the uniform design is given, and a demonstration example shows implementation of the uniform design to physical experiments with model unknown. Section 3 introduces some recent development of the uniform design. Some applications of the uniform design will be given in Section 4.

2 Theory and Methodology of The Uniform Design

2.1 Theory

Suppose that the purpose of experimental design is to find a metamodel $g(\boldsymbol{x})$ in (1.2) to approximate the true model $f(\boldsymbol{x})$ in (1.1). How do we measure the closeness of $g(\boldsymbol{x})$ to $f(\boldsymbol{x})$? There are many criteria. A natural idea in engineering requests the metamodel $g(\boldsymbol{x})$ satisfying

$$\text{diff}(f,g) = |f(\boldsymbol{x}) - g(\boldsymbol{x})| < \delta, \qquad \boldsymbol{x} \in T, \tag{2.1}$$

where δ is the given accuracy in the project. For simplicity, without loss of any generality, the experimental region can be assumed to be a unit cube $C^s = [0,1]^s$. Another criterion is

$$\text{p-diff}(f,g) = \int_{C^s} |f(\boldsymbol{x}) - g(\boldsymbol{x})|^p \, d\boldsymbol{x} < \delta, \tag{2.2}$$

where $p > 0$, more often choosing $p = 1$ or $p = 2$. The class of functions $f(\boldsymbol{x})$ can be considered the class of L_2-integrable continuous functions, denoted by $\mathcal{G}_2$. It is not easy to find a unified way to construct metamodel $g(\boldsymbol{x})$ satisfying the criterion (2.1) or (2.2) for each function in $\mathcal{G}_2$. Therefore, the so-called *overall mean model* was suggested. Let $\mathcal{P} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n\}$ is a set of experimental points on C^s. Suppose the experimenter wants to estimate the overall mean

$$\text{mean}(y \,|\, C^s) = \int_{C^s} f(\boldsymbol{x}) \, d\boldsymbol{x}$$

by the sample mean

$$\bar{y}(\mathcal{P}) = \frac{1}{n} \sum_{i=1}^{n} f(\boldsymbol{x}_i). \tag{2.3}$$

We wish to find a design $\mathcal{P}$ such that diff-mean $\equiv |\text{mean}(y \,|\, C^s) - \bar{y}(\mathcal{P})|$ as small as possible. The famous Koksma-Hlawka inequality in quasi-Monte Carlo methods provides a upper bound of the difference

$$\text{diff-mean} = |\text{mean}(y \,|\, C^s) - \bar{y}(\mathcal{P})| \le V(f) D(\mathcal{P}), \tag{2.4}$$

where $D(\mathcal{P})$ is the star discrepancy of $\mathcal{P}$, a measure of uniformity of the set $\mathcal{P}$ over the domain C^s and does not depend on f, and $V(f)$ is the total variation of the function f in the sense of Hardy and Krause (see Niederreiter [30]).

Let $F_{\mathcal{P}}(\boldsymbol{x})$ be the empirical distribution function

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

where $\boldsymbol{x}_i \le \boldsymbol{x}$ means each component of $\boldsymbol{x}_i$ is less than or equals to the corresponding component of $\boldsymbol{x}$, $I(\boldsymbol{x} \,|\, \boldsymbol{x}_i \le \boldsymbol{x})$ is the indicate function such

that it equals to 1 if $\boldsymbol{x}_i \leq \boldsymbol{x}$, otherwise zero. The star discrepancy is defined as

$$D(\mathcal{P}) = \max_{\boldsymbol{x} \in C^s} |F_{\mathcal{P}}(\boldsymbol{x}) - F(\boldsymbol{x})|, \tag{2.5}$$

where $F(\boldsymbol{x})$ is the uniform distribution function on C^s.

The Koksma-Hlawka inequality indicates:

a) The lower the star discrepancy, the better uniformity the set of points has. This suggests to minimize the star discrepancy $D(\mathcal{P})$ on all designs of n runs on C^s, i.e., to find a *uniform design*. Fang and Wang (Fang [4] and Wang and Fang [36]) proposed the uniform design and provides a number of uniform designs. When the number of runs, n increases, roughly speaking, one can find design $\mathcal{P}_n$ such that $D(\mathcal{P}_n)$ decreases.

b) The uniform design is **robust** against the model specification. For example, two models $y = f_1(\boldsymbol{x})$ and $y = f_2(\boldsymbol{x})$ have the same variation $V(f_1) = V(f_2)$, a uniform design may have the same level performance for these two models.

c) If the true model $f(\boldsymbol{x})$ has a large variation, in general, we need more runs to reach the same upper bound of diff-mean.

d) There are many versions of the Koksma-Hlawka inequality, where the star discrepancy $D(\mathcal{P})$ is replaced by another discrepancy and the total variation $V(g)$ is defined according to the definition of the given discrepancy. Hickernell [20] gave a comprehensive discussion and proposed some new measures of uniformity, among of which the centered L_2-discrepancy (CD) and the wrap-around L_2-discrepancy (WD) have good properties and satisfies the Koksma-Hlawka inequality. The CD and WD have nice computational formulas

$$\begin{aligned}(CD(\mathcal{P}))^2 = &\left(\frac{13}{12}\right)^s - \frac{2}{n}\sum_{k=1}^{n}\prod_{j=1}^{s}\left(1 + \frac{1}{2}|x_{kj} - 0.5| - \frac{1}{2}|x_{kj} - 0.5|^2\right) \\ &+ \frac{1}{n^2}\sum_{k=1}^{n}\sum_{j=1}^{n}\prod_{i=1}^{s}\left[1 + \frac{1}{2}|x_{ki} - 0.5| + \frac{1}{2}|x_{ji} - 0.5| - \frac{1}{2}|x_{ki} - x_{ji}|\right],\end{aligned} \tag{2.6}$$

and

$$(WD(\mathcal{P}))^2 = \left(\frac{4}{3}\right)^s + \frac{1}{n^2}\sum_{k=1}^{n}\sum_{j=1}^{n}\prod_{i=1}^{s}\left[\frac{3}{2} - |x_{ki} - x_{ji}|(1 - |x_{ki} - x_{ji}|)\right], \tag{2.7}$$

respectively, where $\boldsymbol{x}_k = (x_{k1}, \ldots, x_{ks})$ is the kth experimental point.

