



# An Introduction to Chemometrics and Multiway Analysis

December 3-7, 2007  
University of New South Wales (UNSW) Sydney, Australia



The Centre for Water and Waste Technology at UNSW is hosting a series of workshops demonstrating data analysis using chemometrics and multiway analysis. The workshops will be led by Professor Rasmus Bro from the University of Copenhagen. Bro has authored well over 100 scientific papers, books, reviews and popular articles on chemometrics, given more than 50 invited presentations all around the world and is at the forefront of algorithm and software development in this area. He has extensive experience teaching chemometrics and regularly conducts training courses in Europe and USA. Bro has been an editor for the *Journal of Chemometrics* since 1999.

## APPLICATIONS

Chemometrics has been successfully applied to a range of chemical, biological and environmental data. For examples of Multiway applications, see Bro's recent article in *Critical Reviews in Analytical Chemistry* (36:279–293, 2007).

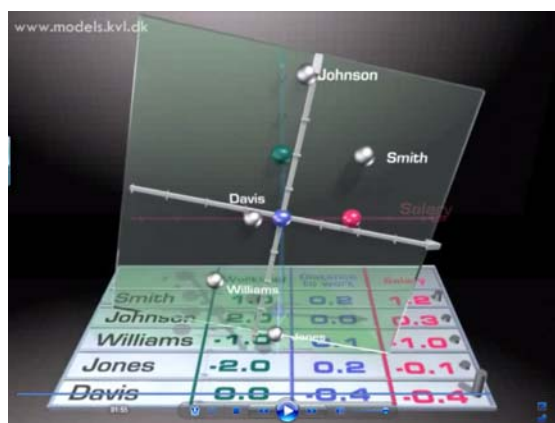
- Fluorescence spectroscopy
- Mass Spectrometry
- Chromatography
- Magnetic resonance (NMR)
- Forensic Science
- Image Analysis
- Process data
- Sensory data
- Environmental analysis
- Psychometric data

## WORKSHOP OVERVIEW

### Day 1-2:

#### Introduction to chemometrics, PCA, PLS and classification

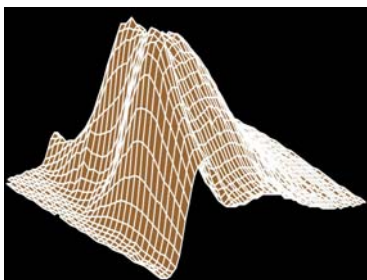
Chemometrics is used to solve problems involving large amounts of data. Within process-analysis and monitoring, chemical analysis, spectroscopy, molecular modelling, sensory analysis and many other fields, large data-tables are obtained that need to be analysed and visualized in order to be able to properly understand the problem at hand. This course will provide insight into the most popular methods for exploring data, building calibration and regression models and for building classification models. These methods are principal component analysis (PCA), partial least squares regression (PLS) and several variants of multivariate classification.



**Audience:** The course is intended for people working with large data sets or who have general interest in learning more about chemometrics and its applications. Some mathematical and statistical expressions will be used in the course and a variety of data will be used as examples. Process analytical applications, sensory data, spectroscopic and general data mining problems will be discussed

### Day 3:

#### Advanced multivariate data analysis, variable selection and pre-processing



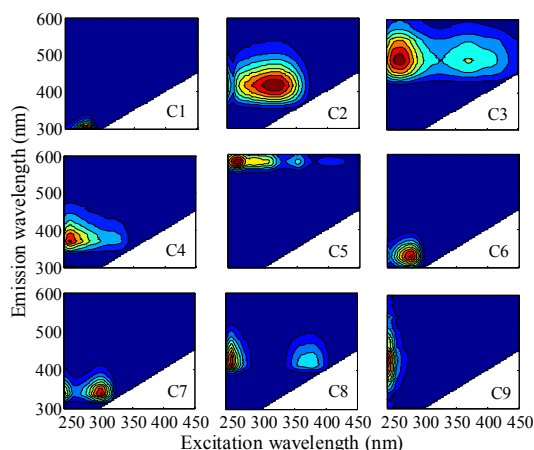
This workshop can be seen as a follow up to the two-day introduction or a preliminary to the multiway workshop. More advanced aspects of multivariate modelling are treated and alternative approaches to variable selection described, including forward selection, genetic algorithm and interval-PLS. It will be shown how to choose which approach is most feasible for a given type of data. Pre-processing of data prior to modelling is an important topic, for example, in order to remove scattering in spectra, baseline variations in chromatography or shifts in NMR spectroscopy. Important methods for pre-processing are described and exemplified with data from various fields.

