

Lecture Notes in Statistics

Volume 212

Series Editors

Peter Bickel

P. J. Diggle

Stephen E. Fienberg

Ursula Gather

Ingram Olkin

Scott Zeger

For further volumes:

<http://www.springer.com/series/694>

Luc Pronzato • Andrej Pázman

Design of Experiments in Nonlinear Models

Asymptotic Normality, Optimality Criteria
and Small-Sample Properties

 Springer

Luc Pronzato
French National Center
for Scientific Research (CNRS)
University of Nice
Sophia Antipolis, France

Andrej Pázman
Department of Applied Mathematics
and Statistics
Comenius University
Bratislava, Slovakia

ISSN 0930-0325

ISBN 978-1-4614-6362-7

ISBN 978-1-4614-6363-4 (eBook)

DOI 10.1007/978-1-4614-6363-4

Springer New York Heidelberg Dordrecht London

Library of Congress Control Number: 2013932292

© Springer Science+Business Media New York 2013

This work is subject to copyright. All rights are reserved by the Publisher, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, reuse of illustrations, recitation, broadcasting, reproduction on microfilms or in any other physical way, and transmission or information storage and retrieval, electronic adaptation, computer software, or by similar or dissimilar methodology now known or hereafter developed. Exempted from this legal reservation are brief excerpts in connection with reviews or scholarly analysis or material supplied specifically for the purpose of being entered and executed on a computer system, for exclusive use by the purchaser of the work. Duplication of this publication or parts thereof is permitted only under the provisions of the Copyright Law of the Publisher's location, in its current version, and permission for use must always be obtained from Springer. Permissions for use may be obtained through RightsLink at the Copyright Clearance Center. Violations are liable to prosecution under the respective Copyright Law.

The use of general descriptive names, registered names, trademarks, service marks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

While the advice and information in this book are believed to be true and accurate at the date of publication, neither the authors nor the editors nor the publisher can accept any legal responsibility for any errors or omissions that may be made. The publisher makes no warranty, express or implied, with respect to the material contained herein.

Printed on acid-free paper

Springer is part of Springer Science+Business Media (www.springer.com)

To Barbara, Lilas, Zélie and Nora,
to Tatiana, Miriam, René, Klára, Kristína, Emma, Filip, David,
and all our friends.

Preface

The final form of this volume differs a lot from our initial project that was born in 2003. Our collaboration that was initiated about 10 years before was then at a pace and we formulated the objective of reviving it through a project that could be conducted over several years (we thought three or four) and could serve as a motivation for maintaining regular exchanges between us. Our initial idea was to write a short monograph that would expose the connections between the asymptotic properties of estimators and experimental design. This corresponds basically to parts which are covered by Chaps. 2–4. The deviation from this initial project was progressive. First, we realized that we had more to say about regression models with heteroscedastic errors than what we expected initially and we found that the investigation of asymptotic normality in the case of singular designs required a rather fundamental revision (Chap. 3). We then quickly agreed that we could not avoid writing a chapter on optimality criteria and optimum experimental design based on asymptotic normality (Chap. 5). Up to that point, the presentation was rather standard, although we gave more emphasis than usual to some particular aspects, like the estimation of a nonlinear function of the model parameters and models with heteroscedastic errors. The results obtained during our collaboration in the 1990s encouraged us to write a chapter on non-asymptotic design approaches (Chap. 6). The motivation for exposing our views on the specific difficulties caused by nonlinear models in LS estimation had always been present in our mind; this project gave us the opportunity to develop and present some of these ideas (Chap. 7). Since this book focused on nonlinear models, having a chapter devoted to the problem raised by the dependency of an optimal experiment on the value of the parameters to be estimated appeared to be essential (Chap. 8). Here some kind of prior for design purposes is unavoidable, with the property that an incorrect prior causes less damage when used for design than for estimation. Finally, we hesitated about indicating or not algorithms for the optimization of the different design criteria that are presented throughout the chapters. This could have led us quite far from the initial project but at the same time was essential for the practical

use of the methods suggested. We reached a compromise solution where all algorithms are gathered in a specific chapter (Chap. 9), where the principles are indicated, in connection with more classical optimization methods. The result is thus much different from what we planned in 2003 and this book covers the following aspects.

