

# Contents

<i>Preface</i>	xi
<i>Note to Readers</i>	xiii
1. A New Beginning . . .	1
2. Elementary Matrix Algebra: Part 1	9
3. Elementary Matrix Algebra: Part 2	17
4. Matrix Algebra and Multiple Linear Regression: Part 1	23
5. Matrix Algebra and Multiple Linear Regression: Part 2	33
6. Matrix Algebra and Multiple Linear Regression: Part 3 – The Concept of Determinants	43
7. Matrix Algebra and Multiple Linear Regression: Part 4 – Concluding Remarks	47
8. Experimental Designs: Part 1	51
9. Experimental Designs: Part 2	57
10. Experimental Designs: Part 3	63
11. Analytic Geometry: Part 1 – The Basics in Two and Three Dimensions	71
12. Analytic Geometry: Part 2 – Geometric Representation of Vectors and Algebraic Operations	77
13. Analytic Geometry: Part 3 – Reducing Dimensionality	81
14. Analytic Geometry: Part 4 – The Geometry of Vectors and Matrices	85
15. Experimental Designs: Part 4 – Varying Parameters to Expand the Design	89
16. Experimental Designs: Part 5 – One-at-a-time Designs	91
17. Experimental Designs: Part 6 – Sequential Designs	93
18. Experimental Designs: Part 7 – $\beta$ , the Power of a Test	97
19. Experimental Designs: Part 8 – $\beta$ , the Power of a Test (Continued)	101
20. Experimental Designs: Part 9 – Sequential Designs Concluded	103
21. Calculating the Solution for Regression Techniques: Part 1 – Multivariate Regression Made Simple	107
22. Calculating the Solution for Regression Techniques: Part 2 – Principal Component(s) Regression Made Simple	109
23. Calculating the Solution for Regression Techniques: Part 3 – Partial Least Squares Regression Made Simple	113
24. Looking Behind and Ahead: Interlude	117
25. A Simple Question: The Meaning of Chemometrics Pondered	119
26. Calculating the Solution for Regression Techniques: Part 4 – Singular Value Decomposition	127
27. Linearity in Calibration	131
28. Challenges: Unsolved Problems in Chemometrics	135
29. Linearity in Calibration: Act II Scene I	141
30. Linearity in Calibration: Act II Scene II – Reader's Comments . . .	145
31. Linearity in Calibration: Act II Scene III	149

32. Linearity in Calibration: Act II Scene IV	159
33. Linearity in Calibration: Act II Scene V	163
34. Collaborative Laboratory Studies: Part 1 – A Blueprint	167
35. Collaborative Laboratory Studies: Part 2 – using ANOVA	179
36. Collaborative Laboratory Studies: Part 3 – Testing for Systematic Error	183
37. Collaborative Laboratory Studies: Part 4 – Ranking Test	185
38. Collaborative Laboratory Studies: Part 5 – Efficient Comparison of Two Methods	187
39. Collaborative Laboratory Studies: Part 6 – MathCad Worksheet Text	193
40. Is Noise Brought by the Stork? Analysis of Noise: Part 1	223
41. Analysis of Noise: Part 2	227
42. Analysis of Noise: Part 3	235
43. Analysis of Noise: Part 4	243
44. Analysis of Noise: Part 5	253
45. Analysis of Noise: Part 6	271
46. Analysis of Noise: Part 7	277
47. Analysis of Noise: Part 8	285
48. Analysis of Noise: Part 9	293
49. Analysis of Noise: Part 10	299
50. Analysis of Noise: Part 11	313
51. Analysis of Noise: Part 12	317
52. Analysis of Noise: Part 13	323
53. Analysis of Noise: Part 14	329
54. Derivatives in Spectroscopy: Part 1 – The Behavior of the Derivative	339
55. Derivatives in Spectroscopy: Part 2 – The “True” Derivative	351
56. Derivatives in Spectroscopy: Part 3 – Computing the Derivative	359
57. Derivatives in Spectroscopy: Part 4 – Calibrating with Derivatives	371
58. Comparison of Goodness of Fit Statistics for Linear Regression: Part 1 – Introduction	379
59. Comparison of Goodness of Fit Statistics for Linear Regression: Part 2 – The Correlation Coefficient	385
60. Comparison of Goodness of Fit Statistics for Linear Regression: Part 3 – Computing Confidence Limits for the Correlation Coefficient	393
61. Comparison of Goodness of Fit Statistics for Linear Regression: Part 4 – Confidence Limits for Slope and Intercept	399
62. Correction and Discussion Regarding Derivatives	413
63. Linearity in Calibration: Act III Scene I – Importance of Nonlinearity	421
64. Linearity in Calibration: Act III Scene II – A Discussion of the Durbin-Watson Statistic, a Step in the Right Direction	427
65. Linearity in Calibration: Act III Scene III – Other Tests for Nonlinearity	435
66. Linearity in Calibration: Act III Scene IV – How to Test for Nonlinearity	439
67. Linearity in Calibration: Act III Scene V – Quantifying Nonlinearity	451
68. Linearity in Calibration: Act III Scene VI – Quantifying Nonlinearity, Part II, and a News Flash	459
69. Connecting Chemometrics to Statistics: Part 1 – The Chemometrics Side	471
70. Connecting Chemometrics to Statistics: Part 2 – The Statistics Side	477
71. Limitations in Analytical Accuracy: Part 1 – Horwitz’s Trumpet	481

72. Limitations in Analytical Accuracy: Part 2 – Theories to Describe the Limits in Analytical Accuracy	487
73. Limitations in Analytical Accuracy: Part 3 – Comparing Test Results for Analytical Uncertainty	491
74. The Statistics of Spectral Searches	497
75. The Chemometrics of Imaging Spectroscopy	503
<i>Glossary of Terms</i>	509
<i>Index</i>	513
<i>Colour Plate Section</i>	