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Nota di contenuto	Chemometrics; Contents; Preface; Supplementary Information; Acknowledgements; 1 Introduction; 1.1 Points of View; 1.2 Software and Calculations; 1.3 Further Reading; 1.3.1 General; 1.3.2 Specific Areas; 1.3.3 Internet Resources; 1.4 References; 2 Experimental Design; 2.1 Introduction; 2.2 Basic Principles; 2.2.1 Degrees of Freedom; 2.2.2 Analysis of Variance and Comparison of Errors; 2.2.3 Design Matrices and Modelling; 2.2.4 Assessment of Significance; 2.2.5 Leverage and Confidence in Models; 2.3 Factorial Designs; 2.3.1 Full Factorial Designs; 2.3.2 Fractional Factorial Designs 2.3.3 Plackett-Burman and Taguchi Designs2.3.4 Partial Factorials at Several Levels: Calibration Designs; 2.4 Central Composite or Response Surface Designs; 2.4.1 Setting Up the Design; 2.4.2 Degrees of Freedom; 2.4.3 Axial Points; 2.4.4 Modelling; 2.4.5 Statistical Factors; 2.5 Mixture Designs; 2.5.1 Mixture Space; 2.5.2 Simplex Centroid; 2.5.3 Simplex Lattice; 2.5.4 Constraints; 2.5.5 Process Variables; 2.6 Simplex Optimisation; 2.6.1 Fixed Sized Simplex; 2.6.2 Elaborations;

2.6.3 Modified Simplex; 2.6.4 Limitations; Problems; 3 Signal Processing; 3.1 Sequential Signals in Chemistry
3.1.1 Environmental and Geological Processes3.1.2 Industrial Process Control; 3.1.3 Chromatograms and Spectra; 3.1.4 Fourier Transforms; 3.1.5 Advanced Methods; 3.2 Basics; 3.2.1 Peakshapes; 3.2.2 Digitisation; 3.2.3 Noise; 3.2.4 Sequential Processes; 3.3 Linear Filters; 3.3.1 Smoothing Functions; 3.3.2 Derivatives; 3.3.3 Convolution; 3.4 Correlograms and Time Series Analysis; 3.4.1 Auto-correlograms; 3.4.2 Cross-correlograms; 3.4.3 Multivariate Correlograms; 3.5 Fourier Transform Techniques; 3.5.1 Fourier Transforms; 3.5.2 Fourier Filters; 3.5.3 Convolution Theorem; 3.6 Topical Methods
3.6.1 Kalman Filters3.6.2 Wavelet Transforms; 3.6.3 Maximum Entropy (Maxent) and Bayesian Methods; Problems; 4 Pattern Recognition; 4.1 Introduction; 4.1.1 Exploratory Data Analysis; 4.1.2 Unsupervised Pattern Recognition; 4.1.3 Supervised Pattern Recognition; 4.2 The Concept and Need for Principal Components Analysis; 4.2.1 History; 4.2.2 Case Studies; 4.2.3 Multivariate Data Matrices; 4.2.4 Aims of PCA; 4.3 Principal Components Analysis: the Method; 4.3.1 Chemical Factors; 4.3.2 Scores and Loadings; 4.3.3 Rank and Eigenvalues; 4.3.4 Factor Analysis
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5.2 Univariate Calibration

Sommario/riassunto

This book is aimed at the large number of people who need to use chemometrics but do not wish to understand complex mathematics, therefore it offers a comprehensive examination of the field of chemometrics without overwhelming the reader with complex mathematics. * Includes five chapters that cover the basic principles of chemometrics analysis.* Provides two chapters on the use of Excel and MATLAB for chemometrics analysis.* Contains 70 worked problems so that readers can gain a practical understanding of the use of chemometrics.