

FRIEDRICH PUKELSHEIM

**OPTIMAL DESIGN
OF EXPERIMENTS**

**WILEY SERIES IN PROBABILITY
AND MATHEMATICAL STATISTICS**

OPTIMAL DESIGN OF EXPERIMENTS

FRIEDRICH PUKELSHEIM

Professor für Stochastik und ihre Anwendungen
Institut für Mathematik der Universität Augsburg
Augsburg, Germany



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Preface

... dans ce meilleur des [modèles] possibles ... tout est au mieux.

Candide (1759), Chapitre I, VOLTAIRE

The working title of the book was a bit long, *Optimality Theory of Experimental Designs in Linear Models*, but focused on two pertinent points. The setting is the *linear model*, the simplest statistical model, where the results are strongest. The topic is *design optimality*, de-emphasizing the issue of design construction. A more detailed *Outline of the Book* follows the Contents.

The design literature is full of fancy nomenclature. In order to circumvent expert jargon I mainly speak of a design ξ being ϕ -optimal for $K'\theta$ in $\tilde{\Xi}$, that is, being optimal under an information function ϕ , for a parameter system of interest $K'\theta$, in a class $\tilde{\Xi}$ of competing designs. The only genuinely new notions that I introduce are *Loewner optimality* (because it refers to the Loewner matrix ordering) and *Kiefer optimality* (because it pays due homage to the man who was a prime contributor to the topic).

The design problems originate from *statistics*, but are solved using special tools from *linear algebra* and *convex analysis*, such as the information matrix mapping of Chapter 3 and the information functions ϕ of Chapter 5. I have refrained from relegating these tools into a set of appendices, at the expense of some slowing of the development in the first half of the book. Instead, the auxiliary material is developed as needed, and it is hoped that the exposition conveys some of the fascination that grows out of merging three otherwise distinct mathematical disciplines.

The result is a *unified optimality theory* that embraces an amazingly wide variety of design problems. My aim is not encyclopedic coverage, but rather to outline typical settings such as D-, A-, and E-optimal polynomial regression designs, Bayes designs, designs for model discrimination, balanced incomplete block designs, or rotatable response surface designs. Pulling together formerly separate entities to build a greater community will always face opponents who fear an assault on their way of thinking. On the contrary, my intention is constructive, to generate a frame for those design problems that share

a common goal. The goal of investigating optimal, theoretical designs is to provide a gauge for identifying efficient, practical designs.

Il meglio è l'inimico del bene.
Dictionnaire Philosophique (1770), Art Dramatique, VOLTAIRE

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The writing of this book became a pleasure when I began experiencing encouragement from so many friends and colleagues, ranging from good advice of how to survive a book project, to the tedious work of weeding out wrong theorems. Above all I would like to thank my Augsburg colleague Norbert Gaffke who, with his vast knowledge of the subject, helped me several times to overcome paralyzing deadlocks. The material of the book called for a number of research projects which I could only resolve by relying on the competence and energy of my co-authors. It is a privilege to have cooperated with Norman Draper, Sabine Rieder, Jim Rosenberger, Bill Studden, and Ben Torsney, whose joint efforts helped shape Chapters 15, 12, 11, 9, 8, respectively.

Over the years, the manuscript has undergone continuous mutations, as a reaction to the suggestions of those who endured the reading of the early drafts. For their constructive criticism I am grateful to Ching-Shui Cheng, Holger Dette, Berthold Heiligers, Harold Henderson, Olaf Krafft, Rudolf Mathar, Wolfgang Näther, Ingram Olkin, Andrej Pázman, Norbert Schmitz, Shayle Searle, and George Styan. The additional chores of locating typos, detecting doubly used notation, and searching for missing definitions was undertaken by Markus Abt, Wolfgang Bischoff, Kenneth Nordström, Ingolf Terveer, and the students of various classes I taught from the manuscript. Their labor turned a manuscript that initially was everywhere dense in error into one which I hope is finally everywhere dense in content.

