CHEMOMETRICS FOR PATTERN RECOGNITION



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Kurt Varmuza

Chemometrics for Pattern Recognition Richard G. Brereton, 2009-06-29 Over the past decade pattern recognition has been one of the fastest growth points in chemometrics This has been catalysed by the increase in capabilities of automated instruments such as LCMS GCMS and NMR to name a few to obtain large quantities of data and in parallel the significant growth in applications especially in biomedical analytical chemical measurements of extracts from humans and animals together with the increased capabilities of desktop computing The interpretation of such multivariate datasets has required the application and development of new chemometric techniques such as pattern recognition the focus of this work Included within the text are Real world pattern recognition case studies from a wide variety of sources including biology medicine materials pharmaceuticals food forensics and environmental science Discussions of methods many of which are also common in biology biological analytical chemistry and machine learning Common tools such as Partial Least Squares and Principal Components Analysis as well as those that are rarely used in chemometrics such as Self Organising Maps and Support Vector Machines Representation in full colour Validation of models and hypothesis testing and the underlying motivation of the methods including how to avoid some common pitfalls Relevant to active chemometricians and analytical scientists in industry academia and government establishments as well as those involved in applying statistics and computational pattern recognition Applied Chemometrics for Scientists Richard G. Brereton, 2007-03-13 The book introduces most of the basic tools of chemometrics including experimental design signal analysis statistical methods for analytical chemistry and multivariate methods It then discusses a number of important applications including food chemistry biological pattern recognition reaction monitoring optimisation of processes medical applications. The book arises from a series of short articles that have been developed over four years on Chemweb www chemweb com Multivariate Pattern Recognition in Chemometrics R.G. Brereton, 1992-09-04 Chemometrics originated from multivariate statistics in chemistry and this field is still the core of the subject The increasing availability of user friendly software in the laboratory has prompted the need to optimize it safely This work comprises material presented in courses organized from 1987 1992 aimed mainly at professionals in industry The book covers approaches for pattern recognition as applied primarily to multivariate chemical data These include data reduction and display techniques principal components analysis and methods for classification and clustering Comprehensive case studies illustrate the book including numerical examples and extensive problems are interspersed throughout the text The book contains extensive cross referencing between various chapters comparing different notations and approaches enabling readers from different backgrounds to benefit from it and to move around chapters at will Worked examples and exercises are given making the volume valuable for courses Tutorial versions of SPECTRAMAP and SIRIUS are optionally available as a Software Supplement at a low price to accompany the text

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chemometrics This new edition of this practical guide on chemometrics emphasizes the principles and applications behind the main ideas in the field using numerical and graphical examples which can then be applied to a wide variety of problems in chemistry biology chemical engineering and allied disciplines Presented in full color it features expansion of the principal component analysis classification multivariate evolutionary signal and statistical distributions sections and new case studies in metabolomics as well as extensive updates throughout Aimed at the large number of users of chemometrics it includes extensive worked problems and chapters explaining how to analyze datasets in addition to updated descriptions of how to apply Excel and Matlab for chemometrics Chemometrics Data Driven Extraction for Science Second Edition offers chapters covering experimental design signal processing pattern recognition calibration and evolutionary data The pattern recognition chapter from the first edition is divided into two separate ones Principal Component Analysis Cluster Analysis and Classification It also includes new descriptions of Alternating Least Squares ALS and Iterative Target Transformation Factor Analysis ITTFA Updated descriptions of wavelets and Bayesian methods are included Includes updated chapters of the classic chemometric methods e g experimental design signal processing etc Introduces metabolomics type examples alongside those from analytical chemistry Features problems at the end of each chapter to illustrate the broad applicability of the methods in different fields Supplemented with data sets and solutions to the problems on a dedicated website www booksupport wiley com Chemometrics Data Driven Extraction for Science Second Edition is recommended for post graduate students of chemometrics as well as applied scientists e g chemists biochemists engineers statisticians working in all areas of data **Chemometrics for Pattern Recognition** ,2015 Chemical Pattern Recognition Oldřich Štrouf, 1986 analysis

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