Nonlinear Regression

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WILEY-
INTERSCIENCE

A JOHN WILEY & SONS, INC., PUBLICATION

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Published by John Wiley & Sons, Inc., Hoboken, New Jersey.
Published simultaneously in Canada.

Library of Congress Cataloging-in-Publication is available.

ISBN 0-471-47135-6

Printed in the United States of America.

10 9 8 7 6 5 4 3 2 1

Preface

Some years ago one of the authors (G.A.F.S.) asked a number of applied statisticians how they got on with fitting nonlinear models. The answers were generally depressing. In many cases the available computing algorithms for estimation had unsatisfactory convergence properties, sometimes not converging at all, and there was some uncertainty about the validity of the linear approximation used for inference. Furthermore, parameter estimates sometimes had undesirable properties. Fortunately the situation has improved over recent years because of two major developments. Firstly, a number of powerful algorithms for fitting models have appeared. These have been designed to handle "difficult" models and to allow for the various contingencies that can arise in iterative optimization. Secondly, there has been a new appreciation of the role of curvature in nonlinear modeling and its effect on inferential procedures. Curvature comes in a two-piece suite: intrinsic curvature, which relates to the geometry of the nonlinear model, and parameter-effects curvature, which depends on the parametrization of the model. The effects of these curvatures have recently been studied in relation to inference and experimental design. Apart from a couple of earlier papers, all the published literature on the subject has appeared since 1980, and it continues to grow steadily. It has also been recognized that the curvatures can be regarded as quantities called connection coefficients which arise in differential geometry, the latter providing a unifying framework for the study of curvature. Although we have not pursued these abstract concepts in great detail, we hope that our book will at least provide an introduction and make the literature, which we have found difficult, more accessible.

As we take most of our cues for nonlinear modeling from linear models, it is essential that the reader be familiar with the general ideas of linear regression. The main results used are summarized in Appendix D. In this respect our book can be regarded as a companion volume to Seber [1977, 1984], which deal with linear regression analysis and multivariate methods.

We originally began writing this book with the intention of covering a wide range of nonlinear topics. However, we found that in spite of a smaller literature than that of linear regression or multivariate analysis, the subject is difficult and diverse, with many applications. We have therefore had to omit a number of important topics, including nonlinear simultaneous equation systems, generalized linear models (and nonlinear extensions), and stochastic approximation. Also, we have been unable to do full justice to the more theoretical econometric literature with its detailed asymptotics (as in Gallant [1987]), and to the wide range of models in the scientific literature at large.

Because of a paucity of books on nonlinear regression when we began this work, we have endeavored to cover both the applied and theoretical ends of the spectrum and appeal to a wide audience. As well as discussing practical examples, we have tried to make the theoretical literature more available to the reader without being too entangled in detail. Unfortunately, most results tend to be asymptotic or approximate in nature, so that asymptotic expansions tend to dominate in some chapters. This has meant some unevenness in the level of difficulty throughout the book. However, although our book is predominantly theoretical, we hope that the balance of theory and practice will make the book useful from both the teaching and the research point of view. It is not intended to be a practical manual on how to do nonlinear fitting; rather, it considers broad aspects of model building and statistical inference.

One of the irritations of fitting nonlinear models is that model fitting generally requires the iterative optimization (minimization or maximization) of functions. Unfortunately, the iterative process often does not converge easily to the desired solution. The optimization algorithms in widespread use are based upon modifications of and approximations to the Newton(–Raphson) and Gauss–Newton algorithms. In unmodified form both algorithms are unreliable. Computational questions are therefore important in nonlinear regression, and we have devoted three chapters to this area. We introduce the basic algorithms early on, and demonstrate their weaknesses. However, rather than break the flow of statistical ideas, we have postponed a detailed discussion of how these algorithms are made robust until near the end of the book. The computational chapters form a largely self-contained introduction to unconstrained optimization.

In Chapter 1, after discussing the notation, we consider the various types of nonlinear model that can arise. Methods of estimating model parameters are discussed in Chapter 2, and some practical problems relating to estimation, like ill-conditioning, are introduced in Chapter 3. Chapter 4 endeavors to summarize some basic ideas about curvature and to bring to notice the growing literature on the subject. In Chapter 5 we consider asymptotic and exact inferences relating to confidence intervals and regions, and hypothesis testing. The role of curvature is again considered, and some aspects of optimal design close the chapter. Autocorrelated errors are the subject of Chapter 6, and Chapters 7, 8, and 9 describe in depth, three broad families of popular models, namely, growth-curve, compartmental, and change-of-phase and spline-regression models. We have not tried to cover every conceivable model, and our coverage thus complements Ratkowsky's [1988] broader description of families of parametric models. Errors-in-variables models are discussed in detail in Chapter 10 for both explicit and implicit nonlinear models, and nonlinear multivariate models are considered briefly in Chapter 11. Almost by way of an appendix, Chapter 12 gives us a glimpse of some of the basic asymptotic theory, and Chapters 13 to 15 provide an introduction to the growing literature on algorithms for optimization and least squares, together with practical advice on the use of such programs. The book closes with five appendices, an author index, an extensive list of references, and a subject index. Appendix A deals with matrix results, Appendix B gives an introduction to some basic concepts of differential geometry and curvature, Appendix C outlines some theory of stochastic differential equations, Appendix D summarizes linear regression theory, and Appendix E discusses a computational method for handling linear equality constraints. A number of topics throughout the book can be omitted at first reading: these are starred in the text and the contents.

We would like to express our sincere thanks to Mrs. Lois Kennedy and her associates in the secretarial office for typing the difficult manuscript. Thanks go also to Betty Fong for the production of many of the figures. We are grateful to our colleagues and visitors to Auckland for many helpful discussions and suggestions, in particular Alastair Scott, Alan Rogers, Jock MacKay, Peter Phillips, and Ray Carroll. Our thanks also go to Miriam Goldberg, David Hamilton, Dennis Cook, and Douglas Bates for help with some queries in Chapter 4.

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May, 1988

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