1. Record Nr. UNINA9910831166903321

Titolo	Chemometrics and numerical methods in LIBS / / edited by Vincenzo Palleschi
Pubbl/distr/stampa	Hoboken, New Jersey : , : John Wiley & Sons, Incorporated, , [2022] ©2022
ISBN	1-119-75961-7 1-119-75957-9 1-119-75956-0
Descrizione fisica	1 online resource (381 pages)
Disciplina	543.015195
Soggetti	Chemometrics Laser-induced breakdown spectroscopy
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Cover -- Title Page -- Copyright Page -- Contents -- List of Contributors -- Preface -- Introduction and Brief Summary of the LIBS Development -- Part I Introduction to LIBS -- Chapter 1 LIBS Fundamentals -- 1.1 Interaction of Laser Beam with Matter -- 1.2 Basics of Laser-Matter Interaction -- 1.3 Processes in Laser-Produced Plasma -- 1.4 Factors Affecting Laser Ablation and Laser-Induced Plasma Formation -- 1.4.1 Influence of Laser Parameters on the Laser-Induced Plasmas -- 1.4.2 Laser Wavelength () -- 1.4.3 Laser Pulse Duration () -- 1.4.4 Laser Energy (E) -- 1.4.5 Influence of Ambient Gas -- 1.5 Plasma Properties and Plasma Emission Spectra -- References -- Chapter 2 LIBS Instrumentations -- 2.1 Basics of LIBS instrumentations -- 2.2 Lasers in LIBS Systems -- 2.3 Desirable Requirements for Atomic Emission Spectrometers/Detectors -- 2.4 Spectrometers -- 2.4.1 Czerny-Turner Optical Configuration -- 2.4.2 Paschen-Runge Design -- 2.4.3 Echelle Spectrometer Configuration -- 2.5 Detectors -- 2.5.1 Photomultiplier Detectors -- 2.5.2 Solid-State Detectors -- 2.5.3 The Interline CCD Detectors -- 2.5.3.1 The Image Intensifier -- References -- Chapter 3 Applications of LIBS -- 3.1 Industrial Applications -- 3.1.1 Metal Industry -- 3.1.2 Energy

Production -- 3.2 Biomedical Applications -- 3.3 Geological and Environmental Applications -- 3.4 Cultural Heritage and Archaeology Applications -- 3.5 Other Applications -- References -- Part II Simplications of LIBS Information -- Chapter 4 LIBS Spectral Treatment -- 4.1 Introduction -- 4.2 Baseline Correction -- 4.2.1 Polynomial Algorithm -- 4.2.2 Model-free Algorithm -- 4.2.3 Wavelet Transform Model -- 4.3 Noise Filtering -- 4.3.1 Wavelet Threshold De-noising (WTD) -- 4.3.2 Baseline Correction and Noise Filtering -- 4.4 Overlapping Peak Resolution.
4.4.1 Curve Fitting Method -- 4.4.2 The Wavelet Transform -- 4.5 Features Selection -- 4.5.1 Principal Component Analysis -- 4.5.2 Genetic Algorithm (GA) -- 4.5.3 Wavelet Transformation (WT) -- References -- Chapter 5 Principal Component Analysis -- 5.1 Introduction -- 5.1.1 Laser-Induced Breakdown Spectroscopy (LIBS) -- 5.2 The Principal Component Analysis (PCA) -- 5.3 PCA in Some LIBS Applications -- 5.3.1 Geochemical Applications -- 5.3.2 Food and Feed Applications -- 5.3.3 Microbiological Applications -- 5.3.4 Forensic Applications -- 5.4 Conclusion -- References -- Chapter 6 Time-Dependent Spectral Analysis -- 6.1 Introduction -- 6.2 Time-Dependent LIBS Spectral Analysis -- 6.2.1 Independent Component Analysis -- 6.2.2 3D Boltzmann Plot -- 6.2.2.1 Principles of the Method -- 6.3 Applications -- 6.3.1 3D Boltzmann Plot Coupled with Independent Component Analysis -- 6.3.2 Analysis of a Carbon Plasma by 3D Boltzmann Plot Method -- 6.3.3 Assessment of the LTE Condition Through the 3D Boltzmann Plot Method -- 6.3.4 Evaluation of Self-Absorption -- 6.3.5 Determination of Transition Probabilities -- 6.3.6 3D Boltzmann Plot and Calibration-free Laser-induced Breakdown Spectroscopy -- 6.4 Conclusion -- References -- Part III Classification by LIBS -- Chapter 7 Distance-based Method -- 7.1 Cluster Analysis -- 7.1.1 Introduction -- 7.1.2 Theory -- 7.1.2.1 K-means Clustering -- 7.1.2.2 Hierarchical Clustering -- 7.1.3 Application -- 7.2 Independent Components Analysis -- 7.2.1 Introduction -- 7.2.2 Theory -- 7.2.3 Application -- 7.3 K-Nearest Neighbor -- 7.3.1 Introduction -- 7.3.2 Theory -- 7.3.3 Application -- 7.4 Linear Discriminant Analysis -- 7.4.1 Introduction -- 7.4.2 Theory -- 7.4.2.1 The Calculation Process of LDA .(Two Categories) -- 7.4.3 Application.
7.5 Partial Least Squares Discriminant Analysis -- 7.5.1 Introduction -- 7.5.2 Theory -- 7.5.3 Application -- 7.6 Principal Component Analysis -- 7.6.1 Introduction -- 7.6.2 Theory -- 7.6.3 Application -- 7.7 Soft Independent Modeling of Class Analogy -- 7.7.1 Introduction -- 7.7.2 Theory -- 7.7.3 Application -- 7.8 Conclusion and Expectation -- References -- Chapter 8 Blind Source Separation in LIBS -- 8.1 Introduction -- 8.2 Data Model -- 8.3 Analyzing LIBS Data via Blind Source Separation -- 8.3.1 Second-order BSS -- 8.3.2 Maximum Noise Fraction -- 8.3.3 Independent Component Analysis -- 8.3.4 ICA for Noisy Data -- 8.4 Numerical Examples -- 8.5 Final Remarks -- References -- Chapter 9 Artificial Neural Networks for Classification -- 9.1 Introduction and Scope -- 9.2 Artificial Neural Networks (ANNs) -- 9.3 Cost Functions and Training -- 9.4 Backpropagation -- 9.5 Convolutional Neural Networks -- 9.6 Evaluation and Tuning of ANNs -- 9.7 Regularization -- 9.8 State-of-the-art LIBS Classification Using ANNs -- 9.9 Summary -- Acknowledgments -- References -- Chapter 10 Data Fusion: LIBS + Raman -- 10.1 Introduction -- 10.2 Data Fusion Background -- 10.3 Data Treatment -- 10.4 Working with Images -- 10.4.1 Vectors Concatenation -- 10.4.2 Vectors Co-addition -- 10.4.3 Vectors Outer Sum -- 10.4.4 Vectors Outer Product -- 10.4.5 Data Analysis -- 10.5

