

Contents

Preface *vii*

List of Abbreviations *xi*

1	What is Chemometrics?	1
1.1	The Computer-Based Laboratory	3
1.2	Statistics and Data Interpretation	11
1.3	Computer-Based Information Systems/Artificial Intelligence	12
	General Reading	13
	Questions and Problems	13
2	Basic Statistics	15
2.1	Descriptive Statistics	16
2.2	Statistical Tests	28
2.3	Analysis of Variance	45
	General Reading	56
	Questions and Problems	57
3	Signal Processing and Time Series Analysis	61
3.1	Signal Processing	62
3.2	Time Series Analysis	91
	General Reading	99
	Questions and Problems	100
4	Optimization and Experimental Design	101
4.1	Systematic Optimization	102
4.2	Objective Functions and Factors	103
4.3	Experimental Design and Response Surface Methods	111
4.4	Sequential Optimization: Simplex Method	135

General Reading 142
Questions and Problems 142

**5 Pattern Recognition and
Classification 145**

- 5.1 Preprocessing of Data 147
- 5.2 Unsupervised Methods 151
- 5.3 Supervised Methods 198
- General Reading 226
- Questions and Problems 227

6 Modeling 231

- 6.1 Univariate Linear Regression 232
- 6.2 Multiple Linear Regression 249
- 6.3 Nonlinear Methods 281
- General Reading 293
- Questions and Problems 293

7 Analytical Databases 295

- 7.1 Representation of Analytical Information 296
- 7.2 Library Search 309
- 7.3 Simulation of Spectra 316
- General Reading 318
- Questions and Problems 318

**8 Knowledge Processing and Soft
Computing 321**

- 8.1 Artificial Intelligence and Expert Systems 321
- 8.2 Neural Networks 330
- 8.3 Fuzzy Theory 352
- 8.4 Genetic Algorithms and Other Global Search
Strategies 365
- General Reading 375
- Questions and Problems 377

**9 Quality Assurance and Good Laboratory
Practice 379**

- 9.1 Validation and Quality Control 380
- 9.2 Accreditation and Good Laboratory Practice 384
- General Reading 386
- Questions and Problems 386

Appendix 387

Index 403