

Scientific Computing and Automation (Europe) 1990



Scientific Computing And Automation Europe 1990 Data Handling In Science And Technology Volume 6

I.E. Frank, Roberto Todeschini



Scientific Computing And Automation Europe 1990 Data Handling In Science And Technology Volume 6:

Scientific Computing and Automation (Europe) 1990 E.J. Karjalainen, 1990-12-17 This book comprises a large selection of papers presented at the second European Scientific Computing and Automation meeting SCA 90 Europe which was held in June 1990 in Maastricht The Netherlands The increasing use of computers for making measurements interpreting data and filing results brings a new unity to science SCA concentrates on common computer based tools which are useful in several disciplines Practical problems in laboratory automation robotics and information management with LIMS are covered in depth The process of designing and acquiring a LIMS is described and standards for data transfer between instruments between LIMS and instruments and between different LIMS are discussed The applications of statistics and expert systems are covered in several chapters Strategies for drug design are discussed with various practical examples Finally the display of scientific results as images and computer based animations is demonstrated by several examples with their color illustrations The book should be of interest to those managing R D projects doing research in laboratories acquiring or planning LIMS designing instruments and laboratory automation systems and those involved in data analysis of scientific results

Robustness of Analytical Chemical Methods and Pharmaceutical Technological Products M.M.W.B. Hendriks, J.H. de Boer, A.K. Smilde, 1996-12-11 In analytical chemistry and pharmaceutical technology attention is increasingly focussed on improving the quality of methods and products This book aims at fostering the awareness of the potential of existing mathematical and statistical methods to improve this quality It provides procedures and ideas on how to make a product or a method less sensitive to small variations in influencing factors Major issues covered are robustness and stability improvement and ruggedness testing General strategies and a theoretical introduction to these methods are described and thorough overviews of methods used in both application areas and descriptions of practical applications are given Features of this book Gives a good overview of mathematical and statistical methods used in two application areas i e pharmaceutical technology and analytical chemistry Illustrates the different approaches available to attain robustness Gives ideas on how to use methods in practical situations The book is intended for those who develop and optimize and are responsible for the overall quality of analytical methods and pharmaceutical technological products and procedures

Handbook of Chemometrics and Qualimetrics, 1997-12-12 Handbook of Chemometrics and Qualimetrics *The Data Analysis Handbook* I.E. Frank, Roberto Todeschini, 1994-09-30 Analyzing observed or measured data is an important step in applied sciences The recent increase in computer capacity has resulted in a revolution both in data collection and data analysis An increasing number of scientists researchers and students are venturing into statistical data analysis hence the need for more guidance in this field which was previously dominated mainly by statisticians This handbook fills the gap in the range of textbooks on data analysis Written in a dictionary format it will serve as a comprehensive reference book in a rapidly growing field However this book is more structured than an ordinary dictionary where each entry is a separate self contained

entity The authors provide not only definitions and short descriptions but also offer an overview of the different topics Therefore the handbook can also be used as a companion to textbooks for undergraduate or graduate courses 1700 entries are given in alphabetical order grouped into 20 topics and each topic is organized in a hierarchical fashion Additional specific entries on a topic can be easily found by following the cross references in a top down manner Several figures and tables are provided to enhance the comprehension of the topics and a list of acronyms helps to locate the full terminologies The bibliography offers suggestions for further reading

Practical Data Analysis in Chemistry Marcel

Maeder,Yorck-Michael Neuhold,2007-08-10 The majority of modern instruments are computerised and provide incredible amounts of data Methods that take advantage of the flood of data are now available importantly they do not emulate graph paper analyses on the computer Modern computational methods are able to give us insights into data but analysis or data fitting in chemistry requires the quantitative understanding of chemical processes The results of this analysis allows the modelling and prediction of processes under new conditions therefore saving on extensive experimentation Practical Data Analysis in Chemistry exemplifies every aspect of theory applicable to data analysis using a short program in a Matlab or Excel spreadsheet enabling the reader to study the programs play with them and observe what happens Suitable data are generated for each example in short routines this ensuring a clear understanding of the data structure Chapter 2 includes a brief introduction to matrix algebra and its implementation in Matlab and Excel while Chapter 3 covers the theory required for the modelling of chemical processes This is followed by an introduction to linear and non linear least squares fitting each demonstrated with typical applications Finally Chapter 5 comprises a collection of several methods for model free data analyses Includes a solid introduction to the simulation of equilibrium processes and the simulation of complex kinetic processes Provides examples of routines that are easily adapted to the processes investigated by the reader Model based analysis linear and non linear regression and model free analysis are covered

Methods for Experimental Design J.L.

