Advanced Chemometrics

Schedule:

Week 1: Descriptive statistics. Mathematical characterization of distributions. Probability density function, cumulative distribution function, expected value, mean value, standard deviation, variance. Central Limit Theorem.

Week 2: Statistical Hypothesis Testing I. t-test. Types, applications, practical examples.

Week 3: Statistical Hypothesis Testing II. ANOVA. Types, applications, practical examples.

Week 4: Principal Component Analysis (PCA) I. Theoretical background. Information encoded by principal components. Variance, eigenvalues, loadings, scores. Steps of the transformation.

Week 5: Principal Component Analysis (PCA) II. Practical applications. Information obtained through the transformation. Pitfalls.

Week 6: Cluster Analysis and Linear Discriminant Analysis (LDA).

Week 7: Modeling I. Linear least-squares fitting. Regression analysis.

Week 8: Modeling II. Nonlinear least-squares fitting. Selected methods of numerical mathematics.

Week 9: Design of Experiments (DoE) I. Sensitivity analysis (screening).

Week 10: Design of Experiments (DoE) II. Optimization.

Week 11: Calibration in analytical chemistry. External standard, internal standard, standard addition, and surrogate (matrix-matched) standard methods.

Week 12: Multivariate calibration. Principal component regression (PCR).