CQ Consultancy

Setting the standard in

Chemometrics and Applied Statistics training

Course program 2012

THIS IS WHAT PARTICIPANTS APPRECIATE:

- **Application-oriented course concept**
  - Provide insight (no cookbook approach)
  - Mix of theory and case studies + hands-on exercises on real-life examples
  - Main goal = direct applicability
- **Quality guarantee**
  - +15 years of experience in training and consulting Chemometrics and Applied Statistics
  - Unique money-back guarantee if a course doesn't fulfill your expectations

CQ Consultancy

CQ Consultancy is a competence center in Chemometrics and Applied Statistics. Building on over 15 years of experience, CQ Consultancy offers its services to chemical, pharmaceutical and food industries, through training, consulting and contracting. Due to our lean organisation we offer our services at prices beyond competition, even when compared with in-house alternatives!

COURSE OVERVIEW

- **Design of Experiments (DOE)**
  Efficiently developing processes and products; exploration and optimization

- **Applied Statistics**
  Backing up decisions by means of classical statistical tools and modern alternatives

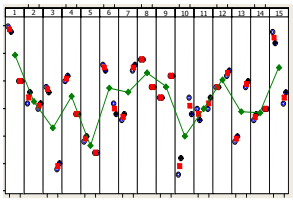
- **Statistical Quality Control (SQC)**
  Statistics-based process monitoring and control: standard and novel approaches.
  Capability Analysis and Measurement System Analysis.

- **Multivariate Data Analysis**
  Acquiring information and insights by analyzing large amounts of (non-designed) data

- **Spectroscopic (NIR) Calibration**
  Spectroscopic regression models as an alternative to lab analyses

IN-COMPANY TRAINING

All trainings listed can be organised in-company, in the language of your choice (English, Dutch, German or French), with the software of your choice, and with the possibility to adapt the exercises and course contents to your needs.



Statistics in Practice

WHY STATISTICS IN PRACTICE?

After years of neglect in industry, statistics is finally being recognized as one of the cornerstones of "good decision making". The statistical analysis and validation of results is no longer merely encouraged but demanded; this is the case both for conclusions from the analytical lab as for research results. This course is intended for anyone who wants to retrieve the information from statistical numbers and graphs so easily produced by software.

COURSE SET-UP

During the first two days all basic statistical concepts and techniques are treated, which will guide the participants through a correct statistical analysis of their results, originating from experiments or other sources. The third day expands the statistical toolbox with such methods as two-way ANOVA, nested designs for the identification of the most important sources of variation (e.g. for an R&r study) and polynomial regression.
Theory will alternate with hands-on computer exercises.

COURSE OBJECTIVE

As a result of this course, participants will acquire a good insight into statistics and they will be able to choose an appropriate technique and interpret the results correctly.

INTENDED AUDIENCE AND PRIOR KNOWLEDGE

This course is intended for anyone who wants to acquire a solid background in statistical thinking and master the application of it to questions that arise in every day's work. Although theoretical details are skipped whenever possible, it is still about statistics. And although no prior knowledge is required, some affinity for numbers is a definite plus.

PRACTICAL

Each course day will be held from 9 am to about 5 pm. The course dates and fees are listed on the application form. The course fee includes handouts and lunches.
To apply, send us back the application form, or apply on-line, at least 20 days before the start of the course .

CQ Consultancy, Thurgauerstrasse 40, CH-8050 Zürich, info@cqplus.ch, www.cqplus.ch

COURSE CONTENTS

Module 1 (2 days)

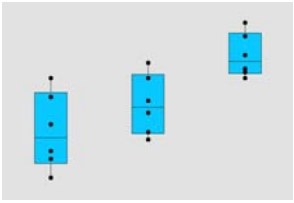
- Descriptive statistics
  - Graphical techniques: scatter plots, histogram, dotplot, boxplot, normal probability plot
  - Descriptive statistics: means, median, variance, IQR, ...
  - Describing the similarity between variables: covariance & correlation
  - Autocorrelation
- Good data collection practice
  - Sampling strategies
  - Paired comparisons
- Dealing with random variables (probability distributions)
  - Properties of distributions of random variables
  - Distributions for discrete and continuous variables: Binomial, Poisson, normal distribution, Weibull, ...
- Functions of random variables: the z-distribution, χ^2, t and the F-distribution
- Confidence intervals for means, difference in means, variances, proportions, capability indices, …
- Hypothesis testing
  - Hypothesis testing with confidence intervals
  - Classical hypothesis testing
  - Statistical significant versus practical relevant
  - Type I and Type II errors
  - Power and sample size calculations
- One-way ANOVA
- Simple Linear Regression

