

BOOK REVIEW

Chemometrics: Data Driven Extraction for Science

by

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The book entitled *Chemometrics Data Driven Extraction for Science*, authored by Brereton G, a professor emeritus at the University of Bristol, UK, describes the chemometrics discipline. In the book, different principles and applications are presented by graphical and numerical presentations, making them easily applicable to solving problems inside different scientific disciplines, such as chemistry, chemical engineering, medicine, and biology.

The book consists of the seven main chapters: Introduction (1), Experimental Design (2), Signal Processing (3), Principal Component Analysis and Unsupervised Pattern Recognition (4), Classification and Supervised Pattern Recognition (5), Calibration (6), Evolutionary Multivariate Signals (7). *Chapter one* presents the origin of chemometrics, its basis, i.e. the three fundamental factors: “applied statistics, statistics in analytical and physical chemistry, and scientific computing”, as well as the contemporary development of the discipline. *The second chapter* introduces the basic principles as the fundamentals for understanding experimental design as the “building blocks”, as well as factorial design, which is understandable by the application of the mentioned building blocks (such as the degrees of freedom, the design matrix, the models, significance testing, etc.). The manner of making composite design and response surface design and mixture designs is also presented. *Chapter three* refers to the need for sequential signals to be analyzed by means of different methods; in this chapter, such methods and processes, and chromatograms and spectra as well, are presented, with a special focus on the presentation of correlograms and time series analysis. *Chapter four* discusses the multivariate data presentation and understanding models (groups of techniques, such as exploratory data analysis, cluster analysis...) at the beginning of the chapter, only to later present the PCA multivariate chemometric technique in the continuation

of the chapter. The presentation of the PCA is illustrated by three case studies. *The fifth chapter* introduces pattern recognition as a widely used application of chemometrics, representing two-, one- and multi-class classifiers. *In chapter six*, calibration is presented as connecting one or several sets of variables together (as part of regression and experimental designs). *In chapter seven*, exploratory data analysis and preprocessing, determining composition and resolution are discussed.

In the book, the data and information are well-organized. It also includes a large number of multiple-choice questions, figures, pattern recognition, case studies of NIR, case studies of metabolomics. The discussion of wavelets and the Bayesian methods in signal analysis is significant. The book also presents chemometric Matlab R2016A (Windows 10), as well as Excel 2016 (Windows 10). The book offers readers to download all the useful content related to the problems presented, Excel add-in, Matlab routines. The author intends the book to the (postgraduate) students of chemometrics or scientists, as well as practicing chemometricians. The publisher's website provides all of them with a significant portion of the material. Therefore, the book is also intended to both beginners in and those with an advanced knowledge of chemometrics, because it offers a familiar approach with examples and questions, the theory useful for the basic understanding beneficial to those who are just becoming familiar with the discipline, and the unfamiliar research based on case studies and numerical data as the new methods that have previously been tested for compliance.

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