Applications -- 10.6 Conclusion -- References -- Part IV Quantitative Analysis -- Chapter 11 Univariate Linear Methods -- 11.1 Standards -- 11.2 Matrix Effect -- 11.3 Normalization -- 11.4 Linear vs Nonlinear Calibration Curves -- 11.5 Figures of Merit of a Calibration Curve -- 11.5.1 Coefficient of Determination -- 11.5.2 Root Mean Squared Error of Calibration -- 11.5.3 Limit of Detection -- 11.6 Inverse Calibration -- 11.7 Conclusion -- References.
Chapter 12 Partial Least Squares -- 12.1 Overview -- 12.2 Partial Least Squares Regression Algorithms -- 12.2.1 Nonlinear Iterative PLS -- 12.2.2 SIMPLS Algorithm -- 12.2.3 Kernel Partial Least Squares -- 12.2.4 Locally Weighted Partial Least Squares -- 12.2.5 Dominant Factor-based Partial Least Squares -- 12.3 Partial Least Squares Discriminant Analysis -- 12.4 Results of Partial Least Squares in LIBS -- 12.4.1 Coal Analysis -- 12.4.2 Metal Analysis -- 12.4.3 Rocks, Soils, and Minerals Analysis -- 12.4.4 Organics Analysis -- 12.5 Conclusion -- References -- Chapter 13 Nonlinear Methods -- 13.1 Introduction -- 13.2 Multivariate Nonlinear Algorithms -- 13.2.1 Artificial Neural Networks -- 13.2.1.1 Conventional Artificial Neural Networks -- 13.2.1.2 Convolutional Neural Networks -- 13.2.2 Other Nonlinear Multivariate Approaches -- 13.2.2.1 The Franzini-Leoni Method -- 13.2.2.2 The Kalman Filter Approach -- 13.2.2.3 Calibration-Free Methods -- 13.3 Conclusion -- References -- Chapter 14 Laser Ablation-based Techniques - Data Fusion -- 14.1 Introduction -- 14.2 Data Fusion of Multiple Analytical Techniques -- 14.2.1 Low-level Fusion -- 14.2.2 Mid-level Fusion -- 14.2.3 High-level Fusion -- 14.3 Data Fusion of Laser Ablation-Based Techniques -- 14.3.1 Introduction -- 14.3.2 Classification of Edible Salts -- 14.3.2.1 LIBS and LA-ICP-MS Measurements of the Salt Samples -- 14.3.2.2 Mid-Level Data Fusion of LIBS and LA-ICP-MS of Salt Samples -- 14.3.2.3 PLS-DA Classification Model for Salt Samples -- 14.3.3 Coal Discrimination Analysis -- 14.3.3.1 LIBS and LA-ICP-TOF-MS Measurements of the Coal Samples -- 14.3.3.2 Mid-Level Data Fusion of LIBS and LA-ICP-TOF-MS of Coal Samples -- 14.3.3.3 PCA Combined with K-means Cluster Analysis for Coal Samples -- 14.3.3.4 PLS-DA and SVM for Coal Samples Analysis.
14.4 Comments and Future Developments -- Acknowledgments -- References -- Part V Conclusions -- Chapter 15 Conclusion -- Index -- EULA.

Sommario/riassunto

"The LIBS community is constantly growing and it now widely recognized that LIBS techniques provide large sets of data statistical methods for simplification and analysis are essential; however, there is still some confusion on the proper application of these methods to LIBS analysis and, most of all, on the procedures that must be applied for the validation of the results obtained. The book will be organized in three parts, dealing with the main applications of chemometrics in LIBS: simplification of the spectral information, classification of spectra, quantitative analysis. Each part will be divided in sections, describing the different techniques with practical examples. For example, in Part 2, the techniques described will be discussed in the perspective of waste sorting by LIBS and LIBS micro-imaging of geological material, to mention just two of the main applications which exploits at the best the chemometric techniques of classification."--