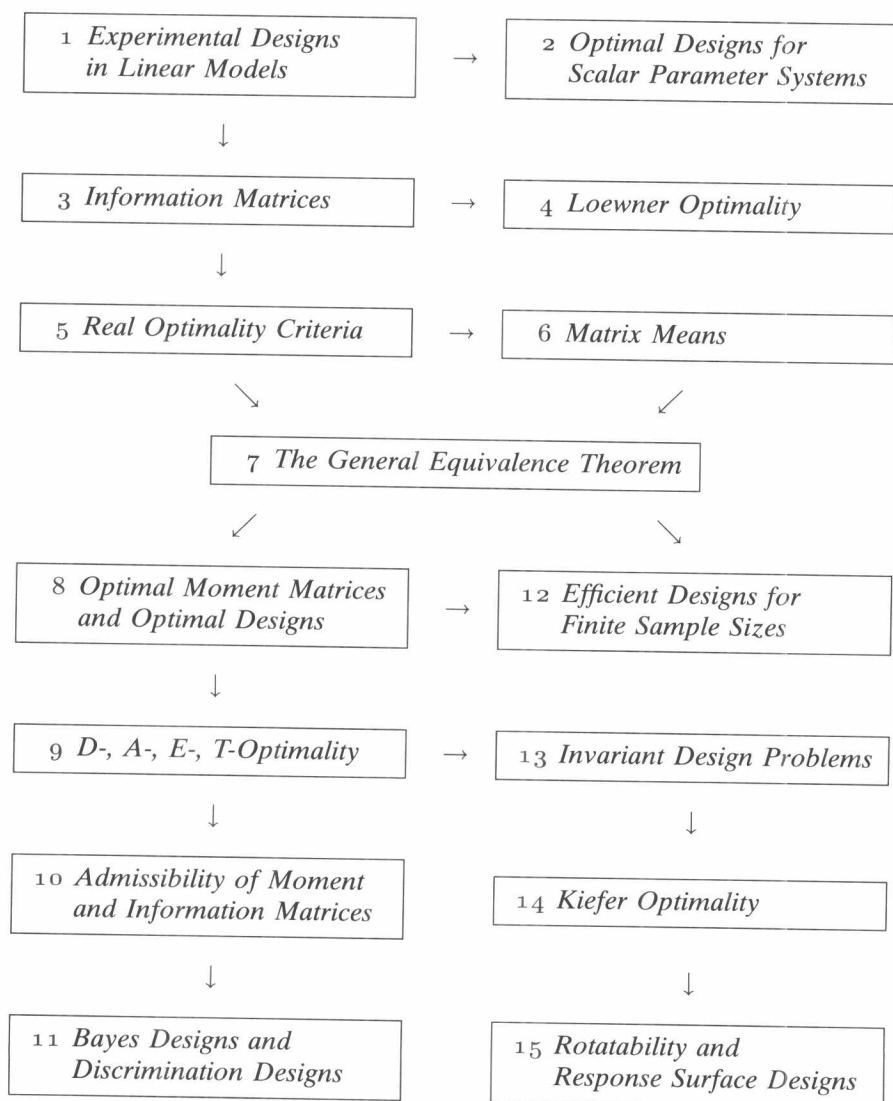
Adalbert Wilhelm carried out most of the calculations for the numerical examples; Inge Dötsch so cheerfully kept retyping what seemed in final form. Ingo Eichenseher and Gerhard Wilhelms contributed the public domain postscript driver *dvilw* to produce the exhibits. Sol Feferman, Timo Mäkeläinen, and Dooley Kiefer kindly provided the photographs of Loewner, Elfving, and Kiefer in the Biographies. To each I owe a debt of gratitude.

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FRIEDRICH PUKELSHEIM

Augsburg, Germany
December 1992

Interdependence of Chapters



Outline of the Book

CHAPTERS 1, 2, 3, 4: LINEAR MODELS AND INFORMATION MATRICES

Chapters 1 and 3 are basic. Chapter 1 centers around the Gauss–Markov Theorem, not only because it justifies the introduction of designs and their moment matrices in Section 1.24. Equally important, it permits us to define in Section 3.2 the information matrix for a parameter system of interest $K'\theta$ in a way that best supports the general theory. The definition is extended to rank deficient coefficient matrices K in Section 3.21. Because of the dual purpose the Gauss–Markov Theorem is formulated as a general result of matrix algebra. First results on optimal designs are presented in Chapter 2, for parameter subsystems that are one-dimensional, and in Chapter 4, in the case where optimality can be achieved relative to the Loewner ordering among information matrices. (This is rare, see Section 4.7.) These results also follow from the General Equivalence Theorem in Chapter 7, whence Chapters 2 and 4 are not needed for their technical details.

