- **Preface**
- **1 Introduction**
- **1.1 Development of Chemometrics**
- **1.2 Application Areas**
- **1.3 How to Use this Book**
- **1.4 Literature and Other Sources of Information**
- **References**
- **2 Experimental Design**
- **2.1 Why Design Experiments in Chemistry?**
- **2.2 Degrees of Freedom and Sources of Error**
- **2.3 Analysis of Variance and Interpretation of Errors**
- **2.4 Matrices, Vectors and the Pseudoinverse**
- **2.5 Design Matrices**
- **2.6 Factorial Designs**
- **2.7 An Example of a Factorial Design**
- **2.8 Fractional Factorial Designs**
- **2.9 Plackett-Burman and Taguchi Designs**
- **2.10 The Application of a Plackett-Burman Design to the Screening of Factors Influencing a Chemical Reaction**
- **2.11 Central Composite Designs**
- **2.12 Mixture Designs**
- **2.13 A Four Component Mixture Design Used to Study Blending of Olive Oils**
- **2.14 Simplex Optimization**
- **2.15 Leverage and Confidence in Models**
- **2.16 Designs for Multivariate Calibration**
- **References**
- **3 Statistical Concepts**
- **3.1 Statistics for Chemists**
- **3.2 Errors**
- **3.3 Describing Data**
- **3.4 The Normal Distribution**
- **3.5 Is a Distribution Normal?**
- **3.6 Hypothesis Tests**
- **3.7 Comparison of Means: the t-Test**
- **3.8 F-Test for Comparison of Variances**
- **3.9 Confidence in Linear Regression**
- **3.10 More about Confidence**
- **3.11 Consequences of Outliers and How to Deal with Them**
- **3.12 Detection of Outliers**
- **3.13 Shewhart Charts**
- **3.14 More about Control Charts**
- **References**
- **4 Sequential Methods**
- **4.1 Sequential Data**
- **4.2 Correlograms**
- **4.3 Linear Smoothing Functions and Filters**
- **4.4 Fourier Transforms**
- **4.5 Maximum Entropy and Bayesian Methods**

- **4.6 Fourier Filters**
- **4.7 Peakshapes in Chromatography and Spectroscopy**
- **4.8 Derivatives in Spectroscopy and Chromatography**
- **4.9 Wavelets**
- **References**
- **5 Pattern Recognition**
- **5.1 Introduction**
- **5.2 Principal Components Analysis**
- **5.3 Graphical Representation of Scores and Loadings**
- **5.4 Comparing Multivariate Patterns**
- **5.5 Preprocessing**
- **5.6 Unsupervised Pattern Recognition: Cluster Analysis**
- **5.7 Supervised Pattern Recognition**
- **5.8 Statistical Classification Techniques**
- **5.9 K Nearest Neighbour Method**
- **5.10 How Many Components Characterize a Dataset?**
- **5.11 Multiway Pattern Recognition**
- **References**
- **6 Calibration**
- **6.1 Introduction**
- **6.2 Univariate Calibration**
- **6.3 Multivariate Calibration and the Spectroscopy of Mixtures**
- **6.4 Multiple Linear Regression**
- **6.5 Principal Components Regression**
- **6.6 Partial Least Squares**
- **6.7 How Good is the Calibration and What is the Most Appropriate Model?**
- **6.8 Multiway Calibration**
- **References**
- **7 Coupled Chromatography**
- **7.1 Introduction**
- **7.2 Preparing the Data**
- **7.3 Chemical Composition of Sequential Data**
- **7.4 Univariate Purity Curves**
- **7.5 Similarity Based Methods**
- **7.6 Evolving and Window Factor Analysis**
- **7.7 Derivative Based Methods**
- **7.8 Deconvolution of Evolutionary Signals**
- **7.9 Noniterative Methods for Resolution**
- **7.10 Iterative Methods for Resolution**
- **8 Equilibria, Reactions and Process Analytics**
- **8.1 The Study of Equilibria using Spectroscopy**
- **8.2 Spectroscopic Monitoring of Reactions**
- **8.3 Kinetics and Multivariate Models for the Quantitative Study of Reactions**
- **8.4 Developments in the Analysis of Reactions using On-line Spectroscopy**
- **8.5 The Process Analytical Technology Initiative**
- **References**