



UNIVERSITI PUTRA MALAYSIA

***ABSOLUTE DEVIANCE METHOD FOR SYMMETRICAL UNIFORM
DESIGNS***

GRACE LAU CHUI TING

FS 2015 10



**ABSOLUTE DEVIANCE METHOD FOR SYMMETRICAL UNIFORM
DESIGNS**

By

GRACE LAU CHUI TING

**Thesis Submitted to the School of Graduate Studies, Universiti Putra Malaysia, in
Fulfilment of the Requirements for the Degree of Master of Science**

October 2015

All material contained within the thesis, including without limitation text, logos, icons, photographs and all other artwork, is copyright material of Universiti Putra Malaysia unless otherwise stated. Use may be made of any material contained within the thesis for non-commercial purposes from the copyright holder. Commercial use of material may only be made with the express, prior, written permission of Universiti Putra Malaysia.

Copyright © Universiti Putra Malaysia



Abstract of thesis presented to the Senate of Universiti Putra Malaysia in fulfilment of the requirement for the Degree of Master of Science

ABSOLUTE DEVIANCE METHOD FOR SYMMETRICAL UNIFORM DESIGNS

By

GRACE LAU CHUI TING

October 2015

Chair : Anwar Fitrianto, PhD

Faculty : Science

Uniform design is a kind of space filling designs which is widely used in various field due to its great advantages. There are two types of uniform design; symmetrical and asymmetrical. Measure of uniformity and construction methods are essentials for construction of uniform designs. Uniform designs can be achieved by minimizing a discrepancy where the discrepancy is a measure of uniformity. From the various discrepancies that have been suggested, centered L_2 discrepancy and mixture discrepancy are employed in our research. In this research, we focused on the type of symmetrical uniform designs, $U_n(n^s)$ which the factors have same number of levels and the number of experimental runs equal to the number of levels. There are numbers of construction methods of uniform designs or nearly uniform designs in the literature. A design with low discrepancy or a good approximation to uniform design is a nearly uniform design. The existing construction methods such as good lattice point method, optimization searching method and the cutting method exhibited their advantages. However, there are still having areas which need to improve. Moreover, there is no development of new construction methods in the recent years. Therefore, two of the existing construction methods of uniform design; the optimization method and the cutting method are analyzed and modified to a better approach in terms of computation time and uniformity.

The optimization method is modified by proposing the absolute difference equivalence (ADE) approach which coordinate with ruin and recreate (R&R) approach in reducing the size of neighborhood and decreasing the computational load. Ultimately, the size of the neighborhood and the computational time are decreased and the global solution can be obtained. We have shown that ADE approach effectively reduce the size of neighborhood which is determined by the R&R approach.

Furthermore, an optimization part is added to the cutting method to find an appropriate number for experimental runs of the initial design. Conclusively, suggestion tables are given on the number of experimental runs for initial design which results in uniform

designs with more stable uniformity. It shows that choosing the suggested number of experimental runs of initial design produces uniform designs with lower uniformity.

Besides, we proposed a new method called absolute deviance method (ADM) for construction of symmetrical nearly uniform designs. The concept of ADM is from the idea of uniform design which uniformly scattered the points in the experimental domain. The uniformity of the uniform design can be achieved by setting specific pattern of the absolute differences between points. It shows that this new method is an efficient method in constructing symmetrical uniform designs with better uniformity.



© COPYRIGHT

Abstrak tesis yang dikemukakan kepada Senat Universiti Putra Malaysia sebagai memenuhi keperluan untuk Ijazah Master Sains

KAEDAH MUTLAK DEVIANS BAGI REKA BENTUK SERAGAM YANG SIMETRI

Oleh

GRACE LAU CHUI TING

Oktober 2015

Pengerusi: Anwar Fitrianto, PhD

Fakulti: Sains

Reka bentuk yang seragam adalah sejenis ruang isi reka bentuk yang digunakan secara meluas dalam pelbagai bidang kerana kelebihan yang menarik. Terdapat dua jenis reka bentuk seragam; simetri dan asimetri. Ukuran untuk keseragaman dan kaedah pembinaan adalah keperluan bagi pembinaan reka bentuk yang seragam. Reka bentuk yang seragam boleh dicapai dengan mengurangkan percanggahan di mana percanggahan itu adalah ukuran keseragaman. Daripada pelbagai percanggahan yang telah dicadangkan, percanggahan berpusat L_2 dan percanggahan campuran digunakan dalam penyelidikan kami. Dalam kajian ini, kami memberi tumpuan kepada jenis reka bentuk seragam yang simetri, $U_n(n^s)$ di mana faktor-faktor mempunyai bilangan peringkat yang sama dan bilangan percubaan beroperasi sama dengan bilangan peringkat. Terdapat banyak kaedah pembinaan reka bentuk yang seragam atau reka bentuk yang hampir seragam dalam kajian literatur. Reka bentuk dengan percanggahan rendah atau penghampiran yang baik untuk mereka-bentuk seragam adalah reka bentuk yang hampir seragam. Kaedah pembinaan yang sedia ada seperti kaedah titik kekisi yang baik, kaedah pengoptimuman dan kaedah pemotongan mempamerkan kelebihan masing-masing. Walau bagaimanapun, masih ada bahagian-bahagian yang perlu ditingkatkan. Selain itu, tiada pembangunan kaedah pembinaan baru dalam beberapa tahun kebelakangan. Oleh yang demikian, dua kaedah pembinaan yang sedia ada untuk reka bentuk yang seragam; kaedah pengoptimuman dan kaedah pemotongan dianalisa dan diubahsuai kepada kaedah yang lebih baik dari segi pengiraan masa dan keseragaman.

