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Descrizione fisica	1 online resource (272 p.)
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Formato	Materiale a stampa
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Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Statistical Treatment of Analytical Data; Contents; Preface; 1 Introduction; 1.1 Statistics and quality assurance, control and assessment; 1.2 References; 2 Statistical measures of experimental data; 2.1 Mean and standard deviation; 2.2 Graphical distributions of the data - bar charts or histograms; 2.3 Propagation of errors (uncertainties); 2.4 References; 3 Distribution functions; 3.1 Confidence limit of the mean; 3.2 Measurements and distribution functions; 3.3 Mathematical presentation of distribution and; 3.4 Continuous distribution functions; 3.5 Discrete distribution functions 3.6 References4 Confidence limits of the mean; 4.1 Confidence limits; 4.2 The Central Limit Theorem - the distribution of means; 4.3 Confidence limit of the mean; 4.4 Confidence limits of the mean of small samples; 4.5 Choosing the sample size; 5 Significance test; 5.1 Introduction; 5.2 Comparison of an experimental mean with an expected; 5.3 Comparison of two samples; 5.4 Paired t-test; 5.5 Comparing two variances - the F-test; 5.6 Comparison of several

means; 5.7 The chi-squared (χ^2) test; 5.8 Testing for normal distribution - probability paper; 5.9 Non-parametric tests; 5.10 References

6 Outliers 6.1 Introduction; 6.2 Dixon's Q-test; 6.3 The rule of huge error; 6.4 Grubbs test for outliers; 6.5 Youden test for outlying laboratories; 6.6 References; 7 Instrumental calibration - regression analysis; 7.1 Errors in instrumental analysis vs. classical 'wet chemistry' methods; 7.2 Standards for calibration curves; 7.3 Derivation of an equation for calibration curves; 7.4 Least squares as a maximum likelihood estimator; 7.5 Tests for linearity; 7.6 Calculation of the concentration; 7.7 Weighted least squares linear regression; 7.8 Polynomial calibration equations

7.9 Linearization of calibration curves in nuclear measurements 7.10 Non-linear curve fitting; 7.11 Fitting straight-line data with errors in both coordinates; 7.12 Limit of detection; 7.13 References; 8 Identification of analyte by multi-measurement analysis; 8.1 References; 9 Smoothing of spectra signals; 9.1 Introduction; 9.2 Smoothing of spectrum signals; 9.3 Savitzky and Golay method (SG method); 9.4 Studies in noise reduction; 9.5 Extension of SG method; 9.6 References; 10 Peak search and peak integration; 10.1 A statistical method; 10.2 First derivative method

10.3 Second derivative method 10.4 Computer - visual separation of peaks; 10.5 Selection of the fitting interval and integration; 10.6 References; 11 Fourier Transform methods; 11.1 Fourier Transform methods in spectroscopy; 11.2 Mathematics of Fourier Transforms; 11.3 Discrete Fourier Transforms; 11.4 Fast Fourier Transforms (FFT); 11.5 References; 12 General and specific issues in uncertainty analysis; 12.1 Introduction; 12.2 The uncertainty era; 12.3 Uncertainties and the laws of nature; 12.4 The creation of the universe and the law of energy and mass

12.5 Statistical and systematic uncertainties

Sommario/riassunto

Statistical techniques have assumed an integral role in both the interpretation and quality assessment of analytical results. In this book the range of statistical methods available for such tasks are described in detail, with the advantages and disadvantages of each technique clarified by use of examples. With a focus on the essential practical application of these techniques the book also includes sufficient theory to facilitate understanding of the statistical principles involved. Statistical Treatment of Analytical Data is written for professional analytical chemists in

2. Record Nr.	UNINA9910279754703321
Autore	Trangenstein J. A (John Arthur), <1949->
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ISBN	3-319-69107-4
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Collana	Texts in Computational Science and Engineering, , 1611-0994 ; ; 19
Disciplina	512.9436
Soggetti	Computer science - Mathematics Differential equations Mathematical optimization Computational Mathematics and Numerical Analysis Ordinary Differential Equations Optimization
Lingua di pubblicazione	Inglese
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Nota di contenuto	1. Eigenvalues and Eigenvectors -- 2. Iterative Linear Algebra -- 3. Nonlinear Systems -- 4. Constrained Optimization -- References -- Author Index.
Sommario/riassunto	This is the second of three volumes providing a comprehensive presentation of the fundamentals of scientific computing. This volume discusses more advanced topics than volume one, and is largely not a prerequisite for volume three. This book and its companions show how to determine the quality of computational results, and how to measure the relative efficiency of competing methods. Readers learn how to determine the maximum attainable accuracy of algorithms, and how to select the best method for computing problems. This book also discusses programming in several languages, including C++, Fortran and MATLAB. There are 49 examples, 110 exercises, 66 algorithms, 24 interactive JavaScript programs, 77 references to software programs and 1 case study. Topics are introduced with goals, literature references and links to public software. There are descriptions of the current algorithms in LAPACK, GSLIB and MATLAB. This book could be

used for a second course in numerical methods, for either upper level undergraduates or first year graduate students. Parts of the text could be used for specialized courses, such as nonlinear optimization or iterative linear algebra.
