

Advanced Statistics for Analytical Chemists

This course is designed for scientists involved in experimental design, decision making and process optimisation.

The course shows how to use analysis of variance, randomisation and manipulation of controllable variables to reduce variability, time and cost of design and development.

Course Contents

Quality Control Methods

- Shewhart charts for mean values
- Shewhart charts for ranges
- Warning and action lines
- Cusum charts
- Zone control charts (J-charts)
- Specification setting

Experimental Design and Optimisation

- Introduction
- Randomisation and blocking
- Two-way ANOVA
- Latin squares and other designs
- Simulated annealing
- Interactions
- Factorial versus one-at-a-time design
- Factorial design and optimisation
- Optimisation: basic principles and univariate methods
- Optimisation using the alternating variable search method
- The method of steepest ascent
- Simplex optimisation

The Multivariate Analysis

- Introduction
- Initial analysis
- Principal component analysis
- Cluster analysis
- Discriminant analysis
- K-nearest neighbour method
- Disjoint class modelling
- Regression methods
- Multiple linear regression (MLR)
- Principal components regression (PCR)
- Partial least squares (PLS) regression
- Artificial neural networks