Module 2 (1 day)

- Two-way ANOVA
- Random effects and nested ANOVA – Variance Components Analysis (R&r study)
- Polynomial Regression

Some cases & applications:

Detecting and proving a change in a process / Quantifying and judging the difference between two products or systems / Deciding on the equivalence of analysis methods / Setting a specification taking the customers' measurement error into account / Calculating the effect of variation in addition and adjustment of a component on the process performance / Calculating the number of data needed to detect a certain improvement / Investigating the effect of different types of constituents on the product properties / Identifying the major source of variation / Investigating the effect of a process parameter on a characteristic



Applied Statistics

A primer

APPLIED STATISTICS, a (solid) primer

Statistics will never be easy. And to acquire an in-depth understanding requires serious efforts and a considerable amount of time; time which may not be available to you. As an alternative for the three-day course Statistics in Practice, this compact version covers the essential concepts of statistics, from descriptive statistics over probability, hypothesis testing, power and sample size calculations to ANOVA and regression. Although primarily intended as a "foundation" on which further courses are built, this course will result in many eye-openers and at the same time enhance the quality of everyday's decision making.

COURSE SET-UP

The set-up is similar to the first two days of the Statistics in Practice course but some more "advanced" extensions are skipped and only continuous variables will be treated. Theory will alternate with hands-on computer exercises.

COURSE OBJECTIVE

As a result of this course, participants will develop a good feel for statistics and will be able to choose an appropriate technique and interpret the results correctly for the most common types of problems.

INTENDED AUDIENCE AND PRIOR KNOWLEDGE

This course is intended for anyone who wants to acquire a solid background in statistical thinking before taking on the more advanced courses like DOE or multivariate analysis. Although everything discussed is directly applicable in practice, we recommend the three-day Statistics in Practice course if you aim at more than getting a primer.
No prior knowledge is required.

PRACTICAL

Each course day will be held from 8.30 am to about 5 pm. The course dates and fees are listed on the attached application form. The course fee includes handouts and lunches.
To apply, send us back the application form or apply on-line, at least 20 days before the start of the course .

COURSE CONTENTS

Module 1

- Descriptive statistics
  - Graphical techniques: scatter plot, histogram, dotplot, boxplot, normal probability plot
  - Descriptive statistics: means, median, variance, IQR, ...
- Good data collection practice
  - Representative sampling
  - Paired comparisons

Module 2

- Dealing with random variables (probability distributions)
  - Properties of distributions of random variables
  - The normal distribution and its derivatives (the z, χ^2, t and F-distribution).

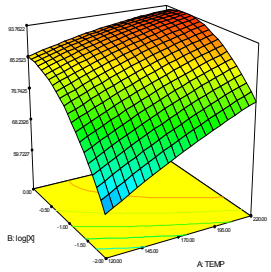
Module 3

- Confidence intervals for means, differences in means and variances
- Hypothesis testing
  - Hypothesis testing with confidence intervals
  - Classical hypothesis testing
  - Statistical significant versus practical relevant
  - Type I and Type II errors
  - Power and sample size calculations

Module 4

- One-way ANOVA
- Describing the similarity between variables: correlation and Simple Linear Regression

Some cases &applications: detecting and proving a change in a process / quantifying and judging the difference between two products or systems / calculating the number of data needed to detect a certain improvement / investigating the effect of different types of a constituent on the product properties / investigating the effect of a process parameter on a characteristic



Design of Experiments

in chemical and related industries

COST-EFFICIENT RESEARCH

Research & Development: searching for new products and improving existing processes. This can be accomplished efficiently and optimally only in one way: the way of Experimental Design. Experimental Design, alias Design of Experiments (DOE) or Statistical Design of Experiments (SDE), not only guarantees reaching the preset goal, but on top costs a minimum number of experiments ... on condition that one takes into account the characteristics of the field of application. The optimal strategy of experimenting will be different in chemical industries as compared to for example the automotive industry. This explains the specific context of this course.

