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Nota di contenuto	Cover -- Statistics and Chemometrics for Analytical Chemistry -- Contents -- Preface to the sixth edition -- Preface to the first edition -- Acknowledgements -- Glossary of symbols -- Introduction -- Analytical problems -- Errors in quantitative analysis -- Types of error -- Random and systematic errors in titrimetric analysis -- Handling systematic errors -- Planning and design of experiments -- Calculators and computers in statistical calculations -- Bibliography and resources -- Exercises -- Statistics of repeated measurements -- Mean and standard deviation -- The distribution of repeated measurements -- Log-normal distribution -- Definition of a 'sample' -- The sampling distribution of the mean -- Confidence limits of the mean for large samples -- Confidence limits of the mean for small samples -- Presentation of results -- Other uses of confidence limits -- Confidence limits of the geometric mean for a log-normal distribution -- Propagation of random errors -- Propagation of systematic errors -- Bibliography -- Exercises -- Significance tests -- Introduction -- Comparison of an experimental mean with a known value -- Comparison of two experimental means -- Paired t -test -- One-sided and two-sided tests -- F-test for the comparison of standard deviations -- Outliers -- Analysis of variance -- Comparison of several

means -- The arithmetic of ANOVA calculations -- The chi-squared test -- Testing for normality of distribution -- Conclusions from significance tests -- Bayesian statistics -- Bibliography -- Exercises -- The quality of analytical measurements -- Introduction -- Sampling -- Separation and estimation of variances using ANOVA -- Sampling strategy -- Introduction to quality control methods -- Shewhart charts for mean values -- Shewhart charts for ranges -- Establishing the process capability -- Average run length: CUSUM charts.
Zone control charts (J-charts) -- Proficiency testing schemes -- Method performance studies (collaborative trials) -- Uncertainty -- Acceptance sampling -- Method validation -- Bibliography -- Exercises -- Calibration methods in instrumental analysis: regression and correlation -- Introduction: instrumental analysis -- Calibration graphs in instrumental analysis -- The product-moment correlation coefficient -- The line of regression of y on x -- Errors in the slope and intercept of the regression line -- Calculation of a concentration and its random error -- Limits of detection -- The method of standard additions -- Use of regression lines for comparing analytical methods -- Weighted regression lines -- Intersection of two straight lines -- ANOVA and regression calculations -- Introduction to curvilinear regression methods -- Curve fitting -- Outliers in regression -- Bibliography -- Exercises -- Non-parametric and robust methods -- Introduction -- The median: initial data analysis -- The sign test -- The Wald-Wolfowitz runs test -- The Wilcoxon signed rank test -- Simple tests for two independent samples -- Non-parametric tests for more than two samples -- Rank correlation -- Non-parametric regression methods -- Introduction to robust methods -- Simple robust methods: trimming and winsorisation -- Further robust estimates of location and spread -- Robust ANOVA -- Robust regression methods -- Re-sampling statistics -- Conclusions -- Bibliography and resources -- Exercises -- Experimental design and optimisation -- Introduction -- Randomisation and blocking -- Two-way ANOVA -- Latin squares and other designs -- Interactions -- Identifying the important factors: factorial designs -- Fractional factorial designs -- Optimisation: basic principles and univariate methods -- Optimisation using the alternating variable search method.
The method of steepest ascent -- Simplex optimisation -- Simulated annealing -- Bibliography and resources -- Exercises -- Multivariate analysis -- Introduction -- Initial analysis -- Principal component analysis -- Cluster analysis -- Discriminant analysis -- K-nearest neighbour method -- Disjoint class modelling -- Regression methods -- Multiple linear regression -- Principal component regression -- Partial least-squares regression -- Natural computation methods: artificial neural networks -- Conclusions -- Bibliography and resources -- Exercises -- Solutions to exercises -- Appendix 1: Commonly used statistical significance tests -- Appendix 2: Statistical tables -- Index.

Sommario/riassunto

This popular textbook gives a clear account of the principles of the main statistical methods used in modern analytical laboratories. Such methods underpin high quality analyses in areas such as the safety of food, water and medicines, environmental monitoring, and chemical manufacturing. The treatment throughout emphasises the underlying statistical ideas, and no detailed knowledge of mathematics is required. There are numerous worked examples, including the use of Microsoft Excel and Minitab, and a large number of student exercises, many of them based on examples from the analytical literature.