Obviously, the overall mean model is too simple and may not reach the task: estimation of the true model $f(\boldsymbol{x})$. But, the overall mean model provides a simple way to develop methodology and theory of the uniform design. It is surprising that the uniform design has an excellent performance for both computer experiments and physical experiments with model unknown.

Wiens [37] concerned with designs for approximately linear regression models and show that the uniform design measure (the uniform distribution on C^s) is maximin in the sense of maximizing the minimum bias in the

regression estimate of σ^2 and is also minimax in the sense of minimizing the maximum bias in the regression estimate of σ^2. Xie and Fang [41] pointed out that the uniform measure is admissible and minimax under the model

$$y = f(x_1, \ldots, x_s) + \epsilon,$$

where f is unknown, but belongs to some function family. Hickernell [21] considered robust regression models

$$y = f(\boldsymbol{x}) + \varepsilon = \text{mean}(y) + h(\boldsymbol{x}) + \varepsilon,$$

where the function $f(\boldsymbol{x})$ is decomposed into the overall mean value of $f(\boldsymbol{x})$ and mis-specification $h(\boldsymbol{x})$. He proposed two models *average mean-square-error model* and *maximum mean-square-error model*. With a certain condition he proved that the uniform design is optimal under these models. His results show that the uniform design is robust for model specification. Hickernell and Liu [22] consider efficiency and robustness of experimental design. They said "Although it is rare for a single design to be both maximally efficient and robust, it is shown here that uniform designs limit the effects of aliasing to yield reasonable efficiency and robustness together."

2.2 Methodology

In this subsection we introduce how to apply the uniform design to real experiments. A uniform design for an experiment of s factors with n runs on the domain C^s is a set of n points such that this set has the minimum discrepancy, the latter can be centered L_2-discrepancy or others. If the domain T is a rectangle in R^s, a linear transformation can transfer n points on C^s into T.

When there is only one factor on the range $[a, b]$ in the experiment with n runs. The uniform design arranges n runs as $\{a+(b-a)\frac{1}{2n}, a+(b-a)\frac{3}{2n}, \ldots, a+(b-a)\frac{2n-1}{2n}\}$.

For multi-factor experiments it is not tractable to find a set of n points, $\mathcal{P} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n\} \subset C^s$, such that it has the minimum discrepancy. Therefore, many authors focus on lattice points and introduce the concept of U-type designs.

Definition 1. A *U-type design* denoted by $U(n; q_1 \times \cdots \times q_s)$ is an $n \times s$ matrix with q_j entries at the jth columns such that the q_j entries 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 $r_1 + \cdots + r_m = s$. When all the number of q_j are equal to q, we write $U(n; q^s)$ and the corresponding designs are called symmetric, otherwise asymmetric or U-type design with mixed levels. Let $\mathcal{U}(n; q_1 \times \cdots \times q_s)$ be the set of all U-type designs $U(n; q_1 \times \cdots \times q_s)$. Similarly we have notations $\mathcal{U}(n; q_1^{r_1} \times \cdots \times q_m^{r_m})$ and $\mathcal{U}(n; q^s)$.

Very often we choose q entries in one column as $\{1, 2, \ldots, q\}$. Sometimes, q entries are chosen as $\{\frac{1}{2q}, \frac{3}{2q}, \ldots, \frac{2q-1}{2q}\}$. Let $\boldsymbol{U} = (u_{ij})$ be a U-type design

in $\mathcal{U}(n; q_1 \times \cdots \times q_s)$ with entries $\{1, \ldots, q_j\}$ at the jth column. Take the transformation

$$x_{ij} = \frac{u_{ij} - 0.5}{q_j}, \qquad i = 1, \ldots, n, \ j = 1, \ldots, s. \tag{2.8}$$

and denote $\boldsymbol{X}_u = (x_{ij})$. Then $\boldsymbol{X}_u$ is a U-type design with entries $\{\frac{1}{2q_j}, \frac{3}{2q_j}, \ldots, \frac{2q_j-1}{2q_j}\}$ at the jth column. The matrix $\boldsymbol{X}_u$ is called the *induced matrix* of $\boldsymbol{U}$. The n rows of the matrix $\boldsymbol{X}_u$ are n points on $[0,1]^s$. Most measures of uniformity are defined on $[0,1]^s$ in the literature. Therefore, we define uniformity of a U-type design $\boldsymbol{U}$ through its induced matrix by

$$D(\boldsymbol{U}) = D(\boldsymbol{X}_u). \tag{2.9}$$

Definition 2. A design $\boldsymbol{U} \in \mathcal{U}(n; q_1 \times \cdots \times q_s)$ is called a uniform design under the pre-decided discrepancy D if

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

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

Under the CD in (2.6) Table 1 and Table 2 give two uniform designs $U_{12}(12^4)$ and $U_6(3^2 \times 2)$, respectively. Table 1 can arrange an experiment having at most 4 12-level factors with 12 runs and Table 2 can apply to an experiment of 6 runs and 3 factors where two have three levels and one has two levels. Figure 2 gives scatter plots for any two columns of $U_{12}(12^4)$. By a visualization we can see that 12 points on any two marginal square are uniformly scattered. How to construct uniform design tables is a challenging job. A comprehensive review on construction of uniform designs can refer to Fang and Lin [11] and Fang, Li and Sudjianto [10]. A number of UD tables can be found on the UD web site at `http://www.math.hkbu.edu.hk/UniformDesign`.

