



Alejandro C. Olivieri

# Introduction to Multivariate Calibration

A Practical Approach

 Springer

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*To my late sister Cristina, wherever she is.*

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# Foreword

The content of this book, written by Prof. Alejandro Olivieri, covers practical and fundamental aspects of multivariate calibration, setting the focus on first-order calibration. It is important to remark that multivariate calibration has become a crucial topic in the analytical world, nowadays being adopted in labs for solving complicated analytical problems, including those found in environmental, biochemical, agro-industry, and food analysis, among other applications.

The book has been divided in 13 chapters, starting in Chap. 1 with an introduction of what chemometrics and multivariate calibration represent in the analytical world. In this chapter, basic concepts are introduced. Then, the following chapters show the evolution that first-order calibration has experienced from the simplest and original methods to the latest algorithms, including artificial neural networks to model nonlinear systems. In addition, several chapters are devoted to explore important subjects as the optimum number of latent variables, comparison of multivariate models, data preprocessing and analytical figures of merit, and topics of supreme importance in the analytical field.

Practical aspects of multivariate calibration are discussed introducing interesting examples. Most of the experimental data used in examples and exercises correspond to methods developed by the author's research group and collaborators. In addition, the examples are intended to guide analytical chemists in their work, appealing to mathematics when it is strictly necessary and showing very smart schematic representations to understand concepts involved in these powerful multivariate chemometric tools.

To follow the explanations given in the chapters dealing with the applications, a free graphical interface software, namely, the MVC1 MATLAB routines, is presented and suggested. The software opens a very interesting scenario, as the user should be able, after the reading of this book, to exploit the usefulness of the available tools to perform calibrations with his/her own laboratory data. Particularly useful in this context is the last chapter with solutions to the homework suggested along the practical application chapters.

Finally, this book may be considered to fill a gap in the subject, with a smart treatment of the advantages and practical limitations of first-order calibration, by a

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combination of both fundamentals and practice, and provides free software, developed by the author, to use the most popular available approaches to deal with current analytical data.

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# Preface

Multivariate calibration is becoming popular in analytical chemistry. Some branches of industry have used it for years; others are gradually incorporating it as the necessary tools, both theoretical and experimental, are disseminated in the academic and industrial fields. Precisely the objective of this book is to contribute to the diffusion of the discipline while providing complementary reading material for undergraduate or postgraduate courses on multivariate calibration in chemistry-related careers.

Every book on multivariate calibration faces a dilemma. Should deep mathematical concepts be employed, as those required for the development of the main tools of the discipline, or should the mathematics be kept at a minimum, describing only in a qualitative manner the different calibration techniques? The following anecdote illustrates the issue.

A journalist once interviewed a physics professor, enquiring about the relativity theory. The professor tried to explain the fundamentals of the theory, using uncommon terms such as *geodesics* and *tensors*. Thus the journalist begged for the use of more understandable terms. The professor then told a story of cowboys firing guns on a moving train and spoke about the speed of the bullets in relation to the train and to the platform.

– Good! –exclaimed the journalist– now I understand.

– Yes, but this is not the relativity theory –said the professor.

The same issue is apparent here: how much mathematics and how much qualitative text to include. Exaggerating the mathematics carries the risk of making the book difficult to understand. Reducing it to zero, on the other hand, leads to a symmetrical loss in the chemometrics. Finding the right balance in a book like this one may be a lost cause, but it is worth trying.

Regarding a chemometrics book introducing complex concepts in a simple manner, an editorial comment used the following words in Latin: *veluti pueris absinthia taetra medentes cum dare conantur, prius oras pocula circum adspirant*

*mellis dulci flavoque liquore*. This is an advice of the poet and philosopher Lucretius to orators:

when the topic is tough, behave as physicians seeking to give a draught of bitter wormwood to a child: first smear some honey along the edge of the cup.

The reader might be left with this same sensation with this book.

Rosario, Argentina

Alejandro C. Olivieri

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## Acknowledgments

To write a book like this one, it is important to have collaborated with Argentinean and foreign scientists over almost two decades and to have taught on the subject in universities and private laboratories. Scientific knowledge helps one to comply with the formalities of the discipline, and teaching practice leads one to recognize the need for printed material about an intrinsically difficult topic. It is therefore appropriate to thank the National University of Rosario and the National Scientific and Technical Research Council (CONICET) for allowing us to develop in the double role of teachers and researchers. That is not all. For this project to come true, other crucial ingredients are required: a brother-in-law (Raul), an experienced editor and excellent critic, and a wife-scientist (Graciela) with patience for consulting and discussion. For them, special thanks.

El libro escrito por el Dr. Alejandro C. Olivieri titulado "Introduction to Multivariate Calibration. A Practical Approach" editado por Springer Nature, una prestigiosa editorial suiza, fue seleccionado por la revista Choice para incluirlo dentro de los "Outstanding Academic Titles for 2019".

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