CHAPTERS 5, 6: INFORMATION FUNCTIONS

Chapters 5 and 6 are reference chapters, developing the concavity properties of prospective optimality criteria. In Section 5.8, we introduce information functions ϕ , which by definition are required to be positively homogeneous, superadditive, nonnegative, nonconstant, and upper semicontinuous. Information functions submit themselves to pleasing functional operations (Section 5.11), of which polarity (Section 5.12) is crucial for the sequel. The most important class of information functions are the matrix means ϕ_p , with parameter $p \in [-\infty; 1]$. They are the topic of Chapter 6, starting from the classical D-, A-, E-criterion as the special cases ϕ_0 , ϕ_{-1} , $\phi_{-\infty}$, respectively.

CHAPTERS 7, 8, 12: OPTIMAL APPROXIMATE DESIGNS AND EFFICIENT DISCRETE DESIGNS

The General Equivalence Theorem 7.14 is the key result of optimal design theory, offering necessary and sufficient conditions for a design's moment matrix M to be ϕ -optimal for $K'\theta$ in \mathcal{M} . The generic result of this type is due to Kiefer and Wolfowitz (1960), concerning D-optimality for θ in $M(\Xi)$. The present theorem is more general in three respects, in allowing for the competing moment matrices to form a set \mathcal{M} which is compact and convex, rather than restricting attention to the largest possible set $M(\Xi)$ of all moment matrices, in admitting parameter subsystems $K'\theta$, rather than concentrating on the full parameter vector θ , and in permitting as optimality criterion any information function ϕ , rather than restricting attention to the classical D-criterion. Specifying these quantities gives rise to a number of corollaries which are discussed in the second half of Chapter 7. The first half is a self-contained exposition of arguments which lead to a proof of the General Equivalence Theorem, based on subgradients and normal vectors to a convex set. Duality theory of convex analysis might be another starting point; here we obtain a duality theorem as an intermediate step, as Theorem 7.12. Yet another approach would be based on directional derivatives; however, their calculus is quite involved when it comes to handling a composition $\phi \circ C_K$ like the one underlying the optimal design problem.

Chapter 8 deals with the practical consequences which the General Equivalence Theorem implies about the support points x_i and the weights w_i of an optimal design ξ . The theory permits a weight w_i to be any real number between 0 and 1, prescribing the proportion of observations to be drawn under x_i . In contrast, a design for sample size n replaces w_i by an integer n_i , as the replication number for x_i . In Chapter 12 we propose the efficient design apportionment as a systematic and easy way to pass from w_i to n_i . This discretization procedure is the most efficient one, in the sense of Theorem 12.7. For growing sample size n , the efficiency loss relative to the optimal design stays bounded of asymptotic order n^{-1} ; in the case of differentiability, the order improves to n^{-2} .

CHAPTERS 9, 10, 11: INSTANCES OF DESIGN OPTIMALITY

D-, A-, and E-optimal polynomial regression designs over the interval $[-1; 1]$ are characterized and exhibited in Chapter 9. Chapter 10 discusses admissibility of the moment matrix of a polynomial regression design, and of the contrast information matrix of a block design in a two-way classification model. Prominent as these examples may be, it is up to Chapter 11 to exploit the power of the General Equivalence Theorem to its fullest. Various sets of competing moment matrices are considered, such as \mathcal{M}_α for Bayes designs, $M(\Xi[a; b])$ for designs with bounded weights, $\mathcal{M}^{(m)}$ for mix-

ture model designs, $\{(M, \dots, M): M \in \mathcal{M}\}$ for mixture criteria designs, and $\mathcal{M}^{(m)} \cap \{\psi \geq \lambda\}$ for designs with guaranteed efficiencies. And they are evaluated using an information function $\phi = \Phi \circ \psi$ that is a composition of a set of m information functions, $\psi = (\psi_1, \dots, \psi_m)$, together with an information function Φ on the nonnegative orthant \mathbb{R}_+^m .

