POINTS OF SIGNIFICANCE

Optimal experimental design

Customize the experiment for the setting instead of adjusting the setting to fit a classical design.

Byran Smucker, Martin Krzywinski and Naomi Altman

To maximize the chance for success in an experiment, good experimental design is needed. However, the presence of unique constraints may prevent mapping the experimental scenario onto a classical design. In these cases, we can use optimal design: a powerful, general-purpose tool that offers an attractive alternative to classical design and provides a framework within which to obtain high-quality, statistically grounded designs under nonstandard conditions. It can flexibly accommodate constraints, is connected to statistical quantities of interest and often mimics intuitive classical designs.

For example, suppose we wish to test the effects of a drug's concentration in the range 0–100 ng/ml on the growth of cells. The cells will be grown with the drug in test tubes, arranged on a rack with four shelves. Our goal may be to determine whether the drug has an effect and precisely estimate the effect size or to identify the concentration at which the response is optimal. We will address both by finding designs that are optimal for regression parameter estimation as well as designs optimal for prediction precision.

To illustrate how constraints may influence our design, suppose that the shelves receive different amounts of light, which might lead to systematic variation between shelves. The shelf would therefore be a natural block. Since we don't expect such systematic variation within a shelf, the order of tubes on a shelf can be randomized. Furthermore, each shelf can only hold nine test tubes. The experimental design question, then, is: What should be the drug concentration in each of the 36 tubes?

If concentration were a categorical factor, we could compare the mean response at nine concentrations—a traditional randomized complete block design (RCBD). However, because concentration is actually continuous, discrete levels unduly limit which concentrations are studied and reduce our ability to detect an effect and estimate the concentration that produces an optimal response. Classical designs, like full factorials or RCBDs, assume an ideal and simple experimental setup, which may be inappropriate for all experimental goals or untenable in the presence of constraints.

Optimal design provides a principled approach to accommodating the entire range of concentrations and making full use of each shelf's capacity. It can incorporate a variety of constraints such as sample size restrictions (e.g., the lab has a limited supply of test tubes), awkward blocking structures (e.g., shelves have different capacities) or disallowed treatment combinations (e.g., certain combinations of factor levels may be infeasible or otherwise undesirable).

To assist in describing optimal design, let's review some terminology. The drug is a 'factor', and particular concentrations are 'levels'. A particular combination of factor levels is a 'treatment' (with just a single factor, a treatment is simply a factor level) applied to an 'experimental unit', which is a test tube. The shelves are 'blocks', which are collections of experimental units that are similar in traits (e.g., light level) that might affect the experimental outcome. The possible set of treatments that could be chosen is the 'design space'. A 'run' is the execution of a single experimental unit, and the 'sample size' is the number of runs in the experiment.

Optimal design optimizes a numerical criterion, which typically relates to the variance or other statistically relevant properties of the design, and uses as input the number of runs, the factors and their possible levels, block structure (if any), and a hypothesized form of the relationship between the response and the factors. Two of the most common criteria are the D-criterion and the I-criterion. They are fundamentally different: the D-criterion relates to the variance of factor effects, and the I-criterion addresses the precision of predictions.

To understand the D-criterion (determinant), suppose we have a quadratic regression model with parameters β_1 and β_2 that relate the factor to the response (for simplicity, ignore β_0, the intercept). Our estimates of these parameters, $\hat{\beta}_1$ and $\hat{\beta}_2$, will have error and, assuming the model error variance is known, the D-optimal design minimizes the area of the ellipse that defines the joint confidence interval for the parameters (Fig. 1). This area will include the true values of both β_1 and β_2 in 95% (or some other desired proportion) of repeated
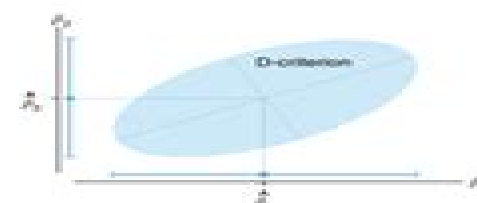

Fig. 1 | The confidence ellipse of a regression model with two parameters, β_1 and β_2. The ellipse can be projected onto each axis to obtain the familiar one-dimensional confidence intervals for each parameter (shown as blue points with error bars). The D-criterion reduces the variance of the parameter estimates and/or the correlation between the estimates by minimizing the area of the ellipse.

executions of the design, and its size and shape are a function of the data's overall variance and the design.