Kaedah pengoptimuman diubahsuai dengan mencadangkan cara perbezaan mutlak kesetaraan (ADE) yang menyelaras dengan cara kehancuran dan mencipta semula (R&R) dalam mengurangkan saiz kawasan kejiranan dan mengurangkan beban pengiraan. Akhirnya, saiz kawasan kejiranan dan masa pengiraan akan berkurangan dan penyelesaian global boleh diperolehi. Kami telah menunjukkan bahawa cara ADE berkesan untuk mengurangkan saiz kejiranan yang ditentukan dengan cara R&R.

Selain itu, langkah pengoptimuman ditambah kepada kaedah pemotongan untuk mencari bilangan yang sesuai untuk percubaan beroperasi reka bentuk permulaan. Akhirnya, jadual cadangan bilangan percubaan beroperasi reka bentuk permulaan disediakan untuk mencapai reka bentuk seragam dengan keseragaman yang lebih stabil. Ia menunjukkan bahawa memilih bilangan percubaan beroperasi reka bentuk permulaan yang dicadangkan menghasilkan reka bentuk yang seragam dengan keseragaman yang lebih baik.

Selain itu, kami mencadangkan satu kaedah baru yang dikenali sebagai kaedah mutlak devians (ADM) bagi pembinaan reka bentuk seragam yang simetri. Konsep ADM adalah dari idea reka bentuk seragam iaitu seragam bertaburan titik-titik di domain eksperimen. Keseragaman reka bentuk seragam dapat dicapai dengan menentukan perbezaan mutlak antara titik-titik. Ia menunjukkan bahawa kaedah baru ini adalah kaedah yang efisien bagi membina reka bentuk seragam yang simetri dengan keseragaman yang lebih baik.

ACKNOWLEDGEMENTS

First and foremost, praise and thanks goes to Almighty God for the many blessings undeservedly bestowed upon me. Indeed His grace is sufficient for me. Secondly, I would like to express my greatest appreciation to my supervisor, Dr. Anwar Fitrianto for the useful comments, remarks and encouragement through the learning process of this master thesis. I want to extend my appreciation to my co-supervisors, Prof. Dr. Habshah binti Midi and Associate Prof. Dr. Leong Wah June for their constructive comments in my thesis.

Not forgetting my friends who have been striving together with during these 2 years of research in Universiti Putra Malaysia. Thanks for your support and make stressful times more bearable.

Last but not least, I would like to thank my loved ones, who have supported me throughout entire process, both by keeping me harmonious and helping me putting pieces together. I will be grateful forever for your love. My gratitude also goes to those who involved directly or indirectly in completion of my thesis. You all have been blessings to me.

This thesis was submitted to the Senate of Universiti Putra Malaysia and has been accepted as fulfilment of the requirement for the degree of Master of Science. The members of the Supervisory Committee were as follows:

Anwar Fitrianto, PhD
Senior Lecturer
Faculty of Science
Universiti Putra Malaysia
(Chairman)

Habshah binti Midi, PhD
Professor
Faculty of Science
Universiti Putra Malaysia
(Member)

Leong Wah June, PhD
Associate Professor
Faculty of Science
Universiti Putra Malaysia
(Member)

BUJANG BIN KIM HUAT, PhD

Professor and Dean
School of Graduate Studies
Universiti Putra Malaysia

Date:

Declaration by Members of Supervisory Committee

This is to confirm that:

- the research conducted and the writing of this thesis was under our supervision;
- supervision responsibilities as stated in the Universiti Putra Malaysia (Graduate Studies) Rules 2003 (Revision 2012-2013) are adhered to.

Signature: _____
Name of Chairman of
Supervisory
Committee: Dr. Anwar Fitrianto

Signature: _____
Name of Member of
Supervisory
Committee: Prof. Dr. Habshah Binti Midi

Signature: _____
Name of Member of
Supervisory
Committee: Assoc. Prof. Dr. Leong Wah June

TABLE OF CONTENTS

	Page
ABSTRACT	i
ABSTRAK	iii
ACKNOWLEDGEMENTS	v
APPROVAL	vi
DECLARATION	viii
LIST OF TABLES	xii
LIST OF FIGURES	xiv
LIST OF ABBREVIATIONS	xv
CHAPTER	
1 INTRODUCTION	1
1.1 Experimental Design	1
1.2 Uniform Design	3
1.2.1 Uniformity and Discrepancy	4
1.2.2 Construction Methods of Uniform Design	6
1.2.3 Performing Experiments with Uniform Design	6
1.3 Problem Statement	7
1.4 Objectives of Study	7
1.5 Limitation of the Study	7
1.6 Summary	8
1.7 An overview of the thesis	8
2 LITERATURE REVIEW	10
2.1 Uniform Design	10
2.2 Measures of Uniformity	12
2.3 Some Applications of Uniform Design	15
3 A NEW APPROACH TO OBTAIN GLOBAL OPTIMIZATION IN UNIFORM DESIGN	18
3.1 Introduction	18
3.2 Optimization Criteria in Construction of Uniform Design	18
3.2.1 Neighborhood	19
3.2.2 Replacement Rule	20
3.3 Methodology	20
3.3.1 Absolute Difference Equivalence Approach	21
3.3.2 Modified Ruin and Recreate Approach	22
3.3.3 Global Absolute Difference Equivalence Search	24
3.4 Performance of Global Absolute Difference Equivalence Search	28

