

1. Record Nr.	UNINA9910876853903321
Autore	Brereton Richard G
Titolo	Applied chemometrics for scientists // Richard G. Brereton
Pubbl/distr/stampa	Chichester, England ; ; Hoboken, NJ, : John Wiley & Sons, c2007
ISBN	1-280-83864-7 9786610838646 0-470-05778-5 0-470-05777-7
Descrizione fisica	1 online resource (397 p.)
Classificazione	35.05
Disciplina	542.30151 543.015195
Soggetti	Chemometrics Chemistry, Analytic
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	Applied Chemometrics for Scientists; Contents; Preface; 1 Introduction; 1.1 Development of Chemometrics; 1.1.1 Early Developments; 1.1.2 1980s and the Borderlines between Other Disciplines; 1.1.3 1990s and Problems of Intermediate Complexity; 1.1.4 Current Developments in Complex Problem Solving; 1.2 Application Areas; 1.3 How to Use this Book; 1.4 Literature and Other Sources of Information; References; 2 Experimental Design; 2.1 Why Design Experiments in Chemistry?; 2.2 Degrees of Freedom and Sources of Error; 2.3 Analysis of Variance and Interpretation of Errors 2.4 Matrices, Vectors and the Pseudoinverse 2.5 Design Matrices; 2.6 Factorial Designs; 2.6.1 Extending the Number of Factors; 2.6.2 Extending the Number of Levels; 2.7 An Example of a Factorial Design; 2.8 Fractional Factorial Designs; 2.9 Plackett-Burman and Taguchi Designs; 2.10 The Application of a Plackett-Burman Design to the Screening of Factors Influencing a Chemical Reaction; 2.11 Central Composite Designs; 2.12 Mixture Designs; 2.12.1 Simplex Centroid Designs; 2.12.2 Simplex Lattice Designs; 2.12.3 Constrained Mixture Designs 2.13 A Four Component Mixture Design Used to Study Blending of Olive

Oils 2.14 Simplex Optimization; 2.15 Leverage and Confidence in Models; 2.16 Designs for Multivariate Calibration; References; 3 Statistical Concepts; 3.1 Statistics for Chemists; 3.2 Errors; 3.2.1 Sampling Errors; 3.2.2 Sample Preparation Errors; 3.2.3 Instrumental Noise; 3.2.4 Sources of Error; 3.3 Describing Data; 3.3.1 Descriptive Statistics; 3.3.2 Graphical Presentation; 3.3.3 Covariance and Correlation Coefficient; 3.4 The Normal Distribution; 3.4.1 Error Distributions; 3.4.2 Normal Distribution Functions and Tables 3.4.3 Applications 3.5 Is a Distribution Normal?; 3.5.1 Cumulative Frequency; 3.5.2 Kolmogorov-Smirnov Test; 3.5.3 Consequences; 3.6 Hypothesis Tests; 3.7 Comparison of Means: the t-Test; 3.8 F-Test for Comparison of Variances; 3.9 Confidence in Linear Regression; 3.9.1 Linear Calibration; 3.9.2 Example; 3.9.3 Confidence of Prediction of Parameters; 3.10 More about Confidence; 3.10.1 Confidence in the Mean; 3.10.2 Confidence in the Standard Deviation; 3.11 Consequences of Outliers and How to Deal with Them; 3.12 Detection of Outliers; 3.12.1 Normal Distributions; 3.12.2 Linear Regression 3.12.3 Multivariate Calibration 3.13 Shewhart Charts; 3.14 More about Control Charts; 3.14.1 Cusum Chart; 3.14.2 Range Chart; 3.14.3 Multivariate Statistical Process Control; References; 4 Sequential Methods; 4.1 Sequential Data; 4.2 Correlograms; 4.2.1 Auto-correlograms; 4.2.2 Cross-correlograms; 4.2.3 Multivariate Correlograms; 4.3 Linear Smoothing Functions and Filters; 4.4 Fourier Transforms; 4.5 Maximum Entropy and Bayesian Methods; 4.5.1 Bayes' Theorem; 4.5.2 Maximum Entropy; 4.5.3 Maximum Entropy and Modelling; 4.6 Fourier Filters; 4.7 Peakshapes in Chromatography and Spectroscopy 4.7.1 Principal Features

---

#### Sommario/riassunto

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](http://www.chemweb.com)).

---