CHAPTERS 13, 14, 15: OPTIMAL INVARIANT DESIGNS

As with other statistical problems, invariance considerations can be of great help in reducing the dimensionality and complexity of the general design problem, at the expense of handling some additional theoretical concepts. The foundations are laid in Chapter 13, investigating various groups and their actions as they pertain to an experimental domain design τ , a regression range design $\xi = \tau \circ f^{-1}$, a moment matrix $M(\xi)$, an information matrix $C_K(M)$, or an information function $\phi(C)$. The idea of “increased symmetry” or “greater balancedness” is captured by the matrix majorization ordering of Section 14.1. This concept is brought together with the Loewner matrix ordering to create the Kiefer ordering of Section 14.2: An information matrix C is at least as good as another matrix D , $C \gg D$, when relative to the Loewner ordering, C is above some intermediate matrix which is majorized by D . The concept is due to Kiefer (1975) who introduced it in a block design setting and called it *universal optimality*. We demonstrate its usefulness with balanced incomplete block designs (Section 14.9), optimal designs for a linear fit over the unit cube (Section 14.10), and rotatable designs for response surface methodology (Chapter 15).

The final *Comments and References* include historical remarks and mention the relevant literature. I do not claim to have traced every detail to its first contributor and I must admit that the book makes no mention of many other important design topics, such as numerical algorithms, orthogonal arrays, mixture designs, polynomial regression designs on the cube, sequential and adaptive designs, designs for nonlinear models, robust designs, etc.

Contents

1. Experimental Designs in Linear Models	1
1.1. Deterministic Linear Models, 1	
1.2. Statistical Linear Models, 2	
1.3. Classical Linear Models with Moment Assumptions, 3	
1.4. Classical Linear Models with Normality Assumption, 4	
1.5. Two-Way Classification Models, 4	
1.6. Polynomial Fit Models, 6	
1.7. Euclidean Matrix Space, 7	
1.8. Nonnegative Definite Matrices, 9	
1.9. Geometry of the Cone of Nonnegative Definite Matrices, 10	
1.10. The Loewner Ordering of Symmetric Matrices, 11	
1.11. Monotonic Matrix Functions, 12	
1.12. Range and Nullspace of a Matrix, 13	
1.13. Transposition and Orthogonality, 14	
1.14. Square Root Decompositions of a Nonnegative Definite Matrix, 15	
1.15. Distributional Support of Linear Models, 15	
1.16. Generalized Matrix Inversion and Projections, 16	
1.17. Range Inclusion Lemma, 17	
1.18. General Linear Models, 18	
1.19. The Gauss–Markov Theorem, 20	
1.20. The Gauss–Markov Theorem under a Range Inclusion Condition, 21	
1.21. The Gauss–Markov Theorem for the Full Mean Parameter System, 22	
1.22. Projectors, Residual Projectors, and Direct Sum Decomposition, 23	

- 1.23. Optimal Estimators in Classical Linear Models, 24
- 1.24. Experimental Designs and Moment Matrices, 25
- 1.25. Model Matrix versus Design Matrix, 27
- 1.26. Geometry of the Set of All Moment Matrices, 29
- 1.27. Designs for Two-Way Classification Models, 30
- 1.28. Designs for Polynomial Fit Models, 32
 - Exercises, 33

2. Optimal Designs for Scalar Parameter Systems 35

- 2.1. Parameter Systems of Interest and Nuisance Parameters, 35
- 2.2. Estimability of a One-Dimensional Subsystem, 36
- 2.3. Range Summation Lemma, 37
- 2.4. Feasibility Cones, 37
- 2.5. The Ice-Cream Cone, 38
- 2.6. Optimal Estimators under a Given Design, 41
- 2.7. The Design Problem for Scalar Parameter Subsystems, 41
- 2.8. Dimensionality of the Regression Range, 42
- 2.9. Elfving Sets, 43
- 2.10. Cylinders that Include the Elfving Set, 44
- 2.11. Mutual Boundedness Theorem for Scalar Optimality, 45
- 2.12. The Elfving Norm, 47
- 2.13. Supporting Hyperplanes to the Elfving Set, 49
- 2.14. The Elfving Theorem, 50
- 2.15. Projectors for Given Subspaces, 52
- 2.16. Equivalence Theorem for Scalar Optimality, 52
- 2.17. Bounds for the Optimal Variance, 54
- 2.18. Eigenvectors of Optimal Moment Matrices, 56
- 2.19. Optimal Coefficient Vectors for Given Moment Matrices, 56
- 2.20. Line Fit Model, 57
- 2.21. Parabola Fit Model, 58
- 2.22. Trigonometric Fit Models, 58
- 2.23. Convexity of the Optimality Criterion, 59
 - Exercises, 59

