FRIEDRICH PUKELSHEIM

OPTIMAL DESIGN OF EXPERIMENTS

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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 Ξ*, that is, being optimal under an information function ϕ, for a parameter system of interest $K'\theta$, in a class Ξ 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

ACKNOWLEDGMENTS

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.

Finally I wish to acknowledge the support of the Volkswagen-Stiftung, Hannover, for supporting sabbatical leaves with the Departments of Statistics at Stanford University (1987) and at Penn State University (1990), and granting an *Akademie-Stipendium* to help finish the project.

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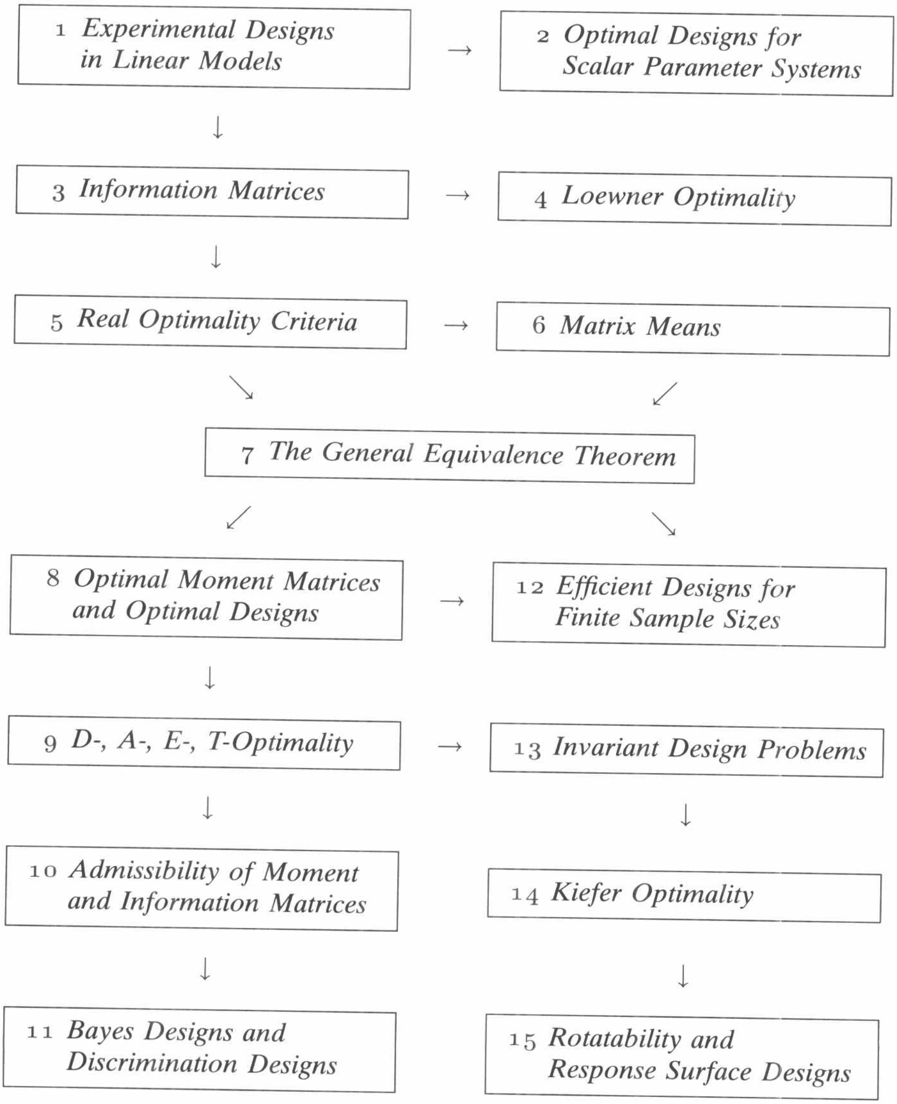
Interdependence of Chapters



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 quantitites 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 $\mathcal{M}_\alpha$ for Bayes designs, $M(\Xi[a;b])$ for designs with bounded weights, $\mathcal{M}^{(m)}$ for mixture model designs, $\{(M, \ldots, M): M \in \mathcal{M}\}$ for mixture criteria designs, and $\mathcal{M}^{(m)} \cap \{\boldsymbol{\psi} \geq \lambda\}$ for designs with guaranteed efficiencies. And they are evaluated using an information function $\phi = \Phi \circ \boldsymbol{\psi}$ that is a composition of a set of m information functions, $\boldsymbol{\psi} = (\psi_1, \ldots, \psi_m)$, 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.

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