3.5	Conclusion	32
4	MODIFYING THE CUTTING METHOD TO OBTAIN UNIFORM DESIGNS WITH BETTER UNIFORMITY	33
4.1	Introduction	33
4.2	Details of the Cutting Method in Uniform Design	34
4.2.1	Good Lattice Point Method with a Power Generator	34
4.2.2	The Cutting Method	36
4.3	Methodology	41
4.4	Performance of the Modified Cutting Method in comparison with Original Cutting Method	46
4.5	Conclusion	48
5	CONSTRUCTION OF UNIFORM DESIGNS USING ABSOLUTE DEVIANCE METHOD	50
5.1	Introduction	50
5.2	Some reviews of Construction Methods of Uniform Design	50
5.3	Methodology	52
5.3.1	The proposed Absolute Deviance Method for two factors Uniform Design	54
5.3.2	The proposed Absolute Deviance Method for higher dimensions Uniform Design	63
5.4	Comparison between the proposed Absolute Deviance Method and other construction method	65
5.5	Conclusion	68
6	CONCLUSION AND FUTURE WORKS	69
	REFERENCES	71
	APPENDICES	75
	BIODATA OF STUDENT	76
	LIST OF PUBLICATIONS	77

LIST OF TABLES

Table		Page
2.1	Four factors UD with five levels and five experimental runs, $U_5(5^4)$	11
3.1	CD and MD values for $U_3(3^2)$ formed from the particular set of points	21
3.2	Possible set of points which will be considered for reconstruction of $U_4(4^2)$	23
3.3	The sets of points that will be considered for reconstruction of $U_4(4^2)$	24
3.4	First candidate design of $U_4(4^2)$ by modified R&R approach	24
3.5	Initial design, X_o with 0.1350 CD value and 0.1821 MD value in searching $U_4(4^2)$	26
3.6	Results of two GADES optimization process in searching $U_4(4^2)$ under CD and MD respectively	27
3.7	The CD and MD values, size of neighborhood, total time and the number of iteration to obtain two factors UD with $n = 4, 5, \dots, 9$ for both ORR and GADES algorithms	28
4.1	Second candidate design, U^2 of $U_7(7^2)$ by $GLP_{7,2}^{power} = (1, 2)$	35
4.2	CD values for all six candidate designs of $U_7(7^2)$	36
4.3(a)	$U_7(7^2)$ by $GLP_{7,2}^{power} = (1, 3)$	36
4.3(b)	$U_7(7^2)$ by $GLP_{7,2}^{power} = (1, 5)$	36
4.4(a)	Sorted C based on first column of C , $C^{(1)}$	38
4.4(b)	Sorted C based on second column of C , $C^{(2)}$	38
4.5	Elements position and its value of $C^{(2,1)}$	39
4.6	UD which is formed by relabeling the elements in $C^{(2,1)}$, $U^{(2,1)}$	39
4.7	CD values for all 14 candidate designs of $U_4(4^2)$ by the cutting method	40
4.8(a)	Fifth subset of $C^{(1)}$, $C^{(1,5)}$	40
4.8(b)	Seventh subset of $C^{(1)}$, $C^{(1,7)}$	40
4.9	Two factors UD with four experimental runs, $U_4(4^2)$	41
4.10	CD values for two factors UD by the cutting method	42

4.11	CD value of UD _s and suggested number of experimental runs of initial design, p , by the modified cutting method	45
5.1	Absolute differences between points for factor 2 of $U_5(5^2)$	52
5.2(a)	Set of points with its absolute difference between points and the corresponding CD values for $U_4(4^2)$	53
5.2(b)	Set of points with its absolute difference between points and the corresponding CD values for $U_5(5^2)$	53
5.3	Possible sets of absolute differences for $n = 5$	55
5.4	The set of five points obtained from $A_1 = \{2, 2\}$	57
5.5	Validity of the sets of five points formed	57
5.6	$U_5(5^2)$, D_1 with $A_2 = \{2, 3\}$ as selected absolute difference set	57
5.7	Possible sets of absolute differences for $n = 6$	60
5.8	The set of six points obtained from $A_1 = \{4, 4\}$	61
5.9	Validity of the sets of six points formed	62
5.10	$U_6(6^2)$, D_1 and D_2 with its CD value	62
5.11	$U_5(5^3)$, D_1	64
5.12	$U_6(6^3)$, D_1 and D_2 with its CD value	64

LIST OF FIGURES

Figure		Page
3.1	Size of neighborhood in searching UDs by the ORR and GADES algorithm	29
3.2 (a)	Time in seconds to obtain UDs by the ORR and GADES algorithm under CD criterion	30
3.2 (b)	Time in seconds to obtain UDs by the ORR and GADES algorithm under MD criterion	30
3.3 (a)	Number of iteration to obtain UDs by the ORR and GADES algorithm under CD criterion	31
3.3 (b)	Number of iteration to obtain UDs by the ORR and GADES algorithm under MD criterion	31
4.1	CD values of two factors UDs generated by TA algorithm, original cutting method and modified cutting method	46
4.2	CD values of three factors UDs generated by TA algorithm, original cutting method and modified cutting method	47
4.3	CD values of four factors UDs generated by TA algorithm, original cutting method and modified cutting method	47
4.4	CD values of five factors UDs generated by TA algorithm, original cutting method and modified cutting method	48
5.1	CD values for two factors UDs generated by GLP, optimization (TA), modified cutting method, original cutting method and our proposed ADM	65
5.2	CD values for three factors UDs generated by GLP, optimization (TA), modified cutting method, original cutting method and our proposed ADM	66
5.3	CD values for four factors UDs generated by GLP, optimization (TA), modified cutting method, original cutting method and our proposed ADM	67
5.4	CD values for five factors UDs generated by GLP, optimization (TA), modified cutting method, original cutting method and our proposed ADM	67