Asymptotic Normality. The first three chapters expose the necessary background on asymptotic properties of estimators in nonlinear models. The presentation is mathematically rigorous, with detailed proofs indicated in an appendix to improve readability. The stress here is on deriving asymptotic properties of estimators from properties of the experimental design, in particular the “design measure” which is a basic notion in classical experimental design since the pioneering work of Jack Kiefer in the early 1960s. For nonlinear models, this is not covered in other books on design and considered in a few research papers only; in general, the published proofs of asymptotic properties of estimators require many assumptions of different types, which are usually rather technical and not directly related to the design. Besides that, some results in Chap. 3 are new, e.g., on singular designs and on models with misspecification or with parameterized variance.

Optimality Criteria. The next chapters concern optimum design more directly. Readers only interested in the application of optimal design methodology can possibly start by reading Chap. 5, where the classical theory is presented together with several new aspects and results. The optimality criteria considered in Chap. 5 are related to the asymptotic behavior of estimators. Optimality criteria obtained under non-asymptotic considerations (small-sample situation) are considered in Chap. 6, while Chap. 7 concerns the connection between design and identifiability/estimability issues, including new extensions of some classical optimality criteria. Nonlinear models have the particularity that an optimal design depends on the value of the parameters to be estimated; this is considered in detail in Chap. 8. Once an optimality criterion is chosen, we still need to optimize it; algorithms are presented in Chap. 9 that cover all situations presented in Chaps. 5–8.

Small-sample Properties. The small-sample differential-geometric approach to the subject is considered in Chap. 6; it mainly corresponds to results obtained by the second author in a series of research papers. Chapter 7 contains results on situations when the nonlinearity of the model is such that the estimator can be totally erroneous because of too small a sample at hand. This subject is not much considered in the literature, even in research papers, although it may be of crucial importance in applications.

Several academic friends gave a substantial support through exchanges of different forms; a special mention goes to Radoslav Harman, Werner Müller, Éric Thierry, Henry Wynn, and Anatoly Zhigljavsky. We thank Jean-Pierre Gauchi, Rainer Schwabe, and particularly Henry Wynn, for their help and

encouragement in reviewing our manuscript. Of course all possible mistakes remain ours. Our friends and families gave a remarkable level of support. The first author expresses his deepest thanks to the Bittner clan in St. Peter in der Au (Austria) whose kind hospitality provided a perfect environment for precious periods of intensive work during winter and summer holidays. The second author thanks the I3S Laboratory for the friendly working atmosphere during his many visits at Sophia Antipolis.

A long-term project like this one necessarily involves supports and grants of different sources. In particular, the research of Andrej Pázman has been partly supported by the VEGA grants Nb. 1/3016/06, 1/0077/09, and 2/0038/12. The work of Luc Pronzato was partially supported by the IST Programme of the European Community, under the PASCAL Network of Excellence, IST-2002-506778; he also benefited from invitations by the Isaac Newton Institute for Mathematical Sciences, Cambridge, UK, in summer 2008 and 2011. Andrej Pázman benefited from several invitations from the University of Nice Sophia Antipolis. The institutions of both authors, CNRS for Luc Pronzato and the Comenius University for Andrej Pázman, are gratefully acknowledged for the freedom they allowed through the years.