Goupy,1993-05-05 A method for organizing and conducting scientific experiments is described in this volume which enables experimenters to reduce the number of trials run while retaining all the parameters that may influence the result The choice of ideal experiments is based on mathematical concepts but the author adopts a practical approach and uses theory only when necessary Written for experimenters by an experimenter it is an introduction to the philosophy of scientific investigation Researchers with limited time and resources at their disposal will find this text a valuable guide for solving specific problems efficiently The presentation makes extensive use of examples and the approach and methods are graphical rather than numerical All calculations can be performed on a personal computer readers are assumed to have no previous knowledge of the subject The presentation is such that the beginner may acquire a thorough understanding of the basic concepts However there is also sufficient material to challenge the advanced student The book is therefore suitable for both first and advanced courses The many examples can also be used in detail for self study or as a reference

Design and

Optimization in Organic Synthesis R. Carlson, 1991-11-21 This is the first general textbook on experimental design and optimization in organic synthesis The book presents a unified methodology for carrying out systematic studies when the objective is to develop efficient and optimum synthetic methods Strategies are included both for exploring the experimental conditions and for systematic studies of entire reaction systems substrates reagents and solvents The methodology is based on multivariate statistical techniques The following topics are treated in depth classical two level designs for screening experiments gradient methods steepest ascent simplex methods as well as response surface techniques for optimization principal components analysis and PLS modelling The book is intended as a hands on text for chemists and engineers engaged in developing synthetic methods in industrial research e g in fine chemicals and pharmaceuticals production as well as for advanced undergraduate students graduate students and researchers in an academic environment *Experimental Design: A Chemometric Approach* S.N. Deming, S.L. Morgan, 1993-06-04 Now available is the second edition of a book which has been described as an exceptionally lucid easy to read presentation would be an excellent addition to the collection of every analytical chemist I recommend it with great enthusiasm Analytical Chemistry N R Draper reviewed the first edition in Publication of the International Statistical Institute discussion is careful sensible amicable and modern and can be recommended for the intended readership The scope of the first edition has been revised enlarged and expanded Approximately 30% of the text is new The book first introduces the reader to the fundamentals of experimental design Systems theory response surface concepts and basic statistics serve as a basis for the further development of matrix least squares and hypothesis testing The effects of different experimental designs and different models on the variance covariance matrix and on the analysis of variance ANOVA are extensively discussed Applications and advanced topics such as confidence bands rotatability and confounding complete the text Numerous worked examples are presented The clear and practical approach adopted by the authors makes the book applicable to a wide audience It will appeal particularly to those with a practical need scientists engineers managers research workers who have completed their formal education but who still need to know efficient ways of carrying out experiments It will also be an ideal text for advanced undergraduate and graduate students following courses in chemometrics data acquisition and treatment and design of experiments **Advanced LIMS Technology** J.E.H. Stafford, 2012-12-06 Laboratory Information Management Systems LIMS are either custom built or off the shelf solutions to the problems of controlling the flow of data through laboratories In this book commercial relevance is ensured by authors from major industrial organizations who demonstrate by example successful application of the technology This book provides an excellent up to date overview of this intensely competitive field Data Analysis for Hyphenated Techniques E.J. Karjalainen, U.P. Karjalainen, 1996-03-14 Based on a concrete set of working MATLAB programs the book begins with a short program of snippets describing basic principles and proceeds to a complete application program filling a central analytical need obtaining pure spectra from the observed overlapping spectra with standard deviations for

the solutions obtained. The strength of the book is the open nature of the programs. All programs can be read, tested, and modified by the user. The mathematical principles needed for the proper treatment of experimental data are thoroughly described. The first part of the book describes how data is collected, converted, and prepared for the actual deconvolution. Practical working algorithms such as the Savitzky-Golay smoothing method are emphasized. The reader can see how searches in spectral libraries can be greatly speeded up by proper formulation of the calculation. Basic signal processing is described by illustrative examples. The main part of the book describes the deconvolution of overlapping chromatographic peaks. Principle component analysis is described and used as a useful tool. The main emphasis is a discussion of a deconvolution method, OSCAR (Optimization by Stepwise Constraining of Alternating Regression), developed by the authors. The results can be validated as OSCAR calculates confidence intervals for the spectra and elution curves. For users who do not want to enter the programs by hand, a separate CD-ROM is available. It contains the programs and extensive sample data files. The CD-ROM has instructional multimedia showing step by step how the programs are used for the problems in the book. The MATLAB programs and datafiles can be directly run on Windows and Macintosh computers having a MATLAB interpreter.

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