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## Chemometrics

By Otto, Matthias

Wiley-VCH, 2007. Book Condition: New. Brand New, Unread Copy in Perfect Condition. A+ Customer Service! Summary: 1 What is Chemometrics? 1.1 The Computer-based Laboratory. 1.2 Statistics and Data Interpretation. 1.3 Computer-based Information Systems/Artificial Intelligence. 1.4 General Reading. 2 Basic Statistics. 2.1 Descriptive Statistics. 2.2 Statistical Tests. 2.3 Analysis of Variance. 2.4 General Reading. 3 Signal Processing and Time-Series Analysis. 3.1 Signal Processing. 3.2 Time Series Analysis. 3.3 General Reading. 4 Optimization and Experimental Design. 4.1 Objective Functions and Factors. 4.2 Experimental Designs and Response Surface Methods. 4.2.1 Fundamentals. 4.2.2 Two-level designs: screening designs. 4.2.3 Three-level designs: response surface designs. 4.3 Sequential Optimization: Simplex Method. 4.4 General Reading. 5 Pattern Recognition and Classification. 5.1 Preprocessing of Data. 5.2 Unsupervised Methods. 5.2.1 Factorial methods. 5.2.2 Cluster analysis. 5.2.3 Graphical methods. 5.3 Supervised Methods. 5.3.1 Linear learning machine. 5.3.2 Discriminant analysis. 5.3.3 -nearest neighbor method. 5.3.4 SIMCA. 5.3.5 Support vector machines. 5.4 General Reading. 6 Modeling. 6.1 Univariate Linear Regression. 6.2 Multiple Linear Regression. 6.2.1 Ordinary test squares regression. 6.2.2 Biased parameter estimations: PCR and PLS. 6.2.3 Applications for multicomponent analysis. 6.2.4 Regression diagnostics. 6.2.5 Multiway regression (modeling). 6.3 Nonlinear Methods. 6.3.1 Nonlinear regression analysis. 6.3.2 Nonparametric methods. 6.4 General Reading. 7 Analytical...


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