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Theory and Application of Uniform Experimental Designs

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Foreword

Experiment is essential to scientific and industrial areas. How do we conduct experiments so as to lessen the number of trials while still achieving effective results? In order to solve this frequently encountered problem, there exists a special technique called experimental design. The better the design, the more effective the results.

In the 1960s, Prof. Loo-Keng Hua introduced J. Kiefer's method, the "golden ratio optimization method," in China, also known as the Fibonacci method. This method and orthogonal design which were popularly used in industry promoted by Chinese mathematical statisticians are the two types of experimental designs. After these methods became popular, many technicians and scientists used them and made a series of achievements, resulting in huge social and economic benefits. With the development of science and technology, these two methods were not enough. The golden ratio optimization method is the best method to deal with a single variable, assuming the real problem has only one interesting factor. However, this situation is almost impossible. This is why we only consider one most important factor and fix the others. Therefore, the golden ratio optimization method is not a very accurate approximation method. Orthogonal design is based on Latin square theory and group theory and can be used to do multifactor experiments. Consequently, the number of trials is greatly reduced for all combinations of different levels of factors. However, for some industrial or expensive scientific experiments, the number of trials is still too high and cannot be facilitated.

In 1978, due to the need for missile designs, a military unit proposed a five-factor experiment, where the level of every factor should be higher than 18 and the total number of trials should be not larger than 50. Neither the golden ratio optimization method nor orthogonal design could be applied. Several years before 1978, Prof. Kai-Tai Fang asked me about an approximate calculation of a multiple integration problem. I introduced him to use the number-theoretical methods for solving that problem, which inspired him to think of using number-theoretical methods in the design of the problem. After a few months of research, we put forward a new type of experimental designs that is known as uniform design. This method had been successfully applied to the design of missiles. After our article was published in the early 1980s, uniform design has been widely applied in China and has resulted in a series of gratifying achievements.

Uniform design belongs to the quasi-Monte Carlo methods or number-theoretical methods, developed for over 60 years. When the calculation of a single variable problem (the original problem) is generalized to a multivariable problem, the calculation complexity is often related to the number of variables. Even if computational technology advances greatly, this method is still impossible in application. Ulam and Von Neumann proposed the Monte Carlo method (i.e., statistical stimulation) in the 1950s. The general idea of this method is to put an analysis problem into a probability problem with the same solution and then use a statistical simulation to deal with the latter. This solves some difficult analysis, including the approximate calculation of multiple definite integrals. The key to the Monte Carlo method is to find a set of random numbers to serve as a statistical simulation sample. Thus, the accuracy of this method lies in the uniformity and independence of random numbers.

In the late 1950s, some mathematicians tried to use deterministic methods to find evenly distributed points in space in order to replace the random numbers used in the Monte Carlo method. The set of points that had been found was by using number theory. According to the measure defined by Weyl, the uniformity (of a uniform design) is good, but the independence is relatively poor. By using these points to replace the random numbers used in the Monte Carlo method, we usually get more precise results. This kind of method is called a quasi-Monte Carlo method, or the number-theoretical method. Mathematicians successfully applied this method into approximate numerical calculations for multiple integrals.

In statistics, pseudo-random numbers can be regarded as representative points of the uniform distribution (in cubed units). Numerical integration requires a large sample, but uniform design just uses small samples. Since the sample is more uniform than orthogonal designs, it is preferred for settling the experiment. Of course, when seeking a small sample, the method of seeking a large sample can be used as a reference.

Uniform design is only one of the applications of the number-theoretical method, which is also widely used in other areas, such as the establishment of multiple interpolation formulas, the approximate solutions of systems of some integrals or differential equations, the global extremes of the functions, the approximate representation points for some multivariate distributions, and some problems for statistical inference, such as multivariate normality test and the sphericity test.

When the Monte Carlo method was first discovered in the late 1950s, Prof. Loo-Keng Hua initiated and led a study of this method in China. Loo-Keng Hua and his pioneering results were summarized in our monograph titled “Applications of Number Theory to Numerical Analysis” published in Springer-Verlag Science Press in 1981. These results are one of the important backgrounds and reference materials for my work with Prof. Kai-Tai Fang.

I have worked with Prof. Kai-Tai Fang for nearly 40 years. As a mathematician and a statistician with long-term valuable experience in popularizing mathematical statistics in Chinese industrial sector, he has excellent insight and experience in applied mathematics. He always provided valuable research questions and possible ways to solve the problem in a timely manner. Our cooperation has been pleasant and fruitful, and the results were summarized in our monograph “Number-Theoretic Methods in Statistics” published by Chapman and Hall in 1994.

