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
CONTENTS

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
   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
   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
3.15. 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

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
6.15. 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**

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
8.15. 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**

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
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, Minimaxity, 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  
11.15. 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  
Exercise, 302  

12. Efficient Designs for Finite Sample Sizes  
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  
Models, 320  
12.13. Minimal Support and Finite Sample Size Optimality, 322  
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  
Exercise, 329
### 13. Invariant Design Problems

13.1. Design Problems with Symmetry, 331  
13.2. Invariance of the Experimental Domain, 335  
13.3. Induced Matrix Group on the Regression Range, 336  
13.4. Congruence Transformations of Moment Matrices, 337  
13.5. Congruence Transformations of Information Matrices, 338  
13.6. Invariant Design Problems, 342  
13.7. Invariance of Matrix Means, 343  
13.8. Invariance of the D-Criterion, 344  
13.9. Invariant Symmetric Matrices, 345  
13.10. Subspaces of Invariant Symmetric Matrices, 346  
13.11. The Balancing Operator, 348  
13.12. Simultaneous Matrix Improvement, 349  

Exercises, 350

### 14. Kiefer Optimality

14.1. Matrix Majorization, 352  
14.2. The Kiefer Ordering of Symmetric Matrices, 354  
14.3. Monotonic Matrix Functions, 357  
14.4. Kiefer Optimality, 357  
14.5. Heritability of Invariance, 358  
14.6. Kiefer Optimality and Invariant Loewner Optimality, 360  
14.7. Optimality under Invariant Information Functions, 361  
14.9. Balanced Incomplete Block Designs, 366  
14.10. Optimal Designs for a Linear Fit over the Unit Cube, 372  

Exercises, 379

### 15. Rotatability and Response Surface Designs

15.1. Response Surface Methodology, 381  
15.2. Response Surfaces, 382  
15.3. Information Surfaces and Moment Matrices, 383  
15.4. Rotatable Information Surfaces and Invariant Moment Matrices, 384  
15.5. Rotatability in Multiway Polynomial Fit Models, 384  
15.6. Rotatability Determining Classes of Transformations, 385  
15.7. First-Degree Rotatability, 386  
15.8. Rotatable First-Degree Symmetric Matrices, 387
CONTENTS

15.9. Rotatable First-Degree Moment Matrices, 388
15.10. Kiefer Optimal First-Degree Moment Matrices, 389
15.11. Two-Level Factorial Designs, 390
15.12. Regular Simplex Designs, 391
15.13. Kronecker Products and Vectorization Operator, 392
15.14. Second-Degree Rotatability, 394
15.15. Rotatable Second-Degree Symmetric Matrices, 396
15.16. Rotatable Second-Degree Moment Matrices, 398
15.17. Rotatable Second-Degree Information Surfaces, 400
15.18. Central Composite Designs, 402
15.19. Second-Degree Complete Classes of Designs, 403
15.20. Measures of Rotatability, 405
15.21. Empirical Model-Building, 406
   Exercises, 406

Comments and References

1. Experimental Designs in Linear Models, 408
2. Optimal Designs for Scalar Parameter Systems, 410
3. Information Matrices, 410
4. Loewner Optimality, 412
5. Real Optimality Criteria, 412
6. Matrix Means, 413
7. The General Equivalence Theorem, 414
8. Optimal Moment Matrices and Optimal Designs, 417
9. D-, A-, E-, T-Optimality, 418
10. Admissibility of Moment and Information Matrices, 421
11. Bayes Designs and Discrimination Designs, 422
12. Efficient Designs for Finite Sample Sizes, 424
13. Invariant Design Problems, 425
14. Kiefer Optimality, 426
15. Rotatability and Response Surface Designs, 426

Biographies

2. Gustav Elfving 1908–1984, 430

Bibliography

Index