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Design of Experiments in Nonlinear Models

Asymptotic Normality, Optimality Criteria and Small-Sample Properties

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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.

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