Springer Series in Statistics

Springer Science+Business Media, LLC

Springer Series in Statistics

Andersen/Borgan/Gill/Keiding: Statistical Models Based on Counting Processes.
Atkinson/Riani: Robust Diagnostic Regression Analysis.
Berger: Statistical Decision Theory and Bayesian Analysis, 2nd edition.
Borg/Groenen: Modern Multidimensional Scaling: Theory and Applications
Brockwell/Davis: Time Series: Theory and Methods, 2nd edition.
Chan/Tong: Chaos: A Statistical Perspective.
Chen/Shao/Ibrahim: Monte Carlo Methods in Bayesian Computation.
David/Edwards: Annotated Readings in the History of Statistics.
Devroye/Lugosi: Combinatorial Methods in Density Estimation.
Efromovich: Nonparametric Curve Estimation: Methods, Theory, and Applications.
Eggermont/LaRiccia: Maximum Penalized Likelihood Estimation, Volume I: Density Estimation.
Fahrmeir/Tutz: Multivariate Statistical Modelling Based on Generalized Linear Models, 2nd edition.
Fan/Yao: Nonlinear Time Series: Nonparametric and Parametric Methods.
Farebrother: Fitting Linear Relationships: A History of the Calculus of Observations 1750-1900.
Federer: Statistical Design and Analysis for Intercropping Experiments, Volume I: Two Crops.
Federer: Statistical Design and Analysis for Intercropping Experiments, Volume II: Three or More Crops.
Ghosh/Ramamoorthi: Bayesian Nonparametrics.
Glaz/Naus/Wallenstein: Scan Statistics.
Good: Permutation Tests: A Practical Guide to Resampling Methods for Testing Hypotheses, 2nd edition.
Gouriéroux: ARCH Models and Financial Applications.
Gu: Smoothing Spline ANOVA Models.
Györfi/Kohler/Krzyżak/ Walk: A Distribution-Free Theory of Nonparametric Regression.
Haberman: Advanced Statistics, Volume I: Description of Populations.
Hall: The Bootstrap and Edgeworth Expansion.
Härdle: Smoothing Techniques: With Implementation in S.
Harrell: Regression Modeling Strategies: With Applications to Linear Models, Logistic Regression, and Survival Analysis
Hart: Nonparametric Smoothing and Lack-of-Fit Tests.
Hastie/Tibshirani/Friedman: The Elements of Statistical Learning: Data Mining, Inference, and Prediction
Hedayat/Sloane/Stufken: Orthogonal Arrays: Theory and Applications.
Heyde: Quasi-Likelihood and its Application: A General Approach to Optimal Parameter Estimation.
Huet/Bouvier/Gruet/Jolivet: Statistical Tools for Nonlinear Regression: A Practical Guide with S-PLUS and R Examples, 2nd edition.
Ibrahim/Chen/Sinha: Bayesian Survival Analysis.
Jolliffe: Principal Component Analysis.

(continued after index)

Thomas J. Santner
Brian J. Williams
William I. Notz

The Design and Analysis of Computer Experiments

Springer

Thomas J. Santner
Department of Statistics
Ohio State University
1958 Neil Avenue
Columbus, OH 43210
USA
tjs@stat.ohio-state.edu

Brian J. Williams
Department of Statistics
Ohio State University
1958 Neil Avenue
Columbus, OH 43210
USA
brianw@rand.org

William I. Notz
Department of Statistics
Ohio State University
1958 Neil Avenue
Columbus, OH 43210
USA
win@stat.ohio-state.edu

Library of Congress Cataloging-in-Publication Data
Santner, Thomas J., 1947–
Design & analysis of computer experiments / Thomas J. Santner, Brian J. Williams, William I. Notz.
p. cm. — (Springer series in statistics)
Includes bibliographical references and index.

1. Experimental design. 2. Physical sciences—Experiments—Computer simulation. I. Title: Design and analysis of computer experiments. II. Williams, Brian J. III. Notz, William. IV. Title. V. Series.
QA279.S235 2003
519.5—dc21 2003045444
ISBN 978-1-4419-2992-1 ISBN 978-1-4757-3799-8 (eBook)
DOI 10.1007/978-1-4757-3799-8

Originally published by Springer-Verlag New York, Inc. in 2003.

Softcover reprint of the hardcover 1st edition 2003

9 8 7 6 5 4 3 2 1 SPIN 10863256

Typesetting: Pages created by the authors using a Springer LaTeX 2e macro package.

www.springer-ny.com

To Gail, Aparna, and Claudia

for their encouragement and patience

Preface

Many physical processes are difficult or even impossible to study by conventional experimental methods. As computing power has increased, it has become possible to model some of these processes by sophisticated computer code. In such cases, the code can serve as a proxy for the physical process. As in a physical experiment, one can vary the inputs to the code and observe how the process output is affected. Such studies are called computer experiments and are becoming increasingly popular surrogates for and adjuncts to physical experiments.

Much of the methodology for designing, modeling, and analyzing computer experiments can only be found in research papers. Our goal in writing this book is to make these methods accessible to a more general audience. To accomplish this, we have tried to keep the mathematics at a level that will be understandable to readers with Masters level training in Statistics. This has been a challenging task. For example, Gaussian process models are a popular way to describe the output of computer experiments, but Gaussian process models are mathematically complex and likely to be unfamiliar to many readers. We provide an introduction to these models and present references for those who wish to study additional mathematical details of such processes. In other chapters, we relegate mathematical details to notes at the chapter end.

To make the book useful to practitioners, we provide software that can be used to fit the models we discuss in this book. Instructions for how to use this software can be found in Appendix C. Samples of the use of the software are interspersed throughout the book. As the program is updated,

new versions (and the expanded user's manual) will be put on line at the web site listed in Appendix C.

We would like to acknowledge the following people for their contributions in bringing this book to completion. Don Bartel and members of the Biomechanics group at Cornell University and the Hospital for Special Surgery galvanized our initial interest in the area of computer experiments to investigate problems of prosthesis design. Several Ohio State graduate students provided valuable criticism on early drafts and help with the computations including Jeff Lehman, Wei Zhao, Ofelia Marin, and Zhenhuan Cui. John Kimmel provided encouragement throughout the process; several anonymous reviewers gave us constructive suggestions. Antonia Orrantia, Frank Ganz, and Frank McGuckin of Springer Verlag were the production and technical assistance team that brought the work to print. Rob Tibshirani provided a useful perl script that helped automate the compilation of the author index. Joseph Hendrickson of the RAND Corporation allowed us to use several of his programs for estimating main and total effects in the sensitivity analysis of Section 7.1. We want to acknowledge the use of the powerful ACED program of Will Welch in several examples as well as the GNU scientific libraries in our own programs. We would like to thank Jerry Sacks for encouraging our interest in computer experiments. Finally, we wish to express our gratitude to the Statistics Group at the RAND Corporation for support of the second author through core funding provided by James Thomson, President and Chief Executive Officer, and Michael Rich, Executive Vice President of RAND.

Contents