On the other hand, the I-criterion (integrated variance) is used when the experimental goal is to make precise predictions of the response, rather than to obtain precise estimates of the model parameters. An I-optimal design chooses the set of runs to minimize the average variance in prediction across the joint range of the factors. The prediction variance is a function of several elements: the data's overall error variance, the factor levels at which we are predicting, and also the design itself. This criterion is more complicated mathematically because it involves integration.

For both criteria, numerical heuristics are used in the optimization but they do not guarantee a global optimum. For most scenarios, however, near-optimal designs are adequate and not hard to obtain.

Returning to our example, suppose we wish to obtain a precise estimate of our drug's effect on the mean response. If we expect that the effect is linear (our model has one parameter of interest, β_1, which is the slope), the D-optimal design places either four or five experimental units in each block at the low level (0 ng/ml) and the

Foundations Of Optimum Experimental Design Mathematics And Its Applications

Rainer Schwabe

Foundations Of Optimum Experimental Design Mathematics And Its Applications:

Artificial Neural Networks – ICANN 2009 Cesare Alippi,Marios M. Polycarpou,Christos Panayiotou,Georgios Ellinas,2009-09-16 This volume is part of the two volume proceedings of the 19th International Conf ence on Artificial Neural Networks ICANN 2009 which was held in Cyprus during September 14 17 2009 The ICANN conference is an annual meeting sp sored by the European Neural Network Society ENNS in cooperation with the ternational Neural Network Society INNS and the Japanese Neural Network Society JNNS ICANN 2009 was technically sponsored by the IEEE Computational Intel gence Society This series of conferences has been held annually since 1991 in various European countries and covers the field of neurocomputing learning systems and related areas Artificial neural networks provide an information processing structure inspired by biological nervous systems They consist of a large number of highly interconnected processing elements with the capability of learning by example The field of artificial neural networks has evolved significantly in the last two decades with active partici tion from diverse fields such as engineering computer science mathematics artificial intelligence system theory biology operations research and neuroscience Artificial neural networks have been widely applied for pattern recognition control optimization image processing classification signal processing etc *Applications of Linear and Nonlinear Models* Erik Grafarend,Joseph L. Awange,2012-08-15 Here we present a nearly complete treatment of the Grand Universe of linear and weakly nonlinear regression models within the first 8 chapters Our point of view is both an algebraic view as well as a stochastic one For example there is an equivalent lemma between a best linear uniformly unbiased estimation BLUUE in a Gauss Markov model and a least squares solution LESS in a system of linear equations While BLUUE is a stochastic regression model LESS is an algebraic solution In the first six chapters we concentrate on underdetermined and overdeterimined linear systems as well as systems with a datum defect We review estimators algebraic solutions of type MINOLESS BLIMBE BLUMBE BLUUE BIQUE BLE BIQUE and Total Least Squares The highlight is the simultaneous determination of the first moment and the second central moment of a probability distribution in an inhomogeneous multilinear estimation by the so called E D correspondence as well as its Bayes design In addition we discuss continuous networks versus discrete networks use of Grassmann Pluecker coordinates criterion matrices of type Taylor Karman as well as FUZZY sets Chapter seven is a speciality in the treatment of an overdetermined system of nonlinear equations on curved manifolds The von Mises Fisher distribution is characteristic for circular or hyper spherical data Our last chapter eight is devoted to probabilistic regression the special Gauss Markov model with random effects leading to estimators of type BLIP and VIP including Bayesian estimation A great part of the work is presented in four Appendices Appendix A is a treatment of tensor algebra namely linear algebra matrix algebra and multilinear algebra Appendix B is devoted to sampling distributions and their use in terms of confidence intervals and confidence regions Appendix C reviews the elementary notions of statistics namely random events and stochastic processes Appendix D introduces the basics of

Groebner basis algebra its careful definition the Buchberger Algorithm especially the C F Gauss combinatorial algorithm