Table 1. $U_{12}(12^4)$

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

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

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

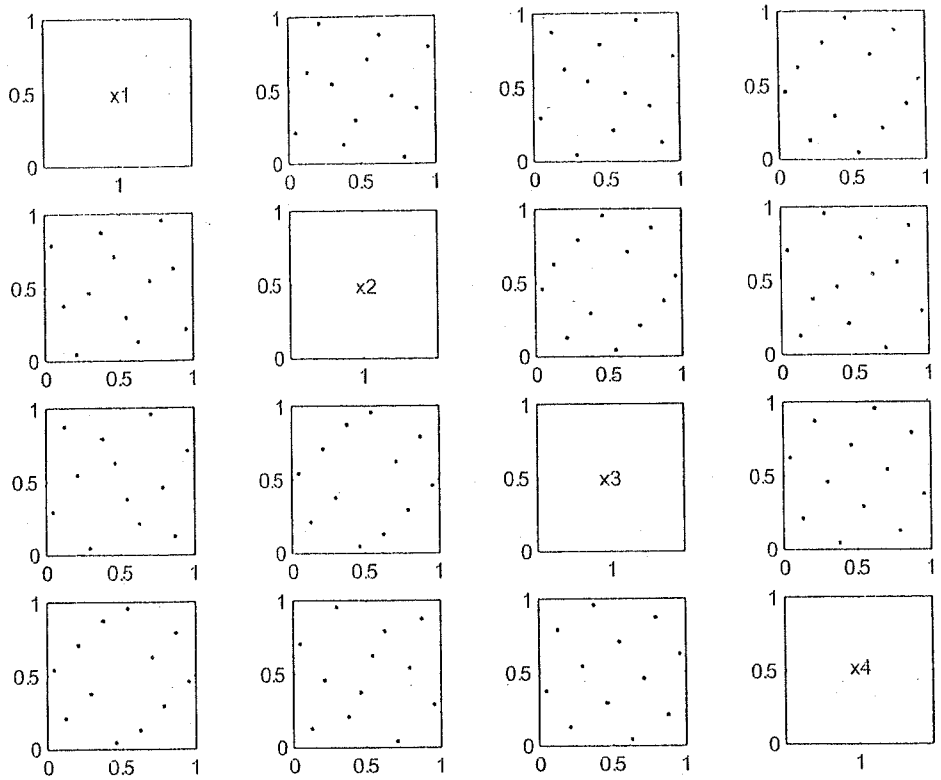

Fig. 2. Scatter plots of any two columns for $U_{12}(12^4)$

2.3 Demonstration example

For illustration applications of the uniform design consider a chemical experiment that is conducted in order to find the best setup to increase the yield. Four factors and 12 levels for each factor are chosen as follows:

x_1, the amount of formaldehyde (mol/mol): 1.0, 1.4, 1.8, 2.2, 2.6, 3.0, 3.4, 3.8, 4.2, 4.6, 5.0, 5.4
x_2, the reaction temperature (hour): 5, 10, 15, 20, 25, 30, 35, 40, 45, 50, 55, 60
x_3, the reaction time (hour): 1.0, 1.5, 2.0, 2.5, 3.0, 3.5, 4.0, 4.5, 5.0, 5.5, 6.0, 6.5
x_4, the amount of potassium (ml): 15, 20, 25, 30, 35, 40, 45, 50, 55, 60, 65, 70

The response variable is designated as the yield (y). This experiment could be arranged with a UD table of the form $U_n(12^4)$, where 12 is a divisor of n. It turns out that the experimenter chooses $U_{12}(12^4)$ design. The 12 levels marked by $1, 2, \ldots, 12$ are transformed into the real levels of the factors. It results in a design listed in Table 3 where the values in the bracket in the columns x_1, x_2, x_3 and x_4 are from the table $U_{12}(12^4)$. Run 12 experiments according to these 12 level-combinations and record the corresponding yield y (see the last column of Table 3).

The experimenters wanted to find a good metamodel such that they could find a level-combination of the factors with a yield that is much higher than

Table 3. Design and response

No	x_1	x_2	x_3	x_4	y
1	1.0 (1)	50 (10)	2.5 (4)	45 (7)	0.0795
2	1.4 (2)	25 (5)	6.0 (11)	25 (3)	0.0118
3	1.8 (3)	5 (1)	4.0 (7)	55 (9)	0.0109
4	2.2 (4)	30 (6)	1.0 (1)	35 (5)	0.0991
5	2.6 (5)	55 (11)	5.5 (10)	65 (11)	0.1266
6	3.0 (6)	45 (9)	4.5 (8)	15 (1)	0.0717
7	3.4 (7)	20 (4)	3.0 (5)	70 (12)	0.1319
8	3.8 (8)	10 (2)	2.0 (3)	20 (2)	0.0900
9	4.2 (9)	35 (7)	6.5 (12)	50 (8)	0.1739
10	4.6 (10)	60 (12)	3.5 (6)	30 (4)	0.1176
11	5.0 (11)	40 (8)	1.5 (2)	60 (10)	0.1836*
12	5.4 (12)	15 (3)	5.0 (9)	40 (6)	0.1424

the current one. We have mentioned that there are many ways to construct a metamodel. In this example, they considered only linear and quadratic regression models.

