Introduction

An average analytical chemist is well trained to deal with most of the problems that could occur during the use of the laboratory instrumentation. They usually do an excellent job adjusting the parameters of their spectrophotometers in order to achieve an as good as possible atomization of the sample. The one who deals with chromatography usually has excellent experience in adjusting the composition of the mobile phase, flow rate etc. in order to achieve the best possible separation of the analytes of interest with shortest possible duration of the analysis. And all of them have excellent practical skills in order to determine which pretreatment could be most suitable for the specific samples. But not many of them are working in the field of analytical chemistry because of their mathematical background, although they are faced with huge amounts of data each and every day. Typically the statistical education of analytical chemist includes low levels training in statistic, linear regression, statistical significance tests, error and mean comparison and all of that with not much of mathematics in it. When some of them are willing to use some more advanced mathematical techniques, they usually face a rookie wall – due to deficiency of background knowledge in the field of mathematics and data analysis. However, it is not necessary to have exact definitions of the mathematical theorems on which the techniques used in chemometrics are based. The important part is to understand the way they work, which kind of data preprocessing is most suitable and which kind of information could be extracted from the experimental data.

For some chemometricians, including the author of this text, the key step in understanding the way different chemometric techniques work is their capability of writing the program for the specific algorithm in some programming language (Visual Basic, C, Matlab, Mathcad, etc.). In the beginning of my work in the field of chemometrics I had to move from easy to use Mathcad environment, where the user interface which looks like writing your code on a sheet of paper, to less user friendly environments of Visual Basic, C and Matlab, because at that time there was no any chemometric code written for Mathcad. Although the programming package Mathcad was not widely used as a tool by the chemometricians, its interface is the most suitable for the novices in this field to learn the basics. That is the main reason why this electronic book called Chemometrics and Mode is presented to the chemical community.

Fig. 1. Table of content of the book.
Content and Description

The book is consisted of several chapters (Fig. 1): (1) Factor Analysis, (2) Signal Processing, (3) Calibration, (4) Chemical Chaos and Theory of Self-Organized Criticality, and (5) Miscellaneous.

The chapter about Factor Analysis [1] is the most detailed one. It is one of the tools considered as basic topics which should be understand by the beginners in the chemometrics. It includes a script used for analysis of factors which influence the grades of the students, by abstract factor analysis which is well explained in order the reader/user to be able to understand the following, let’s say, more complicated versions of factor analysis. A chemical example (purification of reflection infrared spectra from appearing nonlinearities) for the same procedure is also explained. Target Factor Analysis is presented as a tool for determination of, not only a number of factors which have influence in variations of absorbances at different wavenumber (which is possible by abstract factor analysis), but also for qualitative analysis of urinary calculi [1,2]. Further three variations of factor analysis (evolving factor analysis - EFA, window factor analysis – WFA and window target factor analysis – WTFA) which could be employed in chromatography are presented [3]. These methods use the fact that each existing chemical species has a single unique maximum in its evolutionary profile. Beside in chromatography such profiles could be found in reaction kinetics, titrations, variations in pH and so on [3–6] where the instrument response could vary as a function of some parameter. EFA is based on repetitive eigenvalue analysis on set of data matrices generated by evolutionary process. Whenever an absorbing species begins to appear, an eigenvalue from the pool of noise eigenvalue increases in value in relation to its contribution to the enlarged data set. WFA is similar to EFA, however in this case the eigenvalue analysis is preformed on a set of submatrices with constant number of samples in it (or with constant window) from the original one. WTFA (Fig. 2) is variation of WFA with target testing employed to find the desired species in the whole data matrix. The examples on how these algorithms work are presented with examples in chromatography.

Fig. 2. Results from window target factor analysis on simulated chromatograms (a – first eigenvalue target tested with spectra of all six substances present in the chromatogram; b – contour plot of the simulated chromatogram)

The chapter Calibration is maybe the most important part of the book. It is consisted of examples on how linear regression should be performed, calculation of confidence interval as well as calculation of limit of detection [7]. Simple script with the program which performs multiple linear regression is included in this part with an example on prediction of unit cell parameters in cubic perovskites [8, 9]. The most important part of this chapter are the programs developed for principal component regression (PCR) [10, 11] and partial least squares (PLS) regression [11–14] (with cross-validation routine for selection of latent variables) are one of the basic tools for chemometricians – here developed for the first time in Mathcad environment. The examples in this part are presented using data from [15].

At the Signal Processing chapter few different algorithms for smoothing of digitally collected data are presenter. The algorithms for moving average smoothing, moving median smoothing, fast-Fourier transform smoothing and Saviysky-Golay smoothing are developed and also examples of Gaussian kernel smoothing is presented.
In the *Miscellaneous* chapter the procedure for generalization of the resolution function for separation of two chromatographic peaks into certain number of peaks is presented [16]. The procedure could be used for development of automated procedure for determination of optimum parameters for chromatographic separation on more than two analytes. This part also contains the procedure for simulation of square-wave voltammograms of surface redox reactions [17].

The last chapter of this electronic book, *Chemical Chaos*, is the least chemometric part but it is consisted of some interesting theoretical examples of oscillating reactions, some of them are very simple taken form the contemporary books of physical chemistry [18], while other theoretical models are developed by some of the leading groups in the world that work in the field of chemical chaos [19].

The author hopes that this book will be a valuable tool for all young analytical chemists who are willing to extend and learn some of the basic algorithms in the field of chemometrics and data analysis.

The book could be downloaded at: [http://www.hemija.net/chemometrics/](http://www.hemija.net/chemometrics/)

Your suggestions and comments are welcomed. Please leave them at: [http://forum.hemija.net/](http://forum.hemija.net/)

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**References**