A Cornucopia of Chemometrics

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Comprehensive Chemometrics
Chemical and Biochemical data analysis
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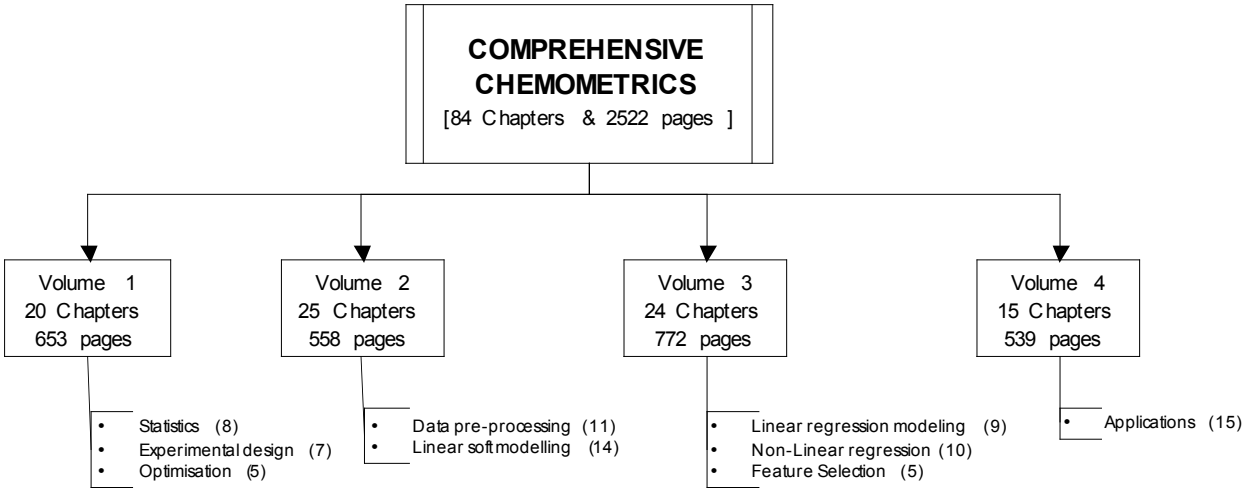
Spectroscopists, like chromatographers, produce large quantities of raw data. Data reduction into something more meaningful is the goal. Selecting the right tool for the job is the challenge. Inevitably the right tool involves heavy duty mathematical and statistical expertise and hence chemometrics.

Many practitioners rely upon sophisticated software routines provided either by instrument suppliers or specialist software packages. Occasionally the brave will venture into the (relatively) uncharted waters of writing their own software in say MatLab. Whatever the approach, there is always a question of understanding what exactly the software is doing. Reaching for the books on statistics and matrix algebra is not usually comforting for those who wish to turn algebra into answers. However for those who did, for many years the ultimate reference, was Massart et al's Handbook of Chemometric and Qualimetics, in two volumes, Parts A & B, published in 1998 of a mere 1580 pages and six authors also published by Elsevier.

This new work is not light reading; figuratively or literally! The good news is that those wishing to avoid back strain can get the physically lighter on-line edition in pdf format. This was a massive undertaking and required a large team to write it. A major collaborative effort involving 3 editors in chief , 10 section editors and an additional 141 additional contributing authors many of whom were involved with more than one of the 84 chapters. The overall scope is shown in the Figure below..



Given the breadth of coverage, chemistry, environmental and life science, engineering and other areas especially in the Applications in Volume 4, this is not intended to be read from cover to cover but as a reference work to allow practitioners to gain an insight into the extraordinary world of chemometric methodologies. There is something here for everyone and the mathematical barrier is lowered somewhat by the excellent use of diagrams and figures particularly the intelligent use of colour for example in a chapter on experimental design 1-14.

Some chapters are more mathematically challenging than others. For example Chapter 1.08 0m Bayesian Methodology in Statistics is not for the faint hearted. In contrast Chapter 1.03 on Proficiency Testing is much more approachable.

Volume 2, in particular, contains much to interest the spectroscopist particularly on data preprocessing and noise reduction. There are also good chapters on the introduction to multivariate curve resolution and principal component analysis. Unsupervised data mining has 6 chapters covering the major clustering techniques.

Overall this is a comprehensive reference work and is well worthy of a place in any analytical science library.

Chris Burgess