COURSE SET-UP

Four courses on DOE are offered: an introductory course (DOE-I: 4 days), a follow-up course (DOE-II: 1.5 days), a course on Principal Properties Design (0.5 day) and a Mixture Design course (1 day). DOE-I is limited to standard designs for continuous variables.

Categorical variables (e.g. type of solvent or type of reactor) and generating and evaluating optimal designs will be discussed in DOE-II.

The Principal Properties Design course deals with how solving / circumventing the problem of multi-level categorical variables.

Designs for problems where the sum of constituents is constant will be discussed in the fourth course.

DOE-I PRACTICAL

Each course day will be held from 9 am to about 5 pm. The course dates and fees are listed on the attached application form. The course fee includes handouts and lunches.
To apply, send us back the application form, or apply on-line, at least 20 days before the start of the course .

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DOE-I

COURSE SET-UP

During the first three days the topics listed below will be theoretically treated, and illustrated with exercises. Day four is actually an Experimental Design "game": the participants go through all phases of a project: from problem analysis over choosing a design, up to analysing simulated data and reporting the results.

COURSE OBJECTIVE

At the end of the course the participants will be able to formalise a problem, find the appropriate design type and, except for complex problems, construct this design. The participants will also master the statistical analysis of standard designs for continuous variables.

INTENDED AUDIENCE AND PRIOR KNOWLEDGE

Those who want to acquire an "active" knowledge in setting up experiments according to Experimental Design theory, as well as people who want to understand both the Experimental Design principles and the results of the statistical analysis.

Participants to DOE-I are assumed to have a thorough understanding of some basic statistical techniques (normal probability plot, confidence intervals, hypothesis tests, Type I & Type II errors, power, ANOVA, regression). The 2-day course 'Applied Statistics – A primer' is ideally suited as a preparation to DOE-I.

The required prior knowledge can however also be obtained by private study. The course material consists of the handouts of the 'Applied Statistics – A primer' course, including problems and solutions. This selfstudy package can be ordered on-line or through the application form.

COURSE CONTENTS

Day 1 - 3

- One Variable At a Time versus Experimental Design
- The concept of interacting variables
- Replication, 2-level blocking variables and randomisation
- 2-level designs: Full Factorial, Fractional Factorial, Minimum-Run designs, Foldover designs, Confounding, Resolution
- Multi-level Response-Surface-Model designs
- Power-analysis: which is the smallest significant effect I can find, how many experiments will it cost to find an effect of a particular size
- Analysing the results with Analysis of Variance
- Residual analysis and graphical validation
- Visualisation of the results
- Response transformation
- Multi-response optimisation

Day 4

- Experimental Design game

DOE-II

Design of Experiments - additional applications

DOE-II deals with several extensions to the standard design approach that offer a solution to frequently occurring problems in practice, such as problems with categorical variables (e.g. type of additive), blocking (e.g. taking into account batch-to-batch variation) and the investigation and optimisation of robustness.

This course also addresses the problem of factors that are subject to combined constraints, for which standard (symmetrical) designs are inadequate.

COURSE SET-UP AND PRIOR KNOWLEDGE

The first day of this course builds further on what was treated in DOE-I.
The second day (a half-day) will mainly focus on generating and evaluating optimal designs, and less on the statistical analysis of experiments.
Theory will be illustrated with hands-on exercises.
Those who participate to DOE-II are assumed to have attended DOE-I.

COURSE OBJECTIVE

With the knowledge acquired in DOE-II, participants will be able to set up a design and to analyse the experimental results for almost all practical problems.

COURSE CONTENTS

Day 1

- Projection properties of designs
- Categorical variables: classical designs and their analysis
- Blocking and split-plot designs
- Hierarchical designs – Variance Components Analysis
- Robustness investigation (minimising the influence of nuisance variables): Taguchi approach and alternatives

Day 2 (morning session only)

- Evaluation of designs: how accurate will the resulting model be, which effects can I determine, condition number, information index, VIF, D/G efficiency, Fraction of Design Space (FDS)
- Optimal designs: optimal configuration of experiments for constrained systems, for which symmetrical designs are inadequate

DOE-II PRACTICAL

Day 1 of this course will be held from 9 am to about 5 pm, day 2 from 9 am to 12.30 pm. The course dates and fees are listed on the attached application form. The course fee includes handouts and lunches.
To apply, send us back the application form, or apply on-line, at least 20 days before the start of the course .