*Audience:* It is assumed that the participant has knowledge of basic chemometric tools such as PCA and PLS, corresponding to Days 1-2 of the workshop.

### Day 4-5:

#### Multiway analysis, PARAFAC and beyond

Threeway analysis is a follow up to the basic chemometric course. The participant will gain knowledge about advanced multiway techniques such as multilinear-PLS and PARAFAC. The methods are useful in classification, calibration and prediction of multiway data. Multiway data occurs, for example, when measurements of each observation give a matrix or data table. Gathering data from several samples will result in a three-way array or "box" of data. Such data can be modelled with very powerful multiway methods that can provide much more information than normal multivariate models. Examples will be given from e.g. fluorescence EEM spectroscopy, hyphenated chromatographic methods and sensory analysis.



*Audience:* It is assumed that the participant has some knowledge on basic chemometric tools such as PCA and PLS, corresponding to Days 1-2 of the workshop.

#### General information for all workshops

All workshops are independent of each other and treat different subjects. They are arranged to build upon progressively more insight on chemometric methods and together provide a whole.

Throughout the course there will be ample opportunity for discussing the participants own data and data analytical problems. Participants will also complete hands-on exercises with real-world data to demonstrate the application of the chemometrics techniques discussed during the course.

MATLAB and PLS\_Toolbox software will be used during practical exercises. The PLS\_Toolbox uses graphical user-interfaces and hence no programming skills are needed. The PLS\_Toolbox and Solo, a standalone version of the toolbox that runs without Matlab, can be purchased by participants at a discounted price.

## Registration Fees

In order that participants receive personalised attention from instructors, numbers of participants will be limited. Registration fees (see below) are due by **15 October, 2007** and include lunch and morning/afternoon teas. Prices include GST (tax). A 10% early bird discount is available to participants who register before 1 September, 2007. Students must provide evidence of full-time university enrolment status in 2007.

	Non-member	RACI Member‡	Academic	Student
Full Course	1980	1870	1320	660
Day 1-2	990	935	660	
Day 3	495	470	330	
Day 4-5	990	935	660	

‡ Discounted registration fees are offered to members of the Royal Australian Chemical Institute (RACI).

## Accommodation (optional)

Inexpensive basic accommodation and optional meals (dinner/breakfast) are available at New College, located on the UNSW campus (<http://www.newcollege.unsw.edu.au/Guest-accommodation.44.0.html>). You are free to make alternative arrangements for food and accommodation if you prefer. Please contact us if you would like to receive information about hotels in the UNSW area.

Single student rooms per person per night		Self-contained flats (Bathroom & Kitchenette) per room per night	
<i>Option</i>	<i>Cost</i>	<i>Option</i>	<i>Cost</i>
Accommodation Only	55.00	Accommodation Only	80.00
Accommodation & Breakfast	60.50	Accommodation & Breakfast	85.00
Accommodation & 2 Meals	66.00	Accommodation & 2 Meals	90.00

## Cancellation Policy

In the event that a participant wishes to cancel registration in a course prior to October 15, any money paid toward the course will be refunded in full subject to a cancellation fee. Cancellations received before 1 September 2007 will incur no fees. Cancellations received between September 1-October 15 will be subject to a \$75 administrative fee. No refunds will be given after October 15, however, you may substitute another person to attend in your place.

In the event that the workshops do not go ahead as advertised, registration fees and fees paid to the New College for accommodation will be returned to participants in full. UNSW accepts no liability for financial losses (e.g. air ticket cancellations) incurred by participants as a result of changes to or cancellation of any of the workshops. We strongly advise that participants travelling from overseas or interstate purchase travel insurance to protect against unforeseen risks.

Further information: [robby@unsw.edu.au](mailto:robby@unsw.edu.au)