LIST OF ABBREVIATIONS

ADE	Absolute Difference Equivalence
ADM	Absolute Deviance Method
CD	Centered L_2 -Discrepancy
CPU	Central Processing Unit
CP	Columnwise-Pairwise
C^s	s -dimensional unit cube
DFSS	Design for Six Sigma
GADES	Global Absolute Difference Equivalence Search
GLP	Good Lattice Point
GWP	Generalized Wordlength Pattern
K-H	Koksma-Hlawka
LCD	Liquid Crystal Display
LHD	Latin Hypercube Designs
LS	Local Search
MD	Mixture Discrepancy
M	Measure of Uniformity
NTM	Number-Theoretic Method
NP	Non deterministic Polynomial-time
n	Number of experimental runs
ORR	Optimization which employed R&R approach
p	Number of experimental runs for initial design
QMCM	Quasi-Monte Carlo Method
q	Number of levels
R&R	Ruin and Recreate
\mathfrak{R}	Experimental domain
s	Number of factors
TA	Threshold Accepting
T	Threshold value
UD	Uniform Design
WD	Wrap-around L_2 -Discrepancy

CHAPTER 1

INTRODUCTION

1.1 Experimental Design

Statistical experimental design has proven track record in history and has been used as statistical tools in various fields. The experimental design was first employed in agriculture and technology. It has been developed rapidly in the past years and played an important role in development of sciences and high technology (Fang & Chan, 2006). Furthermore, it is now widely applied in product and process design. Nowadays experiments are carried out almost everywhere to explore about a process or system. Hence, an experimental design is an efficient choice to obtain a reaction product or process with desirable characteristics.

Responses and factors are the two important types of variables in experimental design. Normally, responses are the dependent variables and factors are the independent variables. A factor is a general type or category of treatments. It is sometimes called input variable or a controllable variable which can be quantitative or qualitative. A quantitative factor is where each level is described by a numerical quality on an equal interval scale, for instance, temperature in degree, time in second, price in Ringgit Malaysia and weight in kilogram. Meanwhile, a qualitative factor is where the levels differ by some qualitative attribute, for example, hair color, gender and blood type. Additionally, treatment is a factor level or combination of factors levels that applied to an experimental unit where experimental unit is defined as a person, object or material that receives a treatment. The response of an experiment depends on the number of factors involved in the experiment.

In general, responses will be denoted by letter y and factors by the letter x :

$$y = f(x_1, x_2, \dots, x_s) + e$$

where $f(\cdot)$ is a function, s is the number of factors and e is the random error. Domain or region of an experiment is the set within which the factors could conceivably change. Let \mathfrak{R} denotes the domain of an experiment. Frequently, super rectangle $[a_1, b_1] \times \dots \times [a_s, b_s]$ or a s -dimensional unit cube $C^s = [0, 1]^s$ is chosen as the experimental domain \mathfrak{R} . The values in $[a_i, b_i]$ are representing the levels of the i^{th} factor (Liang et al., 2001).

The goal of the experimental design is to primarily understand the effect of the factors and their interactions, and followed by modeling the relationship between the response

and the factors with a least number of experiments. A good experimental design should minimize the number of experimental runs to acquire as much information as possible. This requires an orderly and efficient mapping of the experimental domain or space. Reduction cost is achieved when the experimental design is well adopted (Liang et al., 2001).

There are important notes need to be taken into account when implementing the experimental design. First, choosing suitable factors is one of the crucial steps in each experiment. It is always recommended that the number of factors should be minimized. However, it is uneasy task to decide which variable is more significant than the others. Hence, the appropriateness of the factors can be determined by multiple statistic models. Besides, experiments may be carried out at different combinations of different levels of the factors, in order to identify the important factors and how they contribute to the response. Second, the experiment with larger domain should be considered first if possible. The reason is some unexpected results may appear in this way. If the experiment is carried out in a product process, it is advised not to choose a domain that is unsuitably large. Third, the gap between two successive levels of a quantitative factor should be comparatively large with the random errors. For instance, according to a normal distribution $N(0, \sigma^2)$, the random error of measurement of pH is distributed with $\sigma = 0.20$. Then, the gap of $\text{pH} = 0.5$ can be considered, for example by taking $\text{pH} = 5.0, 5.5$ and 6.0 as different levels for an experiment. The gap of two pH levels is relatively large compared to the random error (Fang & Lin, 2003; Liang et al., 2001).

Randomness, balance, orthogonality, efficiency, and robustness under a specific statistical model are the issues that most of the experimental design methods concerned with (Fang, 2002b). Nevertheless, most of the experiments especially in high technology development have the complexities such as multi- factors, large experimental domain, complicated non-linear model, unknown underlying model and no analytic formula of the response surface (Fang & Lin, 2008; Fang, 2002b).

Due to the reason of these complexities, some new experimental designs are required. The space filling design is a good possible choice when the underlying model is unknown where the relationship between the response and the potential contributing factors is not fully known (Fang, 2002b). Space filling designs are valuable for modeling systems that are deterministic or near deterministic. There is bias although there is no variance in experiments on deterministic systems. Bias is the dissimilarity between the approximation model and the true mathematical function. The intention of space filling designs is to resolve the bias. There are two techniques on how to resolve the bias. One approach is to spread the design points out at a consistent distance from each other in the experimental boundaries. The alternative approach is to scatter the points evenly over the experimental region (SAS Institution Inc., 2014). This leads to the terminology “Uniform Design (UD)” which will introduced briefly in next subchapter.