Note that the task for the experimenter is to find the best level-combination of the factors that can maximize the yield. The best result among the 12 responses is $y_{11} = 18.36\%$ at $x_1 = 5.0$, $x_2 = 40$, $x_3 = 1.5$ and $x_4 = 60$. This can be served as a benchmark. Is there any level-combination to produce a larger amount of yield? The simplest approximate model is the first-order regression or its submodel:

$$E(y) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_4 x_4.$$

Unfortunately, we can't find a satisfactory result under this model as well as its submodel. Therefore, a more flexible second-order regression is considered as below

$$E(y) = \beta_0 + \sum_{i=1}^{4} \beta_i x_i + \sum_{i \le j} \beta_{ij} x_i x_j. \tag{2.10}$$

With a technique of model selection, we find a good submodel:

$$\begin{aligned} \hat{y} = {} & 0.0446 + 0.0029 x_2 - 0.0260 x_3 + 0.0071 x_1 x_3 \\ & + 0.000036 x_2 x_4 - 0.000054 x_2^2 \end{aligned} \tag{2.11}$$

with $R^2 = 97.43\%$ and $s^2 = 0.0001$. In the literature, the centered quadratic regression model

$$E(y) = \beta_0 + \sum_{i=1}^{4} \beta_i (x_i - \bar{x}_i) + \sum_{i \le j} \beta_{ij} (x_i - \bar{x}_i)(x_j - \bar{x}_j), \tag{2.12}$$

is also recommended, where $\bar{x}_i$ is the sample mean of x_i. In this data set, $\bar{x}_1 = 3.2$, $\bar{x}_2 = 32.5$, $\bar{x}_3 = 3.75$ and $\bar{x}_4 = 42.5$. Once again, by using some model selection technique, a metamodel is

$$\hat{y} = 0.1277 + 0.0281(x_1 - 3.2) + 0.000937(x_2 - 32.5) + 0.00114(x_4 - 42.5) + 0.00058(x_3 - 3.75)(x_4 - 42.5) - 0.000082(x_2 - 32.5)^2 \quad (2.13)$$

with $R^2 = 97.05\%$ and $s^2 = 0.0002$.

By an ANOVA analysis and statistical diagnostics both models (2.11) and (2.13) are acceptable. Each can give an explanation for relationships among the four factors and the yield, but these relationships may be consistent or may be not consistent as the number of runs is small for such a four factor experiment. The experimenter should be carefully to make his/her own conclusion. The models (2.11) and (2.13) can be used to predict response at any point of the experimental domain. It also can be used for searching the 'best' combination of the factor-value. We maximize y with respect to x_i, $i = 1, \ldots, 4$ under models (2.11) or (2.13), respectively, over the domain, $\mathcal{X}$, that is to find x_i^*, $i = 1, \ldots, 4$ such that

$$\hat{y}(x_1^*, x_2^*, x_3^*, x_4^*) = \max_{\mathcal{X}} \hat{y}(x_1, x_2, x_3, x_4),$$

where $\hat{y}(x_1, x_2, x_3, x_4)$ is given by (2.11) or (2.13) respectively. By some optimization algorithm, it is easily found that under model (2.11), $x_1^* = 5.4$, $x_2^* = 50.2$, $x_3^* = 1$, $x_4^* = 70$ and the corresponding response $\hat{y}(5.4, 50.2, 1, 70) = 19.3\%$ is the maximum; and under model (2.13), $x_1^* = 5.4$, $x_2^* = 43.9$, $x_3^* = 6.5$, $x_4^* = 70$ and the corresponding response $\hat{y}(5.4, 43.9, 6.5, 70) = 26.5\%$ is the maximum. As two optimal points $\boldsymbol{x}_1^* = (5.4, 50.2, 1, 70)$ and $\boldsymbol{x}_2^* = (5.4, 43.9, 6.5, 70)$ do not appear in the plan (Table 3) some additional experiments are necessary for judging which metamodel is closed to the real one.

A simplest way is to implement m runs at these two optimal points $\boldsymbol{x}_1^*$ and $\boldsymbol{x}_2^*$ and to compare their mean yield. In this experiment the experimenter implemented three runs at $\boldsymbol{x}_1^*$ and $\boldsymbol{x}_2^*$ and find that the mean of y is 20.1% at $\boldsymbol{x}_1^*$ and 26.3% at $\boldsymbol{x}_2^*$, respectively. Thus we prefer (2.13), the centered quadratic regression model, as our chosen metamodel. Note that both metamodels recommend $x_1 = 5.4$ and $x_4 = 70$. This fact implies that we should consider increase upper bound of the experimental level for x_1 and x_4. The experimenter should consider a further investigate and arrange a consequent experiment.