3. Information Matrices 61

- 3.1. Subsystems of Interest of the Mean Parameters, 61
- 3.2. Information Matrices for Full Rank Subsystems, 62
- 3.3. Feasibility Cones, 63

- 3.4. Estimability, 64
- 3.5. Gauss–Markov Estimators and Predictors, 65
- 3.6. Testability, 67
- 3.7. F-Test of a Linear Hypothesis, 67
- 3.8. ANOVA, 71
- 3.9. Identifiability, 72
- 3.10. Fisher Information, 72
- 3.11. Component Subsets, 73
- 3.12. Schur Complements, 75
- 3.13. Basic Properties of the Information Matrix Mapping, 76
- 3.14. Range Disjointness Lemma, 79
- 3.15. Rank of Information Matrices, 81
- 3.16. Discontinuity of the Information Matrix Mapping, 82
- 3.17. Joint Solvability of Two Matrix Equations, 85
- 3.18. Iterated Parameter Subsystems, 85
- 3.19. Iterated Information Matrices, 86
- 3.20. Rank Deficient Subsystems, 87
- 3.21. Generalized Information Matrices for Rank Deficient Subsystems, 88
- 3.22. Generalized Inverses of Generalized Information Matrices, 90
- 3.23. Equivalence of Information Ordering and Dispersion Ordering, 91
- 3.24. Properties of Generalized Information Matrices, 92
- 3.25. Contrast Information Matrices in Two-Way Classification Models, 93
- Exercises, 96

4. Loewner Optimality

98

- 4.1. Sets of Competing Moment Matrices, 98
- 4.2. Moment Matrices with Maximum Range and Rank, 99
- 4.3. Maximum Range in Two-Way Classification Models, 99
- 4.4. Loewner Optimality, 101
- 4.5. Dispersion Optimality and Simultaneous Scalar Optimality, 102
- 4.6. General Equivalence Theorem for Loewner Optimality, 103
- 4.7. Nonexistence of Loewner Optimal Designs, 104
- 4.8. Loewner Optimality in Two-Way Classification Models, 105
- 4.9. The Penumbra of the Set of Competing Moment Matrices, 107

- 4.10. Geometry of the Penumbra, 108
- 4.11. Existence Theorem for Scalar Optimality, 109
- 4.12. Supporting Hyperplanes to the Penumbra, 110
- 4.13. General Equivalence Theorem for Scalar Optimality, 111
Exercises, 113

5. Real Optimality Criteria

114

- 5.1. Positive Homogeneity, 114
- 5.2. Superadditivity and Concavity, 115
- 5.3. Strict Superadditivity and Strict Concavity, 116
- 5.4. Nonnegativity and Monotonicity, 117
- 5.5. Positivity and Strict Monotonicity, 118
- 5.6. Real Upper Semicontinuity, 118
- 5.7. Semicontinuity and Regularization, 119
- 5.8. Information Functions, 119
- 5.9. Unit Level Sets, 120
- 5.10. Function–Set Correspondence, 122
- 5.11. Functional Operations, 124
- 5.12. Polar Information Functions and Polar Norms, 125
- 5.13. Polarity Theorem, 127
- 5.14. Compositions with the Information Matrix Mapping, 129
- 5.15. The General Design Problem, 131
- 5.16. Feasibility of Formally Optimal Moment Matrices, 132
- 5.17. Scalar Optimality, Revisited, 133
Exercises, 134

6. Matrix Means

135

- 6.1. Classical Optimality Criteria, 135
- 6.2. D-Criterion, 136
- 6.3. A-Criterion, 137
- 6.4. E-Criterion, 137
- 6.5. T-Criterion, 138
- 6.6. Vector Means, 139
- 6.7. Matrix Means, 140
- 6.8. Diagonality of Symmetric Matrices, 142
- 6.9. Vector Majorization, 144
- 6.10. Inequalities for Vector Majorization, 146
- 6.11. The Hölder Inequality, 147