1.2 Uniform Design

Uniform design (UD) is a kind of space-filling design which applied in industrial experiments, reliability testing and computer experiments. It is symbolized by scattering uniformly of design points in the experimental domain, and hence it is particularly suitable for an experiment with an unknown underlying model and the entire experimental domain has to be fairly explored. Moreover, it is able to explore the relationships between the response and the factors with a reasonable number of experimental runs.

The development of UD was initially motivated by a need in systems engineering and in the other hand to fulfill the needs in computer and industry experiments. Identify between the effects that are caused by particular factors or build an empirical model between the input (factor) variables and the output (response) variables are the problems that continually faced by the engineers (Fang & Lin, 2003). In 1978, three big projects in system engineering raised some problems. In one of those projects, the number of factors was six or more and in order to obtain the output of the system, they had to solve a system differential equation. Unfortunately, each run required a day of calculation from an input to the corresponding output. Therefore, they needed to find a way of experiment so that as much information as possible could be found using relatively few experimental runs. The relationship between the input and output has no analytic formula and is very complicated. The true model is expressed as

$$y = f(x_1, x_2, \dots, x_s) \equiv f(x), \quad x \in \mathfrak{R}$$

where function $f(\cdot)$ is known and has no analytic expression. Then, the engineers wanted to find a simple and approximate model or known as a metamodel with the following expression

$$y = g(x_1, x_2, \dots, x_s) = g(x)$$

such that the difference of $|f(x) - g(x)|$ is small over the experimental domain \mathfrak{R} . The metamodel should be much simpler than the true one where it is easier to compute (Fang & Lin, 2008).

At the same time, Liang et al. (2001) mentioned that a problem of experimental designs was proposed by a Chinese industrial agency. The experimental design had six factors each having at least 12 levels should be considered. However, the costly experiments restricted the experiment to be run not more than 50. It was impossible for the traditional experiment designs such as fractional factorial design to have such an achievable design. Despite that, a satisfactory result was achieved when UD was

applied to the problem; only 31 experimental runs with each factor having 31 levels were arranged.

As stated in Li et al. (2004), they pointed out some advantages of UD over traditional designs such as factorial design and orthogonal design. One of the advantages is the UD can still be carried out in a relatively small number of experimental runs even when the number of factors or the number of levels of the factors is large. Besides, a significant amount of information can be obtained within a small number of experimental runs. The interesting part is, it is robust to the underlying model assumption, which indicates that although the form of regression model is unknown, UD still performs well.

In addition, Liang et al. (2001) also revealed several advantages of UD based on their experience. First of all, samples with high representativeness in the studied experimental domain are able to be produced by UD. Moreover, UD is robust against changes of model and it does not enforce a strong assumption on the model. Then, the greatest possible number of levels for each factor can be also accommodated by UD among all experimental designs.

Based on the authors' description on the UD as above, it can be said that UD acts as an efficient design which can be utilized as a fractional factorial design, a design of computer experiments, a robust design or a design with mixtures.

1.2.1 Uniformity and Discrepancy

Uniformity of space filling acts as an important part and is an essential feature of UD. The concept of UD is based on quasi-Monte Carlo method (QMCM) which seeks sets of points that are uniformly scattered in the experimental domain. Various discrepancies in QMCM have been used as measures of uniformity in the literature, such as the star-discrepancy, the star L_2 -discrepancy, the centered L_2 -discrepancy (CD), wrap-around L_2 -discrepancy (WD) and mixture discrepancy (MD). The UD can be achieved by minimizing a discrepancy. There is more than one definition of discrepancy, and different discrepancies may produce different UDs (Fang & Chan, 2006). The lower the discrepancy, the better uniformity the set of the points has (Fang et al., 2005). For instance, if all of the points were clustered at one corner of the sphere, the uniformity would be violated and the sample mean would represent the population mean rather poorly, the discrepancy would be very large. Hence in order to construct UD, we should find a design with lowest discrepancy with n experimental runs and s input variables or factors. The aim of the UD is to select a set of n points $P \in C^s$ with lowest discrepancy value, $D(P)$. Apart from that, nearly UD is another definition given by Ma & Fang (2004) where a nearly UD is a design with low discrepancy value. For simplicity, UD or nearly UD will be known as UD in this research.

The discrepancies have played an important role in QMCM. The QMCM have been widely used in multivariate numerical integration, numerical simulation, experimental design, optimization, geometric probability, survey sampling and statistical inference. The treatment for most of these statistical problems in the fields mentioned above require low-discrepancy sequences or sets over the specific experimental domain which can be partially overcome by implementing QCMC (Fang, 2002a).

According to Zhou et al. (2013), QMCM were inspired by multidimensional numerical integration. The prior aim of the UD is to obtain the best estimator of the overall mean of I ,

$$I(g) = \int_{C^s} g(x) dx$$

that can be approximated by using the sample mean,

$$\hat{I}(P) = \bar{y}(P) = \frac{1}{n} \sum_{i=1}^n g(x_i)$$

where $P = \{x_1, \dots, x_n\}$ is a set of n experimental points on C^s and $g(\cdot)$ is a known function (Li et al., 2004; Fang, 2002a).

In 1981, Hua & Wang mentioned about the Koksma-Hlawka (K-H) inequality and given that the error bound of the approximation as

$$|I - \hat{I}(P)| \leq V(g)D(P)$$

where $D(P)$ is the discrepancy of P not depending on g and $V(g)$ is a measure of the variation of g . The definition for a function of bounded variation, $V(g)$ was given by Hardy and Krause (Niederreiter, 1992, p.19; Hua & Wang, 1981, p.99), which is independent of the design points. The K-H inequality indicates that, the more uniform a set of points, P distributes over the C^s , the more accurate $\hat{I}(P)$ is an estimate of I .