2.4 Modeling techniques

We have considered the quadratic regression model and the centered quadratic regression model for the above example. It indicates that for an experiment we may have many possible metamodels. Many metamodels can be represented as a linear combination of a set of basis functions: $\{B_1(\boldsymbol{x}), B_2(\boldsymbol{x}), \ldots, B_m(\boldsymbol{x})\}$ defined on the experimental domain. In this case a metamodel g has of the form of $\sum_{j=1}^{m} \beta_j B_j(\boldsymbol{x})$ and

$$y(\boldsymbol{x}) = \sum_{j=1}^{m} \beta_j B_j(\boldsymbol{x}) + \varepsilon(\boldsymbol{x}), \tag{2.14}$$

where $\boldsymbol{x}$ is a point in the domain, β_j's are unknown coefficients to be estimated and $\varepsilon(\boldsymbol{x})$ is the random error. In fact, simply linear model, and both quadratic regression model and centered quadratic regression model are special cases of (2.14). For a univariate x-variable, the power spline basis has the following general form of $\sum_{j=1}^{m} \beta_j B_j(\boldsymbol{x})$ and

$$1,\ x,\ x^2,\ \ldots,\ x^p,\ (x-\kappa_1)_+^p,\ \ldots,\ (x-\kappa_K)_+^p, \tag{2.15}$$

where $\kappa_1, \ldots, \kappa_K$ are a set of selected knots, and a_+ stands for the positive part of a, i.e., $a_+ = aI(a > 0)$. Multivariate spline basis may be constructed from the univariate spline basis using the tensor product approach. The number of basis functions is often large, various techniques of variable selection are very useful for choosing a good submodel of (2.14) as a metamodel.

The Kriging model

$$y(\boldsymbol{x}) = \sum_{j=1}^{m} \beta_j B_j(\boldsymbol{x}) + z(\boldsymbol{x}), \qquad \boldsymbol{x} \in T, \tag{2.16}$$

has been widely used in modeling computer experiments, where $B_j(\boldsymbol{x})$ are given and β_j are unknown parameters; $z(\boldsymbol{x})$ is a stochastic fields, mostly choosing a stationary Gaussian field that has a zero mean function and a given covariance structure with some unknown parameters to be estimated. As we know that Kriging predictor interpolates its training data, this property is much suitable for modeling data from computer experiments where there is no random error, but it is not so good for the data from physical experiments. Therefore, the so-called "empirical Kriging model" is suggested

$$y(\boldsymbol{x}) = \sum_{j=1}^{m} \beta_j B_j(\boldsymbol{x}) + z(\boldsymbol{x}) + \varepsilon(\boldsymbol{x}), \tag{2.17}$$

where $\varepsilon(\boldsymbol{x})$ is a random error and is assumed to be uncorrelated with $z(\boldsymbol{x})$. A comprehensive study on Kriging model and empirical Kriging model can refer to Sacks et al. [32], Santner et al. [33] and Stein [35]. Other modeling techniques involve *neural networks*, *radial basis function model*, *local polynomial regression* and *Bayesian approach*. The reader can refer to Fang et al. [10] for the details.

The following points in modeling should be emphasized:

- There are many possible metamodels for an experiment. One should consider the following aspects and then choose one for the further process: 1) the metamodel gives a good prediction, 2) the response estimator can be easily calculated by the metamodel, 3) the metamodel can be easily explore relationships between the input factors and the output.

- Both computer experiments and physical experiments can share many common modeling techniques.
- The metamodel generated by some methods such as linear regression, quadratic regression, and of the form (2.14) can be easily interpreted, but the metamodel obtained by the neural networks, Kriging model and empirical Kriging model is not easily to directly give a clear exploration. For solving this difficulty the so-called *sensitivity analysis* (SA) has been developed. It studies how the variation in the output of a model can be apportioned, quantitatively, to different sources of variation and how the given model depends upon the information fed into it. The SA is used to provide an understanding of how the model response variables respond to changes in the inputs. A comprehensive study on SA can refer to Saltelli et al. [34].

3 Some Recent Development of The Uniform Design

The uniform design was based on quasi-Monte Carlo methods and its original theoretic proofs were mostly based on the number theory, not on statistics. There are many essential difficulties in development of its own theory:

- The uniformity is a geometrical criterion, it needs some justification in statistical sense;
- Initially, the uniform design theory is based on the quasi-Monte Carlo methods. The useful tool is the number theory. Most statisticians are lack of knowledge of the number theory;
- The overall mean model is far from the request of modeling;
- Construction of uniform design is a NP hard problem. It needs some powerful algorithms in optimization.

There was a rapid development in theory, methodology and applications of the uniform design in the past years, especially in the past ten years. It needs a very large space to review all the new results. Therefore, I mainly focus on relationship among fractional factorial design, supersaturated design and uniform design in this section.

3.1 Fractional factorial designs and supersaturated designs

Let us review some basic knowledge on these designs.

Definition 3. *For an experiment of n runs, s factors each having $q_1, \ldots, q_s$ levels respectively. A factorial design is a set of n level-combinations. A design where all the level-combinations of the factors appear equally often is called a full factorial design or a full design.*

The number of runs in a full factorial design should be $n = k\prod_{j=1}^{s} q_j$, where q_j is the number of levels of the factor j and k is the number replications for all the level-combinations. When all the factors have the same number of levels, q say, $n = kq^s$. In this case the number of runs of a full factorial design increases exponentially as the number of factors increases. Therefore, we consider to implement a subset of all the level-combinations that have a good representation of the complete combinations, this subset is called fractional factorial design (FFD for short). The most important and popularly used FFD is the orthogonal array.