Sophia Antipolis, France
Bratislava, Slovakia

Luc Pronzato
Andrej Pázman

Contents

1	Introduction	1
1.1	Experiments and Their Designs	1
1.2	Models	3
1.3	Parameters	5
1.4	Information and Design Criteria	6
2	Asymptotic Designs and Uniform Convergence	11
2.1	Asymptotic Designs	11
2.2	Uniform Convergence	16
2.3	Bibliographic Notes and Further Remarks	19
3	Asymptotic Properties of the LS Estimator	21
3.1	Asymptotic Properties of the LS Estimator in Regression Models	21
3.1.1	Consistency	22
3.1.2	Consistency Under a Weaker LS Estimability Condition	25
3.1.3	Asymptotic Normality	29
3.1.4	Asymptotic Normality of a Scalar Function of the LS Estimator	36
3.2	Asymptotic Properties of Functions of the LS Estimator Under Singular Designs	37
3.2.1	Singular Designs in Linear Models	38
3.2.2	Singular Designs in Nonlinear Models	38
3.3	LS Estimation with Parameterized Variance	48
3.3.1	Inconsistency of WLS with Parameter-Dependent Weights	48
3.3.2	Consistency and Asymptotic Normality of Penalized WLS	49
3.3.3	Consistency and Asymptotic Normality of Two-stage LS	53

3.3.4	Consistency and Asymptotic Normality of Iteratively Reweighted LS	56
3.3.5	Misspecification of the Variance Function	57
3.3.6	Different Parameterizations for the Mean and Variance	60
3.3.7	Penalized WLS or Two-Stage LS?	65
3.3.8	Variance Stabilization	69
3.4	LS Estimation with Model Error	70
3.5	LS Estimation with Equality Constraints	74
3.6	Bibliographic Notes and Further Remarks	76
4	Asymptotic Properties of M, ML, and Maximum A Posteriori Estimators	79
4.1	M Estimators in Regression Models	79
4.2	The Maximum Likelihood Estimator	83
4.2.1	Regression Models	84
4.2.2	General Situation	86
4.3	Generalized Linear Models and Exponential Families	89
4.3.1	Models with a One-Dimensional Sufficient Statistic	90
4.3.2	Models with a Multidimensional Sufficient Statistic	92
4.4	The Cramér–Rao Inequality: Efficiency of Estimators	94
4.4.1	Efficiency	94
4.4.2	Asymptotic Efficiency	96
4.5	The Maximum A Posteriori Estimator	98
4.6	Bibliographic Notes and Further Remarks	100
5	Local Optimality Criteria Based on Asymptotic Normality	105
5.1	Design Criteria and Their Properties	108
5.1.1	Ellipsoid of Concentration	108
5.1.2	Classical Design Criteria	109
5.1.3	Positive Homogeneity, Concavity, and Isotonicity	114
5.1.4	Equivalence Between Criteria	115
5.1.5	Concavity and Isotonicity of Classical Criteria	116
5.1.6	Classification into Global and Partial Optimality Criteria	118
5.1.7	The Upper Semicontinuity of the c -Optimality Criterion	119
5.1.8	Efficiency	121
5.1.9	Combining Criteria	123
5.1.10	Design with a Cost Constraint	124
5.2	Derivatives and Conditions for Optimality of Designs	125
5.2.1	Derivatives	125
5.2.2	The Equivalence Theorem	131
5.2.3	Number of Support Points	139
5.2.4	Elfving’s Set and Some Duality Properties	140