Hence, the K-H inequality suggests of choosing a set of points which have the lowest discrepancy among all possible designs for a given number of experimental runs and factors. Since $V(g)$ does not depend on the set P , a UD is robust against changes of the function g provided that $V(g)$ remains unchanged (Li et al., 2004; Liang et al., 2001; Fang, et al., 2000a). Therefore, the key idea of QMCM is to generate s set of n points, denoted by P , on the unit cube C^s for given n and s such that $D(P)$ is minimized.

1.2.2 Construction Methods of Uniform Design

The UD can be constructed by minimizing a discrepancy over the design space. There are two types of UD, namely symmetrical and asymmetrical. A symmetrical UD is a design whose factors have same number of levels, while in asymmetrical UD; more levels are allocated for important factors and less levels for less important factors (Fang et al., 2005).

There are numbers of construction method of UDs have been proposed. Good lattice point (GLP) method, extending orthogonal design method, Latin square method, optimization searching method and cutting method are the construction methods for symmetrical UDs, while combinatorial method, pseudo-level technique and collapsing method are the construction methods for asymmetrical UDs. The key steps for the construction of UDs are first to define a suitable measure of uniformity. Then, reduce the computation complexity of searching UDs and apply any construction methods as stated above to generate UD (Fang & Lin, 2003).

1.2.3 Performing Experiments with Uniform Design

Each UD table has a notation $U_n(q^s)$ where U stands for UD, n for the number of experimental runs, s for the number of factors and q for the number of levels. If the quantitative models cannot build merely based on theoretical consideration or past experience, then performing industrial experiments enable the experimenters to get the required data that is used to set up the quantitative models. The obtained models help in quantifying the process, verifying a theory or optimizing the process (Fang & Chan, 2006).

The following steps are necessary to be taken as a procedure for performing industrial experiments with a UD. First, make sure that the goal is clear by identifying the objective of the experiment and the process response to study. Second, choose factors with suitable number of levels for each factor and determine the appropriate experimental domain. Subsequently, decide the number of experimental runs and choose a suitable UD table that accommodates the number of factors, levels and experimental runs. Next, arrange the number of levels for each factor according to the chosen UD table. Then, come to the modeling steps which need to find an appropriate model to fit the data such as regression analysis. Finally, discover the information from the built model and find the „best combination of the factors values that achieved the objective function. It is necessary to make conclusions from the model established in the modeling part in order to fulfill the objective that is specified earlier. If possible, perform further experiments by adding runs to the experiment to verify the results obtained (Fang & Chan, 2006; Fang & Lin, 2003).

1.3 Problem Statement

There are many construction methods of UD in literature. Hence, we are interested to study and improve the existing construction methods of UDs. In optimization method, choice of neighborhood and replacement rule are two important criteria. Ruin and recreate (R&R) approach is one of the choices of neighborhood (Fang et al., 2000b). The R&R approach is not preferable by many authors as it provides a larger size of neighborhood compared to other choice of neighborhood. Large neighborhood requires longer time to complete the optimization process as large neighborhood increases the computational load. However, the possibility to include the global solution is higher in larger neighborhood. Therefore, a solution is needed to improve the R&R approach in case the R&R approach is determined to be the choice of neighborhood.

Besides, the cutting method which was proposed by Ma & Fang (2004) is one of the construction methods of UDs. The cutting method requires an initial design with p experimental runs, which p or $p+1$ is a prime number and p is greater than n . The interesting question is, "Which p as the number of experimental runs for initial design gives the lowest discrepancy?". Thus, we are trying to find out the uncertainty by carrying out this study.

In addition, the cutting method was the latest existing methods of constructing UDs proposed by Ma & Fang, (2004). Some modification were made on the existing construction methods; for instance, Talke & Borkowski (2012) proposed two approaches (generator equivalence and projection) for GLP method to reduce the computational cost. Meanwhile, Jiang & Ai (2014) modified the threshold accepting (TA) algorithm to search UDs without replications. Although modifications were made on the existing construction methods, there is no new method developed in the recent years.

1.4 Objectives of Study

The objectives of the study are i) to reduce the size of neighborhood that is determined by the R&R approach while maintaining the global solution in the neighborhood, ii) to find an appropriate number of experimental runs for the initial design of the cutting method and iii) to provide an efficient method in constructing symmetrical UD with better uniformity.

1.5 Limitation of the Study

Matlab software is chosen as our research tools that assist us in computing the measure of uniformity and constructing the uniform design. For the optimization method which will be discussed in Chapter 3, our findings are limited to n which is less or equal to 9. It is because in R&R approach, we need to obtain all possible permutations of

$\{1, 2, \dots, n\}$ to be the sets of points that will be considered in reconstruction of the design. Unfortunately, Matlab software fails to give the permutations of $\{1, 2, \dots, n\}$ where n is greater or equal to 10 due to the problem of out of memory.

There is also limitation for the absolute deviance method (ADM) which proposed in Chapter 5. Our findings are limited to n which is less or equal to 14 as the file „npermutek in Matlab which we applied has its limitation. The „npermutek file is applied to obtain the permutation n of k with repetition where k is the desired number to be chosen from n . According to the Step 2 in ADM algorithm, Algorithm 5.1 and Algorithm 5.2, on two factors UD for both odd and even experimental runs, we need to choose $\frac{n-1}{2}$ elements (for odd number experimental runs) and $\frac{n-2}{2}$ elements (for even number experimental runs) from $\{2, 3, \dots, n-2\}$, respectively as the elements of absolute differences. Hence, when $n=15$, we need to select 7 elements from $\{2, 3, \dots, 13\}$. The „npermutek file in the Matlab software fails to compute for selecting 7 elements from $\{2, 3, \dots, 13\}$ with the problem of out of memory. Then, for n which is greater than 15, the Matlab software also fails to compute with the reason of maximum variable size allowed by the program is exceeded.