Definition 4. *An orthogonal array (OA) of strength r with n runs and s factors each having q levels, denoted by $OA(n, s, q, r)$, is a FFD where any subdesign of n runs and r factors is a full design. When $r = 2$, the notation $L_n(q^s)$ is often for $OA(n, s, q, 2)$ in the literature.*

Strength two orthogonal arrays are extensively used for planning experiments in various fields and are often expressed as orthogonal design tables. Table 4 presents two $L_9(3^4)$, where left one $L_9(3^4)_1$ can be found in most textbook while the right one $L_9(3^4)_2$ was obtained by Fang and Winker [17]. Both can arrange an experiment of nine runs and at most four factors each having 3 levels. Is is easy to check that these two designs are isomorphic (see section 3.4 for the definition of the isomorphism). From the traditional view these two designs are equivalent. However, it is easy to find that $L_9(3^4)_2$ has a smaller CD-value than $L_9(3^4)_1$ has. Fang and Ma (2000) found some differences in statistical inference between the two designs. This gives an important message that uniformity of the design can provide additional information in statistical ability of the design. The reader can refer Dey and Mukerjee [3] and Hedayat, Sloane and Stufken [19] for the details.

Table 4. Two $L_9(3^4)$ Tables

No	$L_9(3^4)_1$				$L_9(3^4)_2$			
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

The number of runs for orthogonal array $OA(n, s, q, 2)$ is at least q^2. 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 the effect sparsity assumption, supersaturated designs have been suggested and can be effectively used to identify the dominant factors. The reader can refer to Yamada and Lin [43] and Lin [25] for a comprehensive introduction and recent development.

Definition 5. *Supersaturated designs are fractional factorials in which the number of estimated (main or interaction) effects is greater than the number of runs. Consider a design of n runs and s factors each having q levels. The design is called unsaturated if $n-1 > s(q-1)$; saturated if $n-1 = s(q-1)$; and supersaturated if $n-1 < s(q-1)$.*

Note that there are some common aspects among the orthogonal array, supersaturated design and uniform design:

- they are subset of level-combinations of the factors
- they are constructed based on U-type designs
- there are some criteria for comparing designs

Therefore, there should have some relationships among the three kinds of designs. Fang et al. [13] found that many existing orthogonal arrays of strength two are uniform design under CD. Therefore, they proposed a conjecture that any orthogonal design is a uniform design under a certain discrepancy. Late, under the CD Ma, Fang and Lin [28] proved this conjecture is true for a full design q^s if $q = 2$ or q is odd, or $s = 1$ or 2. In general, the conjecture is not true. The study gives some relationship between orthogonality and uniformity.

3.2 Some criteria in experimental designs

Let us review some existing criteria and relationships among the criteria:

A. Minimum aberration and generalized minimum aberration: There are many useful criteria for comparing factorial designs, such as *resolution* (Box, Hunter and Hunter [2]) and minimum aberration (Fries and Hunter [18]). For given a regular factorial design D of s factors, its word-length pattern, denoted by $W(D) = (A_1(D), \ldots, A_s(D))$, gives rich information on its statistical inference ability. A q^{s-k} regular FFD D is an $(s-k)$-dimensional linear subspace of q^s. The k-dimensional orthogonal subspace, denoted by $D^{\perp}$, of D is the *defining contrasts subgroup* of D. The elements of $D^{\perp}$ are called *words*. Let $A_i(D)$ be the number of distinct words of length i in the defining relation of D. Then the sequence $W(D) = \{A_1(D), \ldots, A_s(D)\}$ is called the *word length pattern* of D. Ma and Fang [27] and Xu and Wu [42] independently extended the word length pattern to non-regular FFD. We still use $W(D) = \{A_1(D), \ldots, A_s(D)\}$ for the generalized word length pattern. The *resolution* of D is the smallest i with positive $A_i(D)$ in $W(D)$. Let D_1 and D_2 be two designs. Let t be the smallest integer such that $A_t(D_1) \neq A_t(D_2)$

in their generalized word length patterns. Then D_1 is said to have less generalized aberration than D_2 if $A_t(D_1) < A_t(D_2)$. A design D has *minimum generalized aberration* (MGA) if no other q-level design has less generalized aberration than it. The MA/GMA is the most popularly used criterion in comparing FFDs.

B. $E(s^2)$ criterion: For a U-type design with two levels -1 and 1, let $\boldsymbol{X}$ be the design matrix where each row stands for the level-combination of a run and each column stands for a factor. Let s_{ij} be the (i,j)-element of $\boldsymbol{X}'\boldsymbol{X}$. The $E(s^2)$ criterion, proposed by Booth and Cox [1], is to minimize

$$E(s^2) = \sum_{1\le i<j\le s} s_{ij}^2 \Big/ \binom{s}{2}.$$

Obviously, $E(s^2) = 0$ for any orthogonal array, otherwise $E(s^2) > 0$. For any non-orthogonal design its lower bound was obtained by Nguyen [31]. Namely,

$$E(s^2) \ge \frac{n^2(s-n+1)}{(s-1)(n-1)}. \tag{3.1}$$

C. ave χ^2 criterion: For three-level supersaturated designs, Yamada and Lin [44] defined a measure for dependency between two factors $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$ by

$$\chi^2(\boldsymbol{x}_i, \boldsymbol{x}_j) = \sum_{u,v=1}^{3} \frac{\left(n_{uv}^{(ij)} - n/9\right)^2}{n/9}, \tag{3.2}$$

where $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$ are the ith and jth columns of $\boldsymbol{X}$, $n_{uv}^{(ij)}$ is the number of (u,v)-pairs in $(\boldsymbol{x}_i, \boldsymbol{x}_j)$. Then they defined a criterion for the whole design $\boldsymbol{X}$ by

$$\text{ave}\,\chi^2 = \sum_{1\le i<j\le s} \chi^2(\boldsymbol{x}_i, \boldsymbol{x}_j) \Big/ \binom{s}{2}.$$