   Model Based Parameter Estimation Hans Georg Bock,Thomas Carraro,Willi Jäger,Stefan Körkel,Rolf Rannacher,Johannes P. Schlöder,2013-02-26 This judicious selection of articles combines mathematical and numerical methods to apply parameter estimation and optimum experimental design in a range of contexts These include fields as diverse as biology medicine chemistry environmental physics image processing and computer vision The material chosen was presented at a multidisciplinary workshop on parameter estimation held in 2009 in Heidelberg The contributions show how indispensable efficient methods of applied mathematics and computer based modeling can be to enhancing the quality of interdisciplinary research The use of scientific computing to model simulate and optimize complex processes has become a standard methodology in many scientific fields as well as in industry Demonstrating that the use of state of the art optimization techniques in a number of research areas has much potential for improvement this book provides advanced numerical methods and the very latest results for the applications under consideration   *Artificial Neural Networks for the Modelling and Fault Diagnosis of Technical Processes* Krzysztof Patan,2008-06-24 An unappealing characteristic of all real world systems is the fact that they are vulnerable to faults malfunctions and more generally unexpected modes of haviour This explains why there is a continuous need for reliable and universal monitoring systems based on suitable and e ective fault diagnosis strategies This is especially true for engineering systems whose complexity is permanently growing due to the inevitable development of modern industry as well as the information and communication technology revolution Indeed the design and operation of engineering systems require an increased attention with respect to availability reliability safety and fault tolerance Thus it is natural that fault diagnosis plays a fundamental role in modern control theory and practice This is re ected in plenty of papers on fault diagnosis in many control oriented c ferencesand journals Indeed a largeamount of knowledgeon model basedfault diagnosis has been accumulated through scienti c literature since the beginning of the 1970s As a result a wide spectrum of fault diagnosis techniques have been developed A major category of fault diagnosis techniques is the model based one where an analytical model of the plant to be monitored is assumed to be available   **Optimal Sensor Networks Scheduling in Identification of Distributed Parameter Systems** Maciej Patan,2012-02-23 Sensor networks have recently come into prominence because they hold the potential to revolutionize a wide spectrum of both civilian and military applications An ingenious characteristic of sensor networks is the distributed nature of data acquisition Therefore they seem to be ideally prepared for the task of monitoring processes with spatio temporal dynamics which constitute one of most general and important classes of systems in modelling of the real world phenomena It is clear that careful deployment and activation of sensor nodes are critical for collecting the most valuable information from the observed environment Optimal Sensor Network Scheduling in Identification of Distributed Parameter Systems discusses the characteristic features of the sensor scheduling problem analyzes classical and recent approaches and proposes a wide range

of original solutions especially dedicated for networks with mobile and scanning nodes Both researchers and practitioners will find the case studies the proposed algorithms and the numerical examples to be invaluable *Model Calibration and Parameter Estimation* Ne-Zheng Sun,Alexander Sun,2015-07-01 This three part book provides a comprehensive and systematic introduction to these challenging topics such as model calibration parameter estimation reliability assessment and data collection design Part 1 covers the classical inverse problem for parameter estimation in both deterministic and statistical frameworks Part 2 is dedicated to system identification hyperparameter estimation and model dimension reduction and Part 3 considers how to collect data and construct reliable models for prediction and decision making For the first time topics such as multiscale inversion stochastic field parameterization level set method machine learning global sensitivity analysis data assimilation model uncertainty quantification robust design and goal oriented modeling are systematically described and summarized in a single book from the perspective of model inversion and elucidated with numerical examples from environmental and water resources modeling Readers of this book will not only learn basic concepts and methods for simple parameter estimation but also get familiar with advanced methods for modeling complex systems Algorithms for mathematical tools used in this book such as numerical optimization automatic differentiation adaptive parameterization hierarchical Bayesian metamodeling Markov chain Monte Carlo are covered in details This book can be used as a reference for graduate and upper level undergraduate students majoring in environmental engineering hydrology and geosciences It also serves as an essential reference book for professionals such as petroleum engineers mining engineers chemists mechanical engineers biologists biology and medical engineering applied mathematicians and others who perform mathematical modeling **Handbook of Design and Analysis of Experiments** Angela Dean,Max Morris,John Stufken,Derek Bingham,2015-06-26 This carefully edited collection synthesizes the state of the art in the theory and applications of designed experiments and their analyses It provides a detailed overview of the tools required for the optimal design of experiments and their analyses The handbook covers many recent advances in the field including designs for nonlinear models and algorithms applicable to a wide variety of design problems It also explores the extensive use of experimental designs in marketing the pharmaceutical industry engineering and other areas *Handling Uncertainty and Networked Structure in Robot Control* Lucian Bușoniu,Levente Tamás,2016-02-06 This book focuses on two challenges posed in robot control by the increasing adoption of robots in the everyday human environment uncertainty and networked communication Part I of the book describes learning control to address environmental uncertainty Part II discusses state estimation active sensing and complex scenario perception to tackle sensing uncertainty Part III completes the book with control of networked robots and multi robot teams Each chapter features in depth technical coverage and case studies highlighting the applicability of the techniques with real robots or in simulation Platforms include mobile ground aerial and underwater robots as well as humanoid robots and robot arms Source code and experimental data are available at http extras

