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Nota di contenuto	Multi-way Analysis with Applications in the Chemical Sciences; CONTENTS; Foreword; Preface; Nomenclature and Conventions; 1 Introduction; 1.1 What is multi-way analysis?; 1.2 Conceptual aspects of multi-way data analysis; 1.3 Hierarchy of multivariate data structures in chemistry; 1.4 Principal component analysis and PARAFAC; 1.5 Summary; 2 Array definitions and properties; 2.1 Introduction; 2.2 Rows, columns and tubes; frontal, lateral and horizontal slices; 2.3 Elementary operations; 2.4 Linearity concepts; 2.5 Rank of two-way arrays; 2.6 Rank of three-way arrays 2.7 Algebra of multi-way analysis2.8 Summary; Appendix 2.A; 3 Two- way component and regression models; 3.1 Models for two-way one- block data analysis: component models; 3.2 Models for two-way two- block data analysis: regression models; 3.3 Summary; Appendix 3.A: some PCA results; Appendix 3.B: PLS algorithms; 4 Three-way component and regression models; 4.1 Historical introduction to multi-

way models; 4.2 Models for three-way one-block data: three-way component models; 4.3 Models for three-way two-block data: three-way regression models; 4.4 Summary
Appendix 4.A: alternative notation for the PARAFAC model
Appendix 4.B: alternative notations for the Tucker3 model; 5 Some properties of three-way component models; 5.1 Relationships between three-way component models; 5.2 Rotational freedom and uniqueness in three-way component models; 5.3 Properties of Tucker3 models; 5.4 Degeneracy problem in PARAFAC models; 5.5 Summary; 6 Algorithms; 6.1 Introduction; 6.2 Optimization techniques; 6.3 PARAFAC algorithms; 6.4 Tucker3 algorithms; 6.5 Tucker2 and Tucker1 algorithms; 6.6 Multi-linear partial least squares regression; 6.7 Multi-way covariates regression models; 6.8 Core rotation in Tucker3 models; 6.9 Handling missing data; 6.10 Imposing non-negativity; 6.11 Summary; Appendix 6.A: closed-form solution for the PARAFAC model; Appendix 6.B: proof that the weights in trilinear PLS1 can be obtained from a singular value decomposition; 7 Validation and diagnostics; 7.1 What is validation?; 7.2 Test-set and cross-validation; 7.3 Selecting which model to use; 7.4 Selecting the number of components; 7.5 Residual and influence analysis; 7.6 Summary; 8 Visualization; 8.1 Introduction; 8.2 History of plotting in three-way analysis; 8.3 History of plotting in chemical three-way analysis; 8.4 Scree plots; 8.5 Line plots; 8.6 Scatter plots; 8.7 Problems with scatter plots; 8.8 Image analysis; 8.9 Dendrograms; 8.10 Visualizing the Tucker core array; 8.11 Joint plots; 8.12 Residual plots; 8.13 Leverage plots; 8.14 Visualization of large data sets; 8.15 Summary; 9 Preprocessing; 9.1 Background; 9.2 Two-way centering; 9.3 Two-way scaling; 9.4 Simultaneous two-way centering and scaling; 9.5 Three-way preprocessing; 9.6 Summary; Appendix 9.A: other types of preprocessing; Appendix 9.B: geometric view of centering

Sommario/riassunto

This book is an introduction to the field of multi-way analysis for chemists and chemometricians. Its emphasis is on the ideas behind the method and its practical applications. Sufficient mathematical background is given to provide a solid understanding of the ideas behind the method. There are currently no other books on the market which deal with this method from the viewpoint of its applications in chemistry. Applicable in many areas of chemistry. No comparable volume currently available. The field is becoming increasingly important.

2. Record Nr.	UNINA9910710261003321
Autore	Swaffield J. A. <1943->
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