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Chemometrics in Practical Applications

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Preface

Chemometrics has been defined as "a chemical discipline that uses statistical and mathematical methods to design or select optimum procedures and experiments, and to provide maximum chemical information by analyzing chemical data". Chemometrics can be considered as a part of the wider field chemoinformatics, and has close relationships to bioinformatics.

The start of chemometrics dates back to the 1960s, when multivariate data analysis methods - like for instance the "learning machine" - have been tried for solving rather complicated problems in chemistry, such as the automatic interpretation of molecular spectra. The name chemometrics was first used by Svante Wold in 1972 (in Swedish, kemometria) and it was established in 1974 by Bruce Kowalski. The first years of chemometrics were characterized by rather uncritical use of machine learning methods for complex - often too complex - tasks in chemistry and consequently sometimes accompanied by ignorance and refusal of many chemists. However, in this time also falls the presentation of the PLS regression method by chemometricians, which is now the most used method for evaluation of multivariate data, not only in chemistry. During the next decades chemometricians learned to use multivariate data analysis in a proper and safe way for problems with a realistic chance for success, and also found back to the underlying statistical concepts. Chemometrics contributed with valuable method developments and provided many stimulants in the area. Furthermore, commercial software became available and nowadays several basic chemometric methods, like principal component analysis, multivariate classification, and multiple regression (by PLS and other approaches) are routinely used in chemical research and industry. Admittedly, sometimes without the necessary elementary knowledge about the used methods.

Despite the broad definition of chemometrics, the most important part of it is still the application of multivariate data analysis to chemistry-relevant data. Chemical-physical systems of practical interest are often complicated and relationships between available (measurement) data and desired data (properties, origin) cannot be described by theory. Therefore, a typical chemometric approach is not based on "first principles" but is "data driven" and has the goal to create empirical models. A thorough evaluation of the performance of such models is essential for new cases. Multivariate statistical data analysis has been proven as a powerful tool for analyzing and structuring such data sets from chemistry and biochemistry.

This book is a collection of 14 chapters, divided into three sections. Assignment of the chapters to these sections only indicates the main contents of a chapter because most are interdisciplinary and contains theoretical as well as practical aspects.

In section "Methods" the topics comprise statistical model comparison, treatment of compositional data, methods for the estimation of kinetic parameters, and a new approach for exploratory data analysis. A comprehensive chapter presents an overview of experimental optimization.

Section "Biochemistry" deals with biomarker identification, kinetics of enzyme reactions, selection of substances with anticancer properties, and the use of an electronic nose for the identification of foodborne pathogens.

Section "Technology" focuses on chemometric methods used in food technology, for water quality estimation, for the characterization of nanocomposite materials by NMR spectra, and in chromatographic separation processes.

The topics of this book cover a wide range of highly relevant problems in chemistry and chemical/biological technology. The presented solutions may be of interest to the reader even if not working exactly in the fields described in the chapters. The book is intended for chemists, chemical engineers, and biotechnologists working in research, production or education. Students in these areas will find a source with highly diverse and successful applications of chemometric methods. In this sense, the major goal of this "mosaic of contributions" - presented in a book - is to promote new and adequate use of multivariate data analysis methods in chemistry and related fields.

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