$\text{ave}\,\chi^2 = 0$ for any orthogonal array, otherwise $\text{ave}\,\chi^2 > 0$. Yamada and Matsui [46] obtained a lower bound of $\text{ave}\,\chi^2$ as follows:

$$\text{ave}\,\chi^2 \ge \frac{2n(2s-n+1)}{(n-1)(s-1)}. \tag{3.3}$$

More results can refer to Yamada et al. [45]

D. $E(f_{NOD})$ criterion: For a U-type design $U(n; q_1 \times \cdots \times q_s)$ define

$$f_{NOD}^{ij} = \sum_{u=1}^{q_i}\sum_{v=1}^{q_j} \left(n_{uv}^{(ij)} - \frac{n}{q_i q_j}\right)^2, \tag{3.4}$$

where $n_{uv}^{(ij)}$ is the number of (u,v)-pairs of factor i and factor j and $n/(q_iq_j)$ stands for the average frequency of level-combinations in each pair of factors i and j. A criterion $E(f_{NOD})$ is defined as

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

Fang, Lin and Liu [12] found a lower bound for $E(f_{NOD})$

$$E(f_{NOD}) \ge \frac{n\left(\sum_{j=1}^{m} n/q_j - m\right)^2}{m(m-1)(n-1)} + C(n, q_1, \ldots, q_m), \tag{3.5}$$

where $C(n, q_1, \ldots, q_m) = \frac{nm}{m-1} - \frac{1}{m(m-1)}\left(\sum_{i=1}^{m}\frac{n^2}{q_i} + \sum_{i,j=1, j\ne i}^{m}\frac{n^2}{q_iq_j}\right)$ depends on the design only through $n, q_1, \ldots, q_m$.

E. Various discrepancies: We have introduced the star discrepancy defined in (2.5), the CD in (2.6) and the WD in (2.7). Hickernell and Liu [22] proposed the so-called the *discrete discrepancy* and Fang, Ge and Liu [6] found a lower bound for this criterion. The discrete discrepancy has played an important role for construction of uniform designs based on combinatorial designs. A comprehensive studies can refer to Fang et al. [6, 7, 8, 9].

3.3 Uniformity and word length pattern

The above criteria have been proposed by its own consideration and their lower bounds were obtained by different authors. Are there any relationships among these criteria? There are a lot of new development along this line. An important finding was by Fang and Mukerjee [15], where they obtained an analytic link between the CD and word-length pattern for any regular two-level factorials 2^{s-p} as follows:

$$\left[CD_2(D)\right]^2 = \left(\frac{13}{12}\right)^s - 2\left(\frac{35}{32}\right)^s + \left(\frac{8}{9}\right)^s\left\{1 + \sum_{i=1}^{s}\frac{A_i(D)}{9^i}\right\}. \tag{3.6}$$

Ma and Fang [26] extended the above result to the wrap-around L_2-discrepancy and three-level designs. They found relationships between WD and word-length pattern:

$$(WD_2(D))^2 = \begin{cases} \left(\frac{11}{8}\right)^s \sum_{r=1}^{s}\frac{A_r(D)}{11^r} + \left(\frac{11}{8}\right)^s - \left(\frac{4}{3}\right)^s, & \text{if } q = 2, \\ \left(\frac{73}{54}\right)^s\left[1 + 2\sum_{j=1}^{s}\left(\frac{4}{73}\right)^j A_j(D)\right] - \left(\frac{4}{3}\right)^s, & \text{if } q = 3. \end{cases} \tag{3.7}$$

The formulas (3.6) and (3.7) indicate that 1) the uniformity criterion is essentially consistent with the resolution and minimum aberration criteria;

2) the uniformity can be applied to both regular and non-regular factorial designs with any number of levels, but the resolution and minimum aberration can be applied only to regular designs in the past and designs with lower number of levels ($q = 2$ or 3 in most studies). Those results show the usefulness of the uniformity in factorial designs and some advantages of the uniformity. However, the discrepancy criteria has some weakness. Comparing the resolution criterion the discrepancy do not have such a clear criterion to classify designs into different levels. For overcoming this shortcoming Hickernell and Liu [22] proposed the so-called *projection discrepancy pattern* that has a similar function like the resolution. They indicated that the uniform design limit aliasing. Fang and Qin [16] proposed the *uniformity pattern* and related criteria for two-level designs, here the uniformity pattern likes the generalized word length pattern, but it is easy to computer.

3.4 Uniformity and isomorphism

Two U-type designs $U(n, q^s)$ are called *isomorphic* each other if one can be obtained from the other by relabelling the factors, reordering the runs, or switching the levels of one or more factors. For identifying two such designs a complete search must be done to compare $n!\,(q!)^s s!$ designs. Therefore, to identify the isomorphism of two $d(n, q, s)$ designs is known to be an NP hard problem when n and s increase. Ma, Fang and Lin [27] noted the fact that two isomorphic $U(n, q^s)$ designs should have the same uniformity and the same distribution of projection uniformity in all marginal subdimensions and proposed an efficient algorithm to detect non-isomorphism. Fang and Ge [5] extended the above idea for detecting inequivalence of Hadamard matrices and proposed a new algorithm. A Hadamard matrix, $\boldsymbol{H}$ say, of order n is an $n \times n$ matrix with elements 1 or -1, which satisfies $\boldsymbol{H}'\boldsymbol{H} = n\boldsymbol{I}$. Hadamard matrices have been played important roles in experimental designs and code theory. Two Hadamard matrices are called equivalent if one can be obtained from the other by some sequence of row and column permutations and negations. They applyed the new algorithm to Hadamard matrices of order 36 and discovered that there are at least 382 pairwise inequivalent Hadamard matrices of order 36. This was a new discovery.

