

Contents

Preface	vii
1 Physical Experiments and Computer Experiments	1
1.1 Introduction	1
1.2 Some Examples of Computer Models	3
1.2.1 Evolution of Fires in Enclosed Areas	4
1.2.2 Design of Prosthesis Devices	6
1.2.3 Formation of Pockets in Sheet Metal	8
1.2.4 Other Examples	10
1.3 Organization of the Book	12
2 Preliminaries	15
2.1 Introduction	15
2.2 Defining the Experimental Goal	17
2.2.1 Introduction	17
2.2.2 Research Goals for Homogeneous-Input Codes	17
2.2.3 Research Goals for Mixed-Inputs	19
2.2.4 Experiments with Multiple Outputs	22
2.3 Modeling Output from Computer Experiments	23
2.3.1 Introduction	23
2.3.2 Gaussian Random Function Models	27
2.3.3 The Correlation Function of a Gaussian Random Function Model	31

2.3.4	Using the Correlation Function to Specify a GRF with Given Smoothness Properties	37
2.3.5	Hierarchical Gaussian Random Field Models	45
3	Predicting Output from Computer Experiments	49
3.1	Introduction	49
3.2	Prediction Basics	50
3.2.1	Classes of Predictors	50
3.2.2	Best MSPE Predictors	51
3.2.3	Best Linear Unbiased MSPE Predictors	58
3.3	Prediction for Computer Experiments	61
3.3.1	Prediction When the Correlation Function Is Known	62
3.3.2	Prediction When the Correlation Function Is Unknown	64
3.4	Chapter Notes	82
3.4.1	Proof That (3.2.2182) Is a BLUP (page 57)	
3.4.2	Proof That (3.3.483) Is a BLUP (page 59)	
3.4.3	Implementation Issues	84
3.4.4	Alternate Predictors	86
4	Additional Topics in Prediction Methodology	87
4.1	Predictive Distributions	87
4.1.1	Introduction	87
4.1.2	Predictive Distributions When σ_z^2 , \mathbf{R} , and \mathbf{r}_0 Are Known	88
4.1.3	Predictive Distributions When \mathbf{R} and \mathbf{r}_0 Are Known	94
4.1.4	Prediction Distributions When Correlation Parameters Are Unknown	96
4.2	Prediction for Multiple Response Models	101
4.2.1	Introduction	101
4.2.2	Modeling Multiple Outputs	101
4.2.3	Optimal Predictors for Multiple Outputs	105
4.2.4	Examples	107
4.3	Chapter Notes	116
5	Space-Filling Designs for Computer Experiments	121
5.1	Introduction	121
5.1.1	Some Basic Principles of Experimental Design	121
5.1.2	Design Strategies for Computer Experiments	124
5.2	Designs Based on Methods for Selecting Random Samples	125
5.2.1	Designs Generated by Elementary Methods for Selecting Samples	125
5.2.2	Designs Generated by Latin Hypercube Sampling	127
5.2.3	Properties of Sampling-Based Designs	132
5.2.4	Variations on Latin Hypercube Designs	136
5.3	Designs Based on Measures of Distance	138

5.4	Uniform Designs	141
5.5	Combined Design Criteria	148
5.6	Chapter Notes	151
5.6.1	Details of the Inequality (5.2.2) for Proportional Stratified Sampling with Random Sampling	151
5.6.2	Proof That T_L is Unbiased and of Theorem 5.2.1	153
5.6.3	The Use of LHDs in a Regression Setting	158
5.6.4	Other Space-Filling Designs	159
6	Some Criterion-based Experimental Designs	163
6.1	Introduction	163
6.2	Designs Based on Entropy and Mean Squared Prediction Error Criterion	164
6.2.1	Maximum Entropy Designs	164
6.2.2	Mean Squared Prediction Error Designs	167
6.3	Designs Based on Optimization Criteria	172
6.3.1	Introduction	172
6.3.2	Bernardo Multi-Stage Approximation	172
6.3.3	The Surrogate Management Framework Algorithm	174
6.3.4	Criteria-Based Optimization	177
6.3.5	Heuristic Global Optimization	178
6.3.6	Constrained Global Optimization	185
7	Sensitivity Analysis, Validation, and Other Issues	189
7.1	Sensitivity Analysis	189
7.1.1	Introduction	189
7.1.2	Sensitivity Analyses Based on Scatterplots and Correlations	190
7.1.3	Sensitivity Analyses Based on Regression Modeling	191
7.1.4	Sensitivity Analyses Based on ANOVA-Type Decompositions	193
7.1.5	Summary	198
7.2	Model Validation	199
7.2.1	Introduction	199
7.2.2	Related Problems	201
7.2.3	Assessing Validation	202
A	List of Notation	205
A.1	Abbreviations	205
A.2	Symbols	206
B	Mathematical Facts	209
B.1	The Multivariate Normal Distribution	209
B.2	The Non-Central Student t Distribution	212
B.3	Some Results from Matrix Algebra	213

C PERK: Parametric Empirical Kriging	215
C.1 Introduction	215
C.2 PERK Job File Options and Output	218
C.3 Examples	224
References	251
Author Index	272
Author Index	279