

## MASTER'S THESIS

### Case studies in computer experiments, applications of uniform design and modern modeling techniques

Ho, Wai Man

*Date of Award:*  
2001

[Link to publication](#)

#### **General rights**

Copyright and intellectual property rights for the publications made accessible in HKBU Scholars are retained by the authors and/or other copyright owners. In addition to the restrictions prescribed by the Copyright Ordinance of Hong Kong, all users and readers must also observe the following terms of use:

- Users may download and print one copy of any publication from HKBU Scholars for the purpose of private study or research
- Users cannot further distribute the material or use it for any profit-making activity or commercial gain
- To share publications in HKBU Scholars with others, users are welcome to freely distribute the permanent URL assigned to the publication

**Case Studies in Computer Experiments,  
Applications of Uniform Design and Modern  
Modeling Techniques**

**HO Wai Man**

A thesis submitted in partial fulfillment of the requirements  
for the degree of  
Master of Philosophy

October 2001

Hong Kong Baptist University

# Abstract

Computer Experiments have been widely used in many areas of scientific research. The purpose of computer experiments is to approximate a complex physical system by a mathematical model in order to understand the output or analyze it more efficiently. Computer experiment consists of two parts, experimental design and modeling. The design is a plan to select data (information) for the system. In the past, many designs such as Latin hypercube and uniform design have been used for computer experiments.

In this thesis, we will consider four methodologies on the modeling of computer experiments, Bayesian method, linear regression method, Sliced inverse regression and principal Hessian directions. We will apply them on computer experiments. The data are collected according to uniform design, Latin hypercube design and orthogonal design. The motivation is to compare the estimating ability of these methodologies on computer experiments which is based on different choice of designs. It was found that the higher level of the design can have the better estimating ability. If two designs have the same level for each factor, we will prefer to use one with better uniformity.

Besides the computer experiments, we will consider the foldover design method on 2 level fractional factorial design. With a suitable choice of foldover plan, we can generate a better resolution design (smaller discrepancy design) with larger number of runs. In this thesis, we will introduce a method to find out the better foldover plan for regular fractional factorial design. Moreover, we will introduce a way to reduce the complexity for searching the best foldover plan on both regular and non-regular fractional factorial design.

# Table of Contents

<b>Declaration</b>	<b>i</b>
<b>Abstract</b>	<b>ii</b>
<b>Acknowledgements</b>	<b>iii</b>
<b>Table of Contents</b>	<b>iv</b>
<b>List of Figures</b>	<b>vi</b>
<b>List of Tables</b>	<b>viii</b>
<b>Chapter 1 Introduction</b>	<b>1</b>
1.1 Computer Experiments . . . . .	1
1.1.1 Goals in Computer Experiments . . . . .	3
1.2 Experimental Design . . . . .	5
1.2.1 Discrepancy . . . . .	7
1.2.2 Construction of Uniform Design . . . . .	9
1.3 Modeling . . . . .	10
1.4 Motivation . . . . .	13
<b>Chapter 2 Bayesian Statistical Method</b>	<b>15</b>
2.1 Prior Distribution . . . . .	16
2.2 Correlation Functions . . . . .	18
2.2.1 Restrictions on $R(\bullet)$ . . . . .	18
2.2.2 Some Choices of Correlation Function . . . . .	18
2.3 Posterior Distribution . . . . .	20

2.4	Optimization . . . . .	22
2.4.1	Sequential Number-Theoretic Method for Optimization . . . . .	22
2.5	Example . . . . .	24
2.6	Discussion . . . . .	26
<b>Chapter 3 Linear Regression Method</b>		<b>28</b>
3.1	Methodology . . . . .	28
3.2	Transformation on Variables . . . . .	29
3.2.1	Transformation on Dependent Variables . . . . .	29
3.2.2	Transformation on Independent Variables . . . . .	31
3.2.3	Transformation on Independent Variables by Graphics . . . . .	34
3.3	Example . . . . .	36
<b>Chapter 4 Dimension Reduction</b>		<b>39</b>
4.1	Sliced Inverse Regression (First Moment Based Methods) . . . . .	40
4.2	Sliced Inverse Regression (Second Moment Based Methods) . . . . .	44
4.3	Principal Hessian Directions . . . . .	47
4.4	Example . . . . .	50
<b>Chapter 5 A Case Study</b>		<b>55</b>
5.1	Use of Bayesian Statistical Method . . . . .	57
5.2	Use of Linear Regression Method . . . . .	59
5.3	Use of Dimension Reduction . . . . .	63
<b>Chapter 6 Model Comparison</b>		<b>70</b>
6.1	Bayesian Statistical Method . . . . .	70
6.2	Linear Regression and Dimensional Method . . . . .	72
6.3	Discussions . . . . .	77
<b>Chapter 7 Conclusions</b>		<b>82</b>
<b>Appendix I. Research Contribution</b>		<b>83</b>
<b>Appendix II. Foldover Orthogonal Design</b>		<b>84</b>
I.	Background . . . . .	84

II. Optimal Foldover Plan . . . . .	87
III. Conclusion . . . . .	90
<b>Appendix III. The Uniform Design <math>U_{10}(10^6)</math></b>	<b>91</b>
<b>Appendix IV. The SAS Result for Simple Linear Model of Robot Arm Problem</b>	<b>92</b>
<b>Appendix V. The C+R Plots of Each Variable for Robot Arm Function</b>	<b>93</b>
<b>Appendix VI. The SAS Result for Final Selected Model of Robot Arm Function</b>	<b>94</b>
<b>Appendix VII. The Uniform Design <math>U_{10}(10^8)</math></b>	<b>95</b>
<b>Appendix VIII. The SAS Result for Simple Linear Model of Borehole Problem</b>	<b>96</b>
<b>Appendix IX. The SAS Result for Final Selected Model of Borehole Problem</b>	<b>97</b>
<b>Bibliography</b>	<b>98</b>
<b>Curriculum Vitae</b>	<b>104</b>