PRINCIPAL PROPERTIES DESIGN

In several situations standard designs are inadequate, such as situations where categorical variables need to be investigated at several factor levels (e.g. type of solvent, additive, etc.). Principal Properties Designs are designs that replace categorical variables by continuous descriptors. At the basis of these designs: Principal Component Analysis (PCA).

Though being a multivariate method, in a DOE-context the use of PCA can also be powerful in the analysis of multi-response problems. PCA can reveal the correlation between all responses which helps identifying outlying values and prove unattainable targets (e.g. low value of response Y_1 combined with high values of Y_2 when they exhibit strong positive correlation).

COURSE SET-UP AND PRIOR KNOWLEDGE

In this course the basics of Principal Component Analysis will be discussed, with two illustrations of its use and power in a DOE context.
This session will be closed with hands-on exercises.
Those who participate to this course are assumed to have attended DOE-I.

COURSE OBJECTIVE

The objective of this course is to provide insight in the way multivariate methods can be of aid in setting up designs for multi-level categorical factors, and in analyzing multi-response problems.

COURSE CONTENTS

- Principal Component Analysis: the basics and interpretation of results
- Principal Properties Design
- The analysis of multi-response problems

PRACTICAL

This course will be held from 1.30 pm to 5 pm. The course dates and fees are listed on the attached application form. The course fee includes handouts and lunches.
To apply, send us back the application form, or apply on-line, at least 20 days before the start of the course .

MIXTURE DESIGNS

In this 1-day course designs will be discussed for mixture problems (e.g. polymerblends). Also D-optimal designs will be treated, however only as "black-box".

COURSE SET-UP AND PRIOR KNOWLEDGE

Theory will be illustrated with hands-on exercises.
Participants are assumed to have attended DOE-I. Also the optimal design part of the DOE-II course is recommended as preparation.

COURSE OBJECTIVE

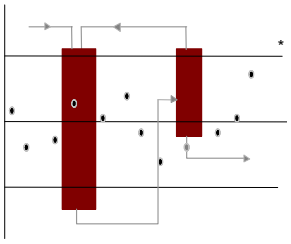
At the end of the course the participants will be able to set up designs for mixture problems and to analyse the experimental results.

COURSE CONTENTS

- The mixture problem
- Designs for regular design regions
- Models for mixture problems: slack variable, Scheffé and Cox models
- Analysis, interpretation and visualisation of mixture models
- Designs for irregular design regions (optimal designs: a black-box approach)
- Irregular regions: Response Surface Modelling

PRACTICAL

This course is offered in-company only.



Statistical Quality Control

in Chemistry and Process industry

WHY A SPECIFIC SQC COURSE?

Where SPC (Statistical Process Control) can be roughly defined as 'control charting', SQC (Statistical Quality Control) has a much broader meaning; it involves SPC, capability analysis as well as Measurement System Analysis (MSA).
However, the way SQC is being treated in most textbooks and courses doesn't focus enough on the typical problems of complex processes, and very often standard methods are not directly applicable. Also the specificity of the measurement system has its implications on the statistics involved, and should be explicitly taken into account.
In this course modifications and extensions to classical SPC are being proposed.

COURSE SET-UP

This two-day course consists of four modules. The statistics module serves as a quick refresher of the material of 'Applied Statistics – A primer' plus a treatment of discrete random variables. In each module, theoretical aspects are alternated with practical exercises. All examples and exercises are based on chemical processes.
The book "Introduction to Statistical Quality Control" by Douglas C. Montgomery is strongly recommended as additional reference material.

COURSE OBJECTIVES

The goal of this course: to offer a thorough introduction to SPC and MSA, with emphasis on typical situations in the process industry: one-at-a-time sampling, short-run processes, batch processes, serial correlations ("drifts") and complex measurements.

INTENDED AUDIENCE AND PRIOR KNOWLEDGE

This course addresses those who are at level with the material treated in 'Applied Statistics – A primer'. No prior knowledge of SQC is required.