5.3	<i>c</i> -Optimum Design in Linearized Nonlinear Models	142
5.3.1	Elfving's Theorem and Related Properties	142
5.3.2	<i>c</i> -Maximin Efficiency and <i>D</i> -Optimality	147
5.3.3	A Duality Property for <i>c</i> -Optimality	148
5.3.4	Equivalence Theorem for <i>c</i> -Optimality	149
5.4	Specific Difficulties with <i>c</i> -Optimum Design in Presence of Nonlinearity	149
5.5	Optimality Criteria for Asymptotic Variance–Covariance Matrices in Product Form	154
5.5.1	The WLS Estimator	154
5.5.2	The Penalized WLS Estimator	156
5.5.3	The LS Estimator with Model Error	157
5.5.4	The M Estimator	159
5.6	Bibliographic Notes and Further Remarks	160
6	Criteria Based on the Small-Sample Precision of the LS Estimator	167
6.1	The Geometry of the Regression Model	168
6.1.1	Basic Notions	168
6.1.2	A Classification of Nonlinear Regression Models	169
6.1.3	Avoiding Failures of LS Estimation	172
6.2	The Probability Density of the LS Estimator in Nonlinear Models with Normal Errors	173
6.2.1	Intrinsically Linear Models	174
6.2.2	Models with $\dim(\theta) = 1$	174
6.2.3	Flat Models	175
6.2.4	Models with Riemannian Curvature Tensor $\mathbf{R}(\theta) \neq 0$	176
6.2.5	Density of the Penalized LS Estimator	176
6.2.6	Marginal Densities of the LS Estimator	177
6.3	Optimality Criteria Based on the p.d.f. of the LS Estimator	178
6.4	Higher-Order Approximations of Optimality Criteria	180
6.4.1	Approximate Bias and Mean-squared Error	182
6.4.2	Approximate Entropy of the p.d.f. of the LS Estimator	183
6.5	Bibliographic Notes and Further Remarks	184
7	Identifiability, Estimability, and Extended Optimality Criteria	187
7.1	Identifiability	188
7.2	LS Estimability of Regression Models	189
7.3	Numerical Issues Related to Estimability in Regression Models	190
7.4	Estimability Function	196
7.4.1	Definition	196
7.4.2	Properties	196

7.4.3	Replications and Design Measures	201
7.4.4	Estimability for Parametric Functions	203
7.5	An Extended Measure of Intrinsic Nonlinearity	207
7.6	Advantages and Drawbacks of Using p -point Designs	211
7.7	Design of Experiments for Improving Estimability	215
7.7.1	Extended (Globalized) E -Optimality	215
7.7.2	Extended (Globalized) c -Optimality	219
7.7.3	Maximum-Entropy Regularization of Estimability Criteria	221
7.7.4	Numerical Examples	222
7.8	Remarks on Estimability for Estimators Other than LS	231
7.9	Bibliographic Notes and Further Remarks	233
8	Nonlocal Optimum Design	235
8.1	Average-Optimum Design	236
8.1.1	Properties	236
8.1.2	A Bayesian Interpretation	238
8.2	Maximin-Optimum Design	244
8.3	Regularization of Maximin Criteria via Average Criteria	248
8.3.1	Regularization via \mathcal{L}_q Norms	248
8.3.2	Maximum-Entropy Regularization	254
8.4	Probability Level and Quantile Criteria	259
8.5	Sequential Design	267
8.5.1	Two-Stage Allocation	268
8.5.2	Full-Sequential D -Optimum Design for LS Estimation in Nonlinear Regression Models	271
9	Algorithms: A Survey	277
9.1	Maximizing a Concave Differentiable Functional of a Probability Measure	277
9.1.1	Vertex-Direction Algorithms	279
9.1.2	Constrained Gradient and Gradient Projection	286
9.1.3	Multiplicative Algorithms	291
9.1.4	D -optimum Design	293
9.2	Exact Design	296
9.2.1	Exchange Methods	298
9.2.2	Branch and Bound	299
9.3	Maximin-Optimum Design	302
9.3.1	Non-Differentiable Optimization of a Design Measure	302
9.3.2	Maximin-Optimum Exact Design	311
9.4	Average-Optimum Design	312
9.4.1	Average-Optimal Design Measures and Stochastic Approximation	312
9.4.2	Average-Optimum Exact Design	313
9.5	Two Methods for Convex Programming	314

9.5.1	Principles for Cutting Strategies and Interior-Point Methods	314
9.5.2	The Ellipsoid Method	315
9.5.3	The Cutting-Plane Method	326
Subdifferentials and Subgradients		335
Computation of Derivatives Through Sensitivity Functions		339
Proofs		343
Symbols and Notation		361
List of Labeled Assumptions		367
References		369
Author Index		389
Subject Index		395