- 6.12. Polar Matrix Means, 149
- 6.13. Matrix Means as Information Functions and Norms, 151
- 6.14. The General Design Problem with Matrix Means, 152
- 6.15. Orthogonality of Two Nonnegative Definite Matrices, 153
- 6.16. Polarity Equation, 154
- 6.17. Maximization of Information versus Minimization of Variance, 155
- Exercises, 156

7. The General Equivalence Theorem

158

- 7.1. Subgradients and Subdifferentials, 158
- 7.2. Normal Vectors to a Convex Set, 159
- 7.3. Full Rank Reduction, 160
- 7.4. Subgradient Theorem, 162
- 7.5. Subgradients of Isotonic Functions, 163
- 7.6. A Chain Rule Motivation, 164
- 7.7. Decomposition of Subgradients, 165
- 7.8. Decomposition of Subdifferentials, 167
- 7.9. Subgradients of Information Functions, 168
- 7.10. Review of the General Design Problem, 170
- 7.11. Mutual Boundedness Theorem for Information Functions, 171
- 7.12. Duality Theorem, 172
- 7.13. Existence Theorem for Optimal Moment Matrices, 174
- 7.14. The General Equivalence Theorem, 175
- 7.15. General Equivalence Theorem for the Full Parameter Vector, 176
- 7.16. Equivalence Theorem, 176
- 7.17. Equivalence Theorem for the Full Parameter Vector, 177
- 7.18. Merits and Demerits of Equivalence Theorems, 177
- 7.19. General Equivalence Theorem for Matrix Means, 178
- 7.20. Equivalence Theorem for Matrix Means, 180
- 7.21. General Equivalence Theorem for E-Optimality, 180
- 7.22. Equivalence Theorem for E-Optimality, 181
- 7.23. E-Optimality, Scalar Optimality, and Eigenvalue Simplicity, 183
- 7.24. E-Optimality, Scalar Optimality, and Elfving Norm, 183
- Exercises, 185

8. Optimal Moment Matrices and Optimal Designs 187

- 8.1. From Moment Matrices to Designs, 187
- 8.2. Bound for the Support Size of Feasible Designs, 188
- 8.3. Bound for the Support Size of Optimal Designs, 190
- 8.4. Matrix Convexity of Outer Products, 190
- 8.5. Location of the Support Points of Arbitrary Designs, 191
- 8.6. Optimal Designs for a Linear Fit over the Unit Square, 192
- 8.7. Optimal Weights on Linearly Independent Regression Vectors, 195
- 8.8. A-Optimal Weights on Linearly Independent Regression Vectors, 197
- 8.9. C-Optimal Weights on Linearly Independent Regression Vectors, 197
- 8.10. Nonnegative Definiteness of Hadamard Products, 199
- 8.11. Optimal Weights on Given Support Points, 199
- 8.12. Bound for Determinant Optimal Weights, 201
- 8.13. Multiplicity of Optimal Moment Matrices, 201
- 8.14. Multiplicity of Optimal Moment Matrices under Matrix Means, 202
- 8.15. Simultaneous Optimality under Matrix Means, 203
- 8.16. Matrix Mean Optimality for Component Subsets, 203
- 8.17. Moore–Penrose Matrix Inversion, 204
- 8.18. Matrix Mean Optimality for Rank Deficient Subsystems, 205
- 8.19. Matrix Mean Optimality in Two-Way Classification Models, 206
Exercises, 209

9. D-, A-, E-, T-Optimality 210

- 9.1. D-, A-, E-, T-Optimality, 210
- 9.2. G-Criterion, 210
- 9.3. Bound for Global Optimality, 211
- 9.4. The Kiefer–Wolfowitz Theorem, 212
- 9.5. D-Optimal Designs for Polynomial Fit Models, 213
- 9.6. Arcsin Support Designs, 217
- 9.7. Equivalence Theorem for A-Optimality, 221
- 9.8. L-Criterion, 222
- 9.9. A-Optimal Designs for Polynomial Fit Models, 223
- 9.10. Chebyshev Polynomials, 226
- 9.11. Lagrange Polynomials with Arcsin Support Nodes, 227