1.6 Summary

Since UD was brought out in 1980, many mathematicians and statisticians made their effort in studying and developing UD. For over thirty years, there are consistently reports in China to show that UD has been widely used and it has been successfully applied in various fields such as agriculture, industry especially in chemistry and chemical engineering, petroleum engineering, quality engineering and system engineering, natural sciences and also on improving technologies of textile industry, pharmaceuticals, fermentation industry and others. It can be seen that UD has been gradually popularized in China and presently has become one of the major experimental designs in China. Despite that, its application in industries worldwide still has to be promoted. The applications of UD showed that the UD is indeed a very promising and powerful experimental design method.

1.7 An Overview of the thesis

Literatures will be reviewed on the UD, measure of uniformity and some applications of UD in Chapter 2.

Optimization method is one of the construction methods of UD which is discussed in Chapter 3. Two important criteria in optimization method such as neighborhood and replacement rule are explained in details. In this research, R&R approach is chosen as the definition of neighborhood. In order to reduce the size of neighborhood that is

obtained by the R&R approach, absolute difference equivalence (ADE) approach is proposed. ADE approach is developed which aims to coordinate with the R&R approach. The modified R&R approach is considering ADE approach in R&R algorithm. After that, an optimization process called global absolute difference equivalence search (GADES) is introduced which implemented modified R&R approach as its neighborhood and a replacement rule that is defined earlier. Then, the performance of the GADES is studied by comparing the UD_s formed from the optimization algorithm which employed R&R approach (later we name it as ORR) with GADES algorithm in terms of uniformity, size of neighborhood, number of iteration and total computational time.

In Chapter 4, another existing construction method called cutting method is presented. Details of the cutting method in UD which include the GLP method with a power generator and the cutting method are discussed with numerical examples provided. Then, the cutting method is modified by searching a suitable p for initial design for the desired UD. After that, the performance of the modified cutting method is compared with the original cutting method.

In Chapter 5, a new construction method of UD, ADM is proposed. At first, the ADM method is concentrating on two factors UD_s. There are two situations with regard to n that needed to be considered, which are when n is an odd or even number. Hence, the algorithms for odd and even experimental runs are different. Then, the ADM to construct UD_s with higher dimensions which is greater than two is proposed as well. The algorithms are implemented in the numerical examples discussed. Finally, the performance of ADM is compared with the existing method, such as GLP method, optimization method, cutting method and the modified cutting method that is proposed in Chapter 4.

REFERENCES

- Bundschuh, P., & Zhu, Y. C. (1993). A method for exact calculation of the discrepancy of low-dimensional finite point sets I. *Abhandlungen Aus Math. Seminar. Univ. Hamburg*, 63, 115–133.
- Chan, L. Y., & Lo, M. L. (2004). Quality Improvement In the Manufacture of Liquid Crystal Displays Using Uniform Design. *International Journal of Materials and Product Technology*, 20(1/2/3), 127–142.
- Chatterjee, K., Li, Z. H., & Qin, H. (2012). Some new lower bounds to centered and wrap-round L_2 -discrepancies. *Statistics & Probability Letters*, 82(7), 1367–1373.
- Fan, J. Q., & Li, G. (2005). *Contemporary Multivariate Analysis and Design of Experiments*. World Scientific.
- Fang, K. T. (1980). The uniform design: application of number-theoretic methods in experimental design (In Chinese). *Acta Math. Appl. Sinica*, 3(4), 363–372.
- Fang, K. T. (2002a). Some Applications of Quasi-Monte Carlo Methods in Statistics. In K. T. Fang, H. Niederreiter, & F. J. Hickernell (Eds.), *Proceedings of a conference held at Hong Kong Baptist University, Hong Kong SAR, China, November 27-December 1, 2000* (pp. 10–26). Springer Berlin Heidelberg.
- Fang, K. T. (2002b). Theory, Method and Applications of the Uniform Design. *International Journal of Reliability, Quality and Safety Engineering*, 09(04), 305–315.
- Fang, K. T., & Chan, L. Y. (2006). Uniform design and its industrial applications. In *Springer Handbook of Engineering Statistics* (pp. 229–247).
- Fang, K. T., Li, R., & Sudjianto, A. (2005). *Design and modeling for computer experiments*. London: Chapman & Hall.
- Fang, K. T., & Lin, D. K. J. (2003). Uniform experimental designs and their applications in industry. *Handbook of Statistics*.
- Fang, K. T., & Lin, D. K. J. (2008). Uniform Design in Computer and Physical Experiments. *The Grammar of Technology Development*, 105–125.