COURSE CONTENTS

Module 1 : Introductory statistics for SQC

- Review of 'Applied Statistics – A primer'
- Probability for discrete variables: Binomial, Poisson, Geometric

Module II : Standard SQC

- Basic concepts
- Traditional control charts: X, X-bar, R, S, S^2, MR2, p, np, c and u
- Moving Average (MA) chart
  Exponentially Weighted MA (EWMA) chart
  Cumulative Sum (CUSUM) charts (classical and tabular)
- Process Capability: meaningful use and required conditions

Module III : SQC in process industry - specific solutions

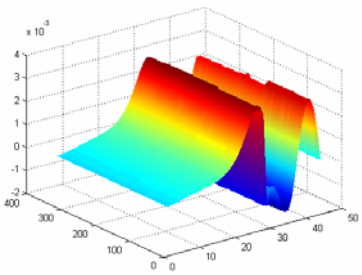
- SQC in the lab
- Control charts for "short run" processes, and "between-within batch" charts
- Serial correlation: detection and remedy
- SPC versus engineering (automatic) process control

Module IV : Measurement System Analysis

- Bias/Accuracy, Resolution and Linearity
- Measurement capability / Precision to Tolerance

PRACTICAL

This course is offered in-company only.



Spectroscopic (NIR) Calibration

WHY SPECTROSCOPIC CALIBRATION?

The last few years more and more companies opt for (on-line) NIR calibration models as an alternative to time-consuming and expensive lab analyses. This is often the case throughout the whole production process: to check the quality of the feedstock at delivery, to obtain timely information on different process streams, and to quantify the quality of the end product.
Due to continuous chemometrical developments, the number of applications of spectroscopic calibration - especially NIR - continues to increase, despite the strong overlap of spectral bands and peaks in the NIR region.

COURSE SET-UP

In this course we will go through the different steps required for a successful Spectroscopic Calibration: from sample selection over validation and interpretation of the models, up to guidelines and recommendations for the maintenance and update of calibration models in the future. Since emphasis will be put on practice, theoretical aspects will be alternated with practical exercises.

COURSE OBJECTIVE

In this course, the participants will develop a feel for the multivariate approach to spectroscopic calibration, gain insight into the underlying methods, learn to perform a multivariate calibration in "normal" situations and recognise problem situations.

INTENDED AUDIENCE AND PRIOR KNOWLEDGE

If your aim is to perform multivariate calibrations and/or to properly interpret the results, this course will satisfy your needs.
No prior knowledge is required.

PRACTICAL

Each course day will be held from 9 am to about 5 pm. The course dates and fees are listed on the attached application form. The course fee includes handouts and lunches.
To apply, send us back the application form, or apply on-line, at least 20 days before the start of the course .

COURSE CONTENTS

Day 1:

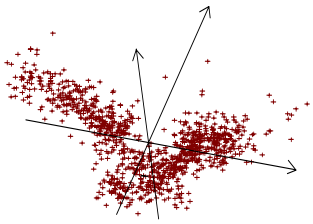
- NIR introduction
- Exploratory Multivariate Analysis
    - Visualisation of information in big data sets
    - Principal Component Analysis (PCA)
    - Cluster analysis: searching for groups of similar samples

Day 2:

- Basic principles of calibration techniques
    - Multiple Linear Regression (MLR)
    - Principal Component Regression (PCR)
    - Partial Least Squares (PLS)
- Interpretation of calibration models
- Model validation
- Preprocessing and scaling of spectra

Day 3:

- Detection of outliers and non-linearities
- Prediction with calibration models
- Selection of calibration samples
- Standardisation of calibration models
- Monitoring the performance of (on-line) calibration models



Multivariate Data Analysis

WHY MULTIVARIATE DATA ANALYSIS?

The massive amounts of (non-designed) collected data, often stored without further analysis, might contain valuable information about wanted and unwanted variation in process factors and product properties. A multivariate approach might reveal the cause of the unwanted variation or phenomena, without any additional experiments or measurements. Taking into account all available information will lead to insights in the often complex interplay of many factors.

COURSE SET-UP

During day 1 qualitative aspects of multivariate data analysis will be treated: exploring the data, searching for correlations, clusters, outliers, ...
In day 2 we come to the model building part: searching for relations between groups of variables. Emphasis will be put on correctly applying and interpreting the different techniques, and not on underlying theory. The course matter can immediately be applied with real-life exercises on PC.