- 9.12. Scalar Optimality in Polynomial Fit Models, I, 229
- 9.13. E-Optimal Designs for Polynomial Fit Models, 232
- 9.14. Scalar Optimality in Polynomial Fit Models, II, 237
- 9.15. Equivalence Theorem for T-Optimality, 240
- 9.16. Optimal Designs for Trigonometric Fit Models, 241
- 9.17. Optimal Designs under Variation of the Model, 243
Exercises, 245

10. Admissibility of Moment and Information Matrices

247

- 10.1. Admissible Moment Matrices, 247
- 10.2. Support Based Admissibility, 248
- 10.3. Admissibility and Completeness, 248
- 10.4. Positive Polynomials as Quadratic Forms, 249
- 10.5. Loewner Comparison in Polynomial Fit Models, 251
- 10.6. Geometry of the Moment Set, 252
- 10.7. Admissible Designs in Polynomial Fit Models, 253
- 10.8. Strict Monotonicity, Unique Optimality, and Admissibility, 256
- 10.9. E-Optimality and Admissibility, 257
- 10.10. T-Optimality and Admissibility, 258
- 10.11. Matrix Mean Optimality and Admissibility, 260
- 10.12. Admissible Information Matrices, 262
- 10.13. Loewner Comparison of Special C-Matrices, 262
- 10.14. Admissibility of Special C-Matrices, 264
- 10.15. Admissibility, Minimality, and Bayes Designs, 265
Exercises, 266

11. Bayes Designs and Discrimination Designs

268

- 11.1. Bayes Linear Models with Moment Assumptions, 268
- 11.2. Bayes Estimators, 270
- 11.3. Bayes Linear Models with Normal-Gamma Prior Distributions, 272
- 11.4. Normal-Gamma Posterior Distributions, 273
- 11.5. The Bayes Design Problem, 275
- 11.6. General Equivalence Theorem for Bayes Designs, 276
- 11.7. Designs with Protected Runs, 277
- 11.8. General Equivalence Theorem for Designs with Bounded Weights, 278
- 11.9. Second-Degree versus Third-Degree Polynomial Fit Models, I, 280

- 11.10. Mixtures of Models, 283
- 11.11. Mixtures of Information Functions, 285
- 11.12. General Equivalence Theorem for Mixtures of Models, 286
- 11.13. Mixtures of Models Based on Vector Means, 288
- 11.14. Mixtures of Criteria, 289
- 11.15. General Equivalence Theorem for Mixtures of Criteria, 290
- 11.16. Mixtures of Criteria Based on Vector Means, 290
- 11.17. Weightings and Scalings, 292
- 11.18. Second-Degree versus Third-Degree Polynomial Fit Models, II, 293
- 11.19. Designs with Guaranteed Efficiencies, 296
- 11.20. General Equivalence Theorem for Guaranteed Efficiency Designs, 297
- 11.21. Model Discrimination, 298
- 11.22. Second-Degree versus Third-Degree Polynomial Fit Models, III, 299
Exercises, 302

12. Efficient Designs for Finite Sample Sizes

304

- 12.1. Designs for Finite Sample Sizes, 304
- 12.2. Sample Size Monotonicity, 305
- 12.3. Multiplier Methods of Apportionment, 307
- 12.4. Efficient Rounding Procedure, 307
- 12.5. Efficient Design Apportionment, 308
- 12.6. Pairwise Efficiency Bound, 310
- 12.7. Optimal Efficiency Bound, 311
- 12.8. Uniform Efficiency Bounds, 312
- 12.9. Asymptotic Order $O(n^{-1})$, 314
- 12.10. Asymptotic Order $O(n^{-2})$, 315
- 12.11. Subgradient Efficiency Bounds, 317
- 12.12. Apportionment of D-Optimal Designs in Polynomial Fit Models, 320
- 12.13. Minimal Support and Finite Sample Size Optimality, 322
- 12.14. A Sufficient Condition for Completeness, 324
- 12.15. A Sufficient Condition for Finite Sample Size D-Optimality, 325
- 12.16. Finite Sample Size D-Optimal Designs in Polynomial Fit Models, 328
Exercises, 329