Applied Chemometrics for Scientists (Book Review)

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Book review

Applied Chemometrics for Scientists
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Professor Brereton is becoming the most prolific author in chemometrics. Hard on the heels of *Chemometrics: Data Analysis for the Laboratory and Chemical Plant* [1,2], we have his latest offering which is based on a series of short (1000 word) articles written for a web site. Between 1999 and 2003 some 114 articles were posted as a 'popular general reference'. The aim was to provide 'bite-size' chunks for folk who needed to know some chemometrics without having the luxury of spending serious time (perhaps at Professor Brereton's lectures) studying the subject. Put like this, there might be some concern about a 'little learning' being a dangerous thing[1], but if scientists are to take shallow drafts, they might as well have them from an acknowledged expert than be at the mercy of Mr Google. Given its origins the text is remarkably coherent; Brereton has done a good job in bringing the strands together. As with many of his books, there is a healthy emphasis on practical examples and applications of the art. This philosophy is spelled out in the Preface where he makes the analogy with organic chemistry which after all the theory rests on making and characterizing real molecules. Presumably this approach explains the rather curious title. If chemometrics is not for scientists, then who is it for (Plumbers, Sculptors … &etc)? The text will make a useful addition to a chemometrics library, whether personal, or institutional. In addition the many scientists who did dip into the web site in the past, might wish to have a complete compilation of the articles.

The introductory chapter records the development from early theory in the 1970s through the time of increasing complexity to the present day, where the interface between chemometrics and bioinformatics is one characterized by enormous quantities of data from hyphenated separation / mass spectrometric methods. From early developments in linear modelling using

[1] The delightful quote from Alexander Pope (1688-1744) from his *An Essay on Criticism* reads "A little learning is a dangerous thing; drink deep, or taste not the Pierian spring: there shallow draughts intoxicate the brain, and drinking largely sobers us again."

principal components analysis and partial least squares for calibration, a wide field of computational algorithms are available that can be classed as machine learning. These include one of Professor Brereton's favourite techniques – the support vector machine.
Along with the theory, the sphere of applications has grown steadily with just about every analytical technique benefiting from some aspect of chemometrics. Industrial process control (Chapters 8 and 9) has always been a user of chemometrics, and particularly the food sector (Chapter 13) has benefitted from soft modelling. Biological chemistry receives two chapters, Biological and Medical Applications of Chemometrics (Chapter 10) and Biological Macromolecules (Chapter 11). The former chapter starts with a description of the "–omics", namely genomics, proteomics and metabolomics. Closely related to metabolomics is disease diagnosis from chemical markers. Chemical taxonomy, defining biological species from a chemical analysis of tissue, fruits or derived products such as essential oils, is a subset of general taxonomy using any observable of a species. Rarely does a single attribute clearly distinguish closely related species, and so discriminant analysis is an obvious approach to take. In discussing how discriminant functions are formed and the concept of the centroid of a population, Brereton introduces the amusing example of mice and elephants discriminated by mass, and shows that a baby elephant is closer to the centroid of the masses of mice, than it is to that of elephants. The chapter on macromolecules is a good addition to the book; the discussion of a description of a molecule in terms of tree diagrams and dendrograms is novel for a chemometrics text. Multivariate image analysis (Chapter 12) again goes into areas that are not always found in chemometrics texts. The chapter ends with brief discussion of multiway methods that can deal with multiple images in time and space (OOO, O= object, for a single measured property), with many variables (OOV, V=variable, would represent a 2D image that has a spectrum recorded at each point), or with two dimensional variables such as 2D fluorescence to give (OVV). Of course multiway analysis is not limited to three dimensions, so all of these cases can be generalized to higher dimensions. The application chapters start with Coupled Chromatography (Chapter 7), which refers to any hyphenated separation technique in which a number of variables are observed at the detector, including mass spectrometry and spectroscopic methods.
These applications have been described first and in more detail, because the book is focussed on specific examples. The initial chapters cover basic theory, statistics, experimental design, methods for handling sequential (in time) data, pattern recognition and calibration. Each of these chapters gives an overview of the subject, necessary because of limitations of space in a single volume. A criticism might be the paucity of references after Chapter 1, which are also somewhat dated, presumably coming from the original articles. It would have been better to have some clearer guidance to further reading.
The text is well presented, with a nice typeface and well produced figures. My copy tended to shed pages from the back after my first visit to the index, something I have noted before with Wiley texts. This will be, however, a good addition to your chemometrics library.

References

[1] R G Brereton, *Chemometrics Data Analysis for the Laboratory and Chemical Plant*. J Wiley, Chichester, 2004.
[2] D B Hibbert, D Ebrahimi, *Chemometrics Data Analysis for the Laboratory and Chemical Plant*. by Richard G. Brereton, Chemometrics and Intelligent Laboratory Systems **75**(1) (2005) 109– 110.