COURSE OBJECTIVE

Multivariate analysis comprises a broad gamma of techniques, but at the same time contains an equally broad gamma of pitfalls. Breaking down the barriers towards multivariate analysis and smoothing the path towards expertise building while at the same time making the participants aware of the problems that arise, are considered to be the main objectives of this course.
At the end of the course participants will be able to select the proper technique to solve a number of problems, analyse the data and correctly interpret the results.

INTENDED AUDIENCE AND PRIOR KNOWLEDGE

This course will be of great help to anyone who is frequently faced with large data tables and who is not familiar with multivariate techniques, who can not make the appropriate choice, or who does not feel confident when trying to interpret the results of these methods.
Prior knowledge is not required.

PRACTICAL

Each course day will be held from 9 am to about 5 pm. The course dates and fees are listed on the attached application form. The course fee includes handouts and lunches.
To apply, send us back the application form, or apply on-line, at least 20 days before the start of the course .

COURSE CONTENTS

Day 1: Exploratory multivariate analysis

- Visualisation of big datasets
- Principal Component Analysis (PCA)
- Cluster analysis: searching for groups of similar samples

Day 2: Quantitative analysis: in search of cause-effect relations

- Multiple Linear Regression (MLR) with uncorrelated variables
- Multiple Linear Regression (MLR) with correlated variables
    - Stepwise regression
    - The collinearity problem
    - An overview of the pitfalls
- Principal Component Regression (PCR)
- Partial Least Squares (PLS)
    - Interpretation of PCR and PLS models
    - Validation of regression models
    - Detection of outliers and non-linearities
    - Prediction with regression models
- Some alternatives

Day 3: Quantitative analysis: the sequel + specific applications

- Feasibility study: does a quantitative analysis make sense?
- Classification (supervised pattern recognition): predicting class membership
    - Classification rules
    - Linear Discriminant Analysis (LDA)
    - Soft Independent Modeling of Class Analogy (SIMCA)
    - PLS-DA
- Specific applications:
    - QSAR / QSPR (Quantitative Structure Activity / Property Relations)
    - Multivariate SPC (M-SPC)
    - Principal Properties Design
    - .....

Course calendar 2012

Course	Course Dates	Language**	Location	Fee
❑ **Statistics in Practice**	❑ May 2, 3, 4	English	Leuven (B)	CHF 1.550
❑ **Applied Statistics – A primer**	❑ November 8- 9	German	Zürich	CHF 1.200*
❑ **Private study package**				CHF 350
❑ **Design of Experiments (DOE-I)**	❑ May 22-25	English	Leuven (B)	CHF 2.400
	❑ December 4-7	German	Zürich	CHF 2.400
❑ **Design of Experiments (DOE-II)**	❑ March 20-21	English	Leuven (B)	CHF 900
❑ **Multivariate Data Analysis**	❑ December 4-6	English	Leuven (B)	CHF 1.450
❑ **Spectroscopic Calibration**	❑ March 27-29	English	Leuven (B)	CHF 1.800
	❑ June 18-20	German	Zürich	CHF 1.800

** The fee is CHF 900 for those who also apply to DOE-I*
*** All course notes are in English*
Fees valid for the listed course dates only
Fees exclusive VAT

Application

Please tick the boxes (title + dates) corresponding to the course(s) you want to apply for.

Mr. / Mrs. First Name : ..... Last name: …….....

Company : …..... Job Title : .....

Address : .....

Phone : ……..... E-mail : ……..…….....

Education / Prior knowledge : ……..……..……..……..……..……

Dietary preferences : .....

Invoice address (if different from above) : .....…….....

VAT Nr. : …….....

The course fee will be paid after receipt of the invoice, **before the first course day**. I have taken note of the general conditions on payment and cancellation.

Date : .....……..... Signature: .....

In case you can not attend a course you applied for, you can always let a colleague take your place, without additional cost. On cancellation until twenty days before the course start, half of the course fee is due. After that the full amount needs to be paid. CQ has the right to cancel a course until 10 days before the start of the course, in which case we will provide a complete refund. CQ also has the right to reject the application of course candidates without further motivation.