1. Record Nr. UNINA9910139922803321

Autore	Brereton Richard G
Titolo	Chemometrics for pattern recognition / / Richard Brereton
Pubbl/distr/stampa	Chichester, West Sussex, U.K. ; ; Hoboken, NJ, : Wiley, 2009
ISBN	1-282-18631-0 9786612186318 0-470-74646-7 0-470-74647-5
Edizione	[1st ed.]
Descrizione fisica	1 online resource (524 p.)
Disciplina	543.01/5195
Soggetti	Chemometrics Pattern perception
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Chemometrics for Pattern Recognition; Contents; Acknowledgements; Preface; 1 Introduction; 1.1 Past, Present and Future; 1.2 About this Book; Bibliography; 2 Case Studies; 2.1 Introduction; 2.2 Datasets, Matrices and Vectors; 2.3 Case Study 1: Forensic Analysis of Banknotes; 2.4 Case Study 2: Near Infrared Spectroscopic Analysis of Food; 2.5 Case Study 3: Thermal Analysis of Polymers; 2.6 Case Study 4: Environmental Pollution using Headspace Mass Spectrometry; 2.7 Case Study 5: Human Sweat Analysed by Gas Chromatography Mass Spectrometry 2.8 Case Study 6: Liquid Chromatography Mass Spectrometry of Pharmaceutical Tablets2.9 Case Study 7: Atomic Spectroscopy for the Study of Hypertension; 2.10 Case Study 8: Metabolic Profiling of Mouse Urine by Gas Chromatography of Urine Extracts; 2.11 Case Study 9: Nuclear Magnetic Resonance Spectroscopy for Salival Analysis of the Effect of Mouthwash; 2.12 Case Study 10: Simulations; 2.13 Case Study 11: Null Dataset; 2.14 Case Study 12: GCMS and Microbiology of Mouse Scent Marks; Bibliography; 3 Exploratory Data Analysis; 3.1 Introduction; 3.2 Principal Components Analysis; 3.2.1 Background 3.2.2 Scores and Loadings3.2.3 Eigenvalues; 3.2.4 PCA Algorithm; 3.2.5 Graphical Representation; 3.3 Dissimilarity Indices, Principal Co-

ordinates Analysis and Ranking; 3.3.1 Dissimilarity; 3.3.2 Principal Co-ordinates Analysis; 3.3.3 Ranking; 3.4 Self Organizing Maps; 3.4.1 Background; 3.4.2 SOM Algorithm; 3.4.3 Initialization; 3.4.4 Training; 3.4.5 Map Quality; 3.4.6 Visualization; Bibliography; 4 Preprocessing; 4.1 Introduction; 4.2 Data Scaling; 4.2.1 Transforming Individual Elements; 4.2.2 Row Scaling; 4.2.3 Column Scaling; 4.3 Multivariate Methods of Data Reduction
4.3.1 Largest Principal Components4.3.2 Discriminatory Principal Components; 4.3.3 Partial Least Squares Discriminatory Analysis Scores; 4.4 Strategies for Data Preprocessing; 4.4.1 Flow Charts; 4.4.2 Level 1; 4.4.3 Level 2; 4.4.4 Level 3; 4.4.5 Level 4; Bibliography; 5 Two Class Classifiers; 5.1 Introduction; 5.1.1 Two Class Classifiers; 5.1.2 Preprocessing; 5.1.3 Notation; 5.1.4 Autoprediction and Class Boundaries; 5.2 Euclidean Distance to Centroids; 5.3 Linear Discriminant Analysis; 5.4 Quadratic Discriminant Analysis; 5.5 Partial Least Squares Discriminant Analysis; 5.5.1 PLS Method
5.5.2 PLS Algorithm5.5.3 PLS-DA; 5.6 Learning Vector Quantization; 5.6.1 Voronoi Tesselation and Codebooks; 5.6.2 LVQ1; 5.6.3 LVQ3; 5.6.4 LVQ Illustration and Summary of Parameters; 5.7 Support Vector Machines; 5.7.1 Linear Learning Machines; 5.7.2 Kernels; 5.7.3 Controlling Complexity and Soft Margin SVMs; 5.7.4 SVM Parameters; Bibliography; 6 One Class Classifiers; 6.1 Introduction; 6.2 Distance Based Classifiers; 6.3 PC Based Models and SIMCA; 6.4 Indicators of Significance; 6.4.1 Gaussian Density Estimators and Chi-Squared; 6.4.2 Hotelling's T2; 6.4.3 D-Statistic
6.4.4 Q-Statistic or Squared Prediction Error

Sommario/riassunto

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