- Fang, K. T., Lin, D. K. J., Winker, P., & Zhang, Y. (2000). Uniform Design: Theory and Application. *Technometrics*, 42(3), 237–248. Retrieved 30 October 2013 <http://amstat.tandfonline.com/doi/abs/10.1080/00401706.2000.10486045>
- Fang, K. T., Ma, C. X., & Winker, P. (2000). Centered L_2 discrepancy of random sampling and Latin hypercube design, and construction of uniform designs. *Mathematics of Computation*, 71(237), 275–297.
- Fang, K. T., & Qin, H. (2003). A note on construction of nearly uniform designs with large number of runs. *Statistics and Probability Letters*, 61(2), 215–224.
- Fang, K. T., & Wang, Y. (1994). *Number-Theoretic Methods in Statistics*. London: Chapman & Hall.
- Fang, K. T., Wang, Y., & Bentler, P. M. (1994). Some Applications of Number-Theoretic Methods in Statistics. *Statistical Science*, 9(3), 416–428.
- Heinrich, S. (1996). Efficient algorithms for computing the L_2 -discrepancy. *Mathematics of Computation*, 65(216), 1621–1634.
- Hickernell, F. J. (1998). A generalized discrepancy and quadrature error bound. *Mathematics of Computation*, 67(221), 299–322.
- Hua, L. K., & Wang, Y. (1981). *Applications of Number Theory to Numerical Analysis*. Berlin and Beijing: Springer-Verlag and Science Press.
- Jiang, B. C., & Ai, M. Y. (2014). Construction of uniform designs without replications. *Journal of Complexity*, 30(1), 98–110.
- Jin, Y. S., Peng, X. F., Liang, Y. Z., & Ma, J. Y. (2008). Uniform design-based sensitivity analysis of circadian rhythm model in Neurospora. *Computers and Chemical Engineering*, 32(8), 1956–1962.
- Koziołek, S., & Derlukiewicz, D. (2012). Method of assessing the quality of the design process of construction equipment with the use of DFSS (design for Six Sigma). *Automation in Construction*, 22, 223–232.
- Lee, C. K., & Cheng, Y. C. (2014). Application of Uniform Design and Quantum-Behaved Particle Swarm Optimization in Solving the Sensitivity Problem a Railway Vehicle System. *Procedia Engineering*, 79, 427–436.

- Li, R., Lin, D. K. J., & Chen, Y. (2004). Uniform design: design, analysis and applications. *International Journal of Materials and Product Technology*, 20, 101–114.
- Li, W. W., & Wu, C. F. J. (1997). Columnwise-Pairwise Algorithms With Applications to the Construction of Supersaturated Designs. *Technometrics*, 39(2), 171–179.
- Liang, Y. Z., Fang, K. T., & Xu, Q. S. (2001). Uniform design and its applications in chemistry and chemical engineering. *Chemometrics and Intelligent Laboratory Systems*, 58(1), 43–57.
- Lo, Y. K., Zhang, W. J., & Han, M. X. (2000). Applications of the uniform design to quality engineering (In chinese). *Journal of Chinese Statistical Association*, 38(4), 411–428.
- Lu, X., Fang, K. T., Xu, Q. F., & Yin, J. X. (2002). Balance Pattern And BP-Optimal Factorial Designs. *Technical Report-324, Hong Kong Baptist University*.
- Ma, C. X., & Fang, K. T. (2001). A note on generalized aberration in factorial designs. *Metrika*, 53(1), 85–93.
- Ma, C. X., & Fang, K. T. (2004). A new approach to construction of nearly uniform designs. *International Journal of Materials and Product Technology*, 20(1/2/3), 115–126.
- Niederreiter, H. (1992). *Random number generation and Quasi-Monte Carlo methods*. Philadelphia, Pennsylvania: Society for Industrial and Applied Mathematics.
- Park, J. S. (1994). Optimal Latin-hypercube designs for computer experiments. *Journal of Statistical Planning and Inference*, 39(1), 95–111.
- SAS Institution Inc. (2014). *JMPR 11 Design of Experiments Guide*. Cary, NC, USA: SAS Institute Inc.
- Schrimpf, G., Schneider, J., Stamm-Wilbrandt, H., & Dueck, G. (2000). Record Breaking Optimization Results Using the Ruin and Recreate Principle. *Journal of Computational Physics*, 159(2), 139–171.
- Song, J., Song, Z. G., & Sun, R. (2012). Study of uniform experiment design method applying to civil engineering. *Procedia Engineering*, 31, 739–745.

- Talke, I. S., & Borkowski, J. J. (2012). Generation of space-filling uniform designs in unit hypercubes. *Journal of Statistical Planning and Inference*, 142(12), 3189–3200.
- Tang, M., Li, J. K., Chan, L. Y., & Lin, D. K. J. (2004). Application of Uniform Design in the Formation of Cement Mixtures. *Quality Engineering*, 16(3), 461–474.
- Wang, Y., & Fang, K. T. (1981). A note on uniform distribution and experimental design. *Kexue Tongbao*, 26(6), 485–489.
- Warnock, T. T. (1972). Computational investigations of low-discrepancy point sets. In *Applications of Number Theory to Numerical Analysis*, Academic Press, New York, 319–343.
- Weyl, H. (1916). Über die Gleichverteilung von Zahlen mod Eins. *Mathematische Annalen*, 77, 313–352.
- Winker, P., & Fang, K. T. (1997). Application of Threshold-Accepting to the Evaluation of the Discrepancy of a Set of Points. *SIAM Journal on Numerical Analysis*, 34(5), 2028.
- Xu, H. Q., & Wu, C. F. J. (2001). Generalized minimum aberration for asymmetrical fractional factorial designs. *Annals of Statistics*, 29(4), 1066–1077.
- Yang, P., & Chen, A. (2006). Application of Uniform Design in Grouting Experiment (In Chinese). *Exploration Engineering (Rock & Soil Drilling and Tunneling)*, 33(3), 9–11.
- Ye, K. Q., Li, W., & Sudjianto, A. (2000). Algorithmic construction of optimal symmetric Latin hypercube designs. *Journal of Statistical Planning and Inference*, 90(1), 145–159.
- Zhou, Y. D., Fang, K. T., & Ning, J. H. (2013). Mixture discrepancy for quasi-random point sets. *Journal of Complexity*, 29(3-4), 283–301.