springer com The text gathers contributions from academic and industry experts and offers a valuable resource for researchers or graduate students in robot control and perception It also benefits researchers in related areas such as computer vision nonlinear and learning control and multi agent systems **Collecting Spatial Data** Werner G. Müller,2007-08-17 The book is concerned with the statistical theory for locating spatial sensors It bridges the gap between spatial statistics and optimum design theory After introductions to those two fields the topics of exploratory designs and designs for spatial trend and variogram estimation are treated Special attention is devoted to describing new methodologies to cope with the problem of correlated observations *Functional Approach to Optimal Experimental Design* Viatcheslav B. Melas,2006-04-20 The present book is devoted to studying optimal experimental designs for a wide class of linear and nonlinear regression models This class includes polynomial trigonometrical rational and exponential models as well as many particular models used in ecology and microbiology As the criteria of optimality the well known D E and c criteria are implemented The main idea of the book is to study the dependence of optimal signs on values of unknown parameters and on the bounds of the design interval Such a study can be performed on the base of the Implicit Fu tion Theorem the classical result of functional analysis The idea was rst introduced in the author s paper Melas 1978 for nonlinear in parameters exponential models Recently it was developed for other models in a n ber of works Melas 1995 2000 2001 2004 2005 Dette Melas 2002 2003 Dette Melas Pepelyshev 2002 2003 2004b and Dette Melas Biederman 2002 Thepurposeofthepresentbookistobringtogethertheresultsobtained and to develop further underlying concepts and tools The approach m tioned above will be called the functional approach Its brief description can be found in the Introduction The book contains eight chapters The rst chapter introduces basic concepts and results of optimal design theory initiated mainly by J Kiefer **Optimum Designs for Multi-Factor Models** Rainer Schwabe,2012-12-06 In real applications most experimental situations are influenced by a large number of different factors In these settings the design of an experiment leads to challenging optimization problems even if the underlying relationship can be described by a linear model Based on recent research this book introduces the theory of optimum designs for complex models and develops general methods of reduction to marginal problems for large classes of models with relevant interaction structures **Semidistributive Modules and Rings** A.A. Tuganbaev,2012-12-06 A module M is called distributive if the lattice Lat M of all its submodules is distributive i e Fn G H FnG FnH for all submodules F G and H of the module M A module M is called uniserial if all its submodules are comparable with respect to inclusion i e the lattice Lat M is a chain Any direct sum of distributive resp uniserial modules is called a semidistributive resp serial module The class of distributive resp semidistributive modules properly cont ains the class ofall uniserial resp serial modules In particular all simple resp semisimple modules are distributive resp semidistributive All strongly regular rings for example all factor rings of direct products of division rings and all commutative regular rings are distributive all valuation rings in division rings and all commutative Dedekind rings e g

rings of integral algebraic numbers or commutative principal ideal rings are distributive A module is called a Bezout module or a locally cyclic module ifevery finitely generated submodule is cyclic If all maximal right ideals of a ring A are ideals e g if A is commutative then all Bezout A modules are distributive   Applications of Lie Algebras to Hyperbolic and Stochastic Differential Equations Constantin Vârsan,2012-12-06 The main part of the book is based on a one semester graduate course for students in mathematics I have attempted to develop the theory of hyperbolic systems of differen tial equations in a systematic way making as much use as possible ofgradient systems and their algebraic representation However despite the strong sim ilarities between the development of ideas here and that found in a Lie alge bras course this is not a book on Lie algebras The order of presentation has been determined mainly by taking into account that algebraic representation and homomorphism correspondence with a full rank Lie algebra are the basic tools which require a detailed presentation I am aware that the inclusion of the material on algebraic and homomorphism correspondence with a full rank Lie algebra is not standard in courses on the application of Lie algebras to hyperbolic equations I think it should be Moreover the Lie algebraic structure plays an important role in integral representation for solutions of nonlinear control systems and stochastic differential equations yelding results that look quite different in their original setting Finite dimensional nonlin ear filters for stochastic differential equations and say decomposability of a nonlinear control system receive a common understanding in this framework   Recent Advances in Statistics and Probability J. P. Vilaplana,M. N. Puri,2020-05-18 No detailed description available for Recent Advances in Statistics and Probability   *Recent Advances in Experimental Designs and Related Topics* Stan Altan,Jagbir Singh,2001 Researchers in all disciplines are becoming increasingly aware of the importance of experimental designs and statistical methods in their investigations Use of a sound experimental design is crucial to ensure reliability of data and subsequent findings from a study That is why a design for collecting date is at the core of Statistics Professor Damaraju Raghavarao has made fundamental contributions to both the theory and application of the Design of Experiments This book is dedicated to him and consists of twelve papers on recent developments on different topics in the area of Design of Experiments by distinguished researchers   *Clifford Algebras and Spinor Structures* Rafal Ablamowicz,P. Lounesto,2013-06-29 This volume is dedicated to the memory of Albert Crumeyrolle who died on June 17 1992 In organizing the volume we gave priority to articles summarizing Crumeyrolle s own work in differential geometry general relativity and spinors articles which give the reader an idea of the depth and breadth of Crumeyrolle s research interests and influence in the field articles of high scientific quality which would be of general interest In each of the areas to which Crumeyrolle made significant contribution Clifford and exterior algebras Weyl and pure spinors spin structures on manifolds principle of triality conformal geometry there has been substantial progress Our hope is that the volume conveys the originality of Crumeyrolle s own work the continuing vitality of the field he influenced and the enduring respect for and tribute to him and his accomplishments in the mathematical community It isour pleasure to thank Peter Morgan Artibano