3.5 Majorization framework

Recently, Zhang et al. [47] found a unified approach to describe the above criteria and their lower bounds by the use of the *majorization theory* (Marshall and Olkin [29]).

For two nonnegative vectors $\boldsymbol{x}, \boldsymbol{y} \in R_+^m$ with the same sum of its components. We write $\boldsymbol{x} \preceq \boldsymbol{y}$ if $\sum_{r=1}^{k} x_{[r]} \geq \sum_{r=1}^{k} y_{[r]}$, $k = 1, 2, \ldots, m-1$, where $x_{[1]} \leq x_{[2]} \leq \cdots \leq x_{[m]}$ are ordered numbers of x_i, and $y_{[r]}$ have the same meaning. A real-valued function ψ on R_+^m is called *Schur-convex* if

$\psi(\boldsymbol{x}) \leq \psi(\boldsymbol{y})$ for every pair $\boldsymbol{x}$, $\boldsymbol{y} \in R_+^m$ with $\boldsymbol{x} \preceq \boldsymbol{y}$. The summation/product of several Schur-convex functions is still a Schur-convex function, especially, an important class of Schur-convex functions are *separable convex* functions of the form $\Psi(\boldsymbol{x}) = \sum_{r=1}^m \psi(x_r)$ with $\psi''(x) \geq 0$.

For a U-type design $\mathcal{X}$ of n runs and s factors. Let d_{ij}^H be the *Hamming distance between runs i and k*. Let $\boldsymbol{d}(D)$ be m-dimensional *pairwise distance vector* (PDV) of d_{ij}^H for $1 \leq i < k \leq n$, where $m = n(n-1)/2$. For any design $U(n, q^s)$, the sum of its pairwise distance vector is uniquely determined by $d_{total} = \sum_{1 \leq i < k \leq n} d_{ij}^H = \frac{ns(n-q)}{2q}$. This fact gives possibility that we can apply the majorization theory to find a lower bound. Zhang et al. [47] found that the criteria, like $E(s^2)$, aveχ^2, A_2, A_3 in word length pattern, discrete discrepancy, wrap-around L_2-discrepancy ($q = 2, 3$) and centered L_2-discrepancy ($q = 2$) can be expressed as a separable Schur function of PDV.

Let $\bar{d} = d_{total}/m = \frac{s(n-q)}{q(n-1)}$, and let $\bar{\boldsymbol{d}}(D)$ be a $m \times 1$ vector of $\bar{d}$'s. From the majorization theory we have $\bar{\boldsymbol{d}}(D) \preceq \boldsymbol{d}(D)$. By this way we obtain a lower bound $m\psi(\bar{d})$, when $\bar{d}$ is an integer and the criterion has of the form $\Psi(\boldsymbol{x}) = \sum_{i=1}^m \psi(x_i)$. When $\bar{d}$ is not an integer, let $\bar{d}_i$ and $\bar{d}_f$ be the integral part and fractional part of $\bar{d}$, respectively. For any separable convex function $\sum_{i=1}^m \psi(x_i)$ it has a tight lower bound

$$m(1 - \bar{d}_f)\psi(\bar{d}_i) + m\bar{d}_f(\psi(\bar{d}_i) + 1). \tag{3.8}$$

Denote $\tilde{\boldsymbol{d}}(D)$ with the first $m(1 - \bar{d}_f)$ components of $\bar{d}_i$'s and following $m\bar{d}_f$ components of $1 + \bar{d}_i$'s. We have $\bar{\boldsymbol{d}}(D) \preceq \tilde{\boldsymbol{d}}(D) \preceq \boldsymbol{d}(D)$ by Lemma 5.2.1 of Dey and Mukerjee [3]. This approach gives a unified approach to find a lower bound for the criterion that can be expressed as a separable Schur function of PDV of a U-type design. When $\bar{d}$ is not an integer, the lower bound of (3.8) is new for all the criteria we have mentioned.

4 Applications of The Uniform Design

Since 1980 the uniform design has been widely used for various projects. For example, Ling, Fang and Xu (2001) gave a comprehensive review on applications of UD in chemistry and chemical engineering. There is a large potential applications of the uniform design for grammar of technology development, especially, for grammar of high tech development. Those who can first to develop a new high tech product and who will dominate the market, at least in the first few years. From the literature you can find the following about UD:

- There are more than 500 hundreds case studies published in more than one hundred journals.
- More than one hundred theoretic research papers have been published in various journals.

- Ford Motor Company has used UD for automobile development and "Design for Six Sigma".
- A nationwide society "The Uniform Design Association of China" was established in 1994 and has organized many public lectures, short courses, conferences and workshops.

The users appreciate the UD in the following aspects:

(a) flexibility in design and modeling;
(b) easy to understand and use;
(c) good for nonlinear models;
(d) can be applied on complicated system; and
(e) can be used for several occasions: physical experiments with unknown model, computer experiments, computer-based simulations and experiments with mixtures;
(f) computer aided software is available.

The Ford Motor Company has used the UD for developing new engines. Agus Sudjianto, Engineering Manager in FORD invited the first author of the paper to visit the FORD in 2002: His letter of invitation wrote: "In the past few years, we have tremendous in using Uniform Design for computer experiments. The technique has become a critical enabler for us to execute 'design for Six Sigma' to support new product development, in particular, automotive engine design. Today, computer experiments using uniform design have become standard practices at Ford Motor Company to support early stage of product design before hardware is available." It shows that there is a big potential applications of the uniform design in Six Sigma development. The monograph "Design and Modeling for Computer Experiment" by Fang, Li and Sudjianto presents many experiments that were implemented in the FORD.

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