This book focuses on the theory and application of uniform designs, but also includes many latest results in the past 20 years. I strongly believe that this book will be important for further development and application of uniform designs. I would like to take this opportunity to wish the book success.

Beijing, China

Yuan Wang
Academician of Chinese Academy
of Sciences

Preface

The purpose of this book is to introduce theory, methodology, and applications of the *Uniform experimental design*. The uniform experimental design can be regarded as a fractional factorial design with model uncertainty, a space-filling design for computer experiments, a robust design against the model specification, a supersaturated design and can be applied to experiments with mixtures. The book provides necessary knowledge for the reader who is interested in developing theory of the uniform experimental design.

The *experimental design* is extremely useful in multifactor experiments and has played an important role in industry, high tech, sciences and various fields. Experimental design is a branch of statistics with a long history. It involves rich methodologies and various designs. Comprehensive reviews for various kinds of designs can be found in *Handbook of Statistics, Vol. 13*, edited by S. Ghosh and C. R. Rao.

Most of the traditional experimental designs, like fractional factorial designs and optimum designs, have their own statistical models. The model for a factorial plan wants to estimate the main effects of the factors and some interactions among the factors. The optimum design considers a regression model with some unknown parameters to be estimated. However, the experimenter may not know the underlying model in many case studies. How to choose experimental points on the domain when the underlying model is unknown is a challenging problem. The natural idea is to spread experimental points uniformly distributed on the domain. A design that chooses experimental points uniformly scattered on the domain is called *uniform experimental design* or *uniform design* for simplicity. The uniform design was proposed in 1980 by Fang and Wang (Fang 1980; Wang and Fang 1981) and has been widely used for thousands of industrial experiments with model unknown.

Computer experiments are for simulations of physical phenomena which are governed by a set of equations including linear, nonlinear, ordinary, and partial differential equations or by several softwares. There is no analytic formula to describe the phenomena. The so-called space-filling design becomes a key part of computer simulation. In fact, the uniform design is one of the space-filling designs.

Computer experiment is a hot topic in the past decades. It involves two parts: design and modeling. The book focuses on the theory of construction of uniform designs and connections among the uniform design, orthogonal array, combinatorial design, supersaturated design, and experiments with mixtures. There are many useful techniques in the literature, such as polynomial regression models, Kriging models, wavelets, Bayesian approaches, neural networks as well as various methods for variable selection. This book gives a brief introduction to some of these methods; the reader can refer to Fang et al. (2006) for details of these methods.

There are many other space-filling designs among which the Latin hypercube sampling has been widely used. Santner et al. (2003) and Fang et al. (2006) give the details of the Latin hypercube sampling.

The book involves eight chapters. Chapter 1 gives an introduction to various experiments and their models. The reader can easily understand the key idea and method of the uniform experimental design from a demo experiment. Many basic concepts are also reviewed. Chapter 2 concerns with various measures of uniformity and introduces their definitions, computational formula, and properties. Many useful lower bounds are derived. There are two chapters for the construction of uniform designs. Chapter 3 focuses on the deterministic approach while Chap. 4 on numerical optimization approach. Various useful modeling techniques are briefly recommended in Chap. 5. The uniformity has played an important role not only for construction of uniform designs, but also for many other designs such as factorial plans, block designs, and supersaturated designs. Chapters 6 and 7 present a detailed description on the usefulness of the uniformity. Chapter 8 introduces design and modeling for experiments with mixtures.

The book can be used as a textbook for postgraduate level and as a reference book for scientists and engineers who have been implementing experiments often. We have taught partial contents of the book for our undergraduate students and our postgraduate students.

We sincerely thank our coauthors for their significant contribution to the development of the uniform design, who are Profs. Yuan Wang in the Chinese Academy of Science, Fred Hickernell in the Illinois Institute of Technology, Dennis K. J. Lin in the Pennsylvania State University, R. Mukerjee in Indian Institute of Management Calcatta, P. Winker in Justus-Liebig-Universität Giessen, C. X. Ma in the State University of New York at Buffalo, H. Xu in University of California, Los Angeles, and K. Chatterjee in Visva-Bharati University. Many thanks to Profs. Z. H. Yang, R. C. Zhang, J. X. Yin, R. Z. Li, L. Y. Chan, J. X. Pan, R. X. Yue, M. Y. Xie, Y. Tang, G. N. Ge, Y. Z. Liang, E. Liski, G. L. Tian, J. H. Ning, J. F. Yang, F. S. Sun, A. J. Zhang, Z. J. Ou, and A. M. Elsawah for successful collaboration and their encouragement. We particularly thank Prof. K. Chatterjee who spent so much time to read our manuscript and to give valuable useful comments.

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