Micali Joseph Grifone Marie Crumeyrolle and Kluwer Academic Publishers for their help in preparingthis volume **Abelian Groups and Modules** Alberto Facchini,Claudia Menini,2012-12-06 On the 26th of November 1992 the organizing committee gathered together at Luigi Salce s invitation for the first time The tradition of abelian groups and modules Italian conferences Rome 77 Udine 85 Bressanone 90 needed to be kept up by one more meeting Since that first time it was clear to us that our goal was not so easy In fact the main intended topics of abelian groups modules over commutative rings and non commutative rings have become so specialized in the last years that it looked really ambitious to fit them into only one meeting Anyway since everyone of us shared the same mathematical roots we did want to emphasize a common link So we elaborated the long symposium schedule three days of abelian groups and three days of modules over non commutative rings with a two days bridge of commutative algebra in between Many of the most famous names in these fields took part to the meeting Over 140 participants both attending and contributing the 18 Main Lectures and 64 Communications see list on page xv provided a really wide audience for an Algebra meeting Now that the meeting is over we can say that our initial feeling was right PROBABILITY AND STATISTICS - Volume III Reinhard Viertl ,2009-06-11 Probability and Statistics theme is a component of Encyclopedia of Mathematical Sciences in the global Encyclopedia of Life Support Systems EOLSS which is an integrated compendium of twenty one Encyclopedias The Theme with contributions from distinguished experts in the field discusses Probability and Statistics Probability is a standard mathematical concept to describe stochastic uncertainty Probability and Statistics can be considered as the two sides of a coin They consist of methods for modeling uncertainty and measuring real phenomena Today many important political health and economic decisions are based on statistics This theme is structured in five main topics Probability and Statistics Probability Theory Stochastic Processes and Random Fields Probabilistic Models and Methods Foundations of Statistics which are then expanded into multiple subtopics each as a chapter These three volumes are aimed at the following five major target audiences University and College students Educators Professional practitioners Research personnel and Policy analysts managers and decision makers and NGOs Parallel Processing and Applied Mathematics Roman Wyrzykowski,Jack Dongarra,Marcin Paprzycki,Jerzy Wasniewski,2003-08-01 This book constitutes the thoroughly refereed post proceedings of the 4th International Conference on Parallel Processing and Applied Mathematics PPAM 2002 held in Naleczow Poland in September 2001 The 101 papers presented were carefully reviewed and improved during two rounds of reviewing and revision The book offers topical sections on distributed and grid architectures scheduling and load balancing performance analysis and prediction parallel non numerical algorithms parallel programming tools and environments parallel numerical algorithms applications and evolutionary computing and neural networks **Gaussian Random Functions** M.A. Lifshits,2013-03-09 It is well known that the normal distribution is the most pleasant one can even say an exemplary object in the probability theory It combines almost all conceivable nice properties that a distribution may ever have symmetry stability indecomposability a regular tail

behavior etc Gaussian measures the distributions of Gaussian random functions as infinite dimensional analogues of tht

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Table of Contents Foundations Of Optimum Experimental Design Mathematics And Its Applications

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