



ISOCS Winter School

1-6 February 2009 - Alpbach, Austria

Technical Programme Fundamentals of multivariate data analysis for chemical and biological sensing

Introduction

The School explores the nature of data generated by existing chemical sensors and analytical instrumentation, such as mass spectrometers, optical spectrometers and time of flight ion mass spectrometers, as well as an introduction to more recent protein and DNA sequencing chips.

We will cover such concepts as data exploration, feature extraction and feature selection techniques currently used. We will also look at linear and non-linear methods, supervised and unsupervised techniques, and parametric and non parametric techniques. The School consists of lectures in the morning and the laboratories in the evening during which attendees can apply the techniques on standard data-bases.

The School is ideal for anyone with an interest in data processing and new to the field; for example, PhD students, researchers, technologists and industrialists. The data analysis does not need a high performance computer and can be carried out on a basic laptop or personal computer running the windows operating system.

For further information visit: www.olfactionsociety.org/winterschool.html

Data sets

The laboratory sessions will employ four realistic data sets, chosen to illustrate the types of multivariate techniques available and required by the differing nature of the sensing methods. They will be presented in a standard XML format and will be available to other researchers from the ISOCS website after the course.

- I. Chemical sensor array, simple components, static model, linearly separable classes.
- II. Mass spectra data, simple components, static model, linearly separable.
- III. Chemical sensor array, complex data-set, static model, non-linear class separation so needs ANN.
- IV. Chemical sensor array, simple components, time-series with significant drift, linear filters applied (e.g. auto-regression with moving average).

School Technical Director:	Prof Julian Gardner	University of Warwick, UK
Lecturers:	Dr Udo Weimar	University of Tübingen, Germany
	Prof Krishna Persaud	University of Manchester, UK
	Prof Agustin Gutierrez	University of Barcelona, Spain
	Dr Jan Mitrovics	JLM Innovation, Germany
Laboratory supervisors:	Dr Zoltan Racz	University of Manchester, UK
	Dr Jan Mitrovics	JLM Innovation, Germany
School organizer:	Dr Monika Kwoka	University of Tübingen, Germany

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Schedule

Sunday 1st February

- 15:00 – 18:00 Registration and laptop preparation
18:00 – 20:00 Welcome Reception
20:00 Dinner

Monday 2nd February

Introduction to sensors and data handling

Morning Session: **Theory**

- 08:30 – 09:30 Introduction to chemical sensors and analytical instrumentation **Udo Weimar**
09:30 – 09:50 Coffee break
09:50 – 10:50 Basic statistical analysis of data from a single sensor and initial pre processing **Jan Mitrovics**
10:50 – 11:50 Introduction to data handling and data formats suitable for data analysis **Jan Mitrovics**
12:00 Lunch

Evening Session: **Computer Lab**

- 17:30 – 19:30 Introduction to data formats and data analysis software using database I.
20:00 Dinner

Tuesday 3rd February

Exploratory data analysis and linear multivariate techniques

Morning Session: **Theory**

- 08:30 – 09:30 Signal and data pre-processing: experimental design **Krishna Persaud**
09:30 – 09:50 Coffee break
09:50 – 10:50 Linear regression methods: multi linear regression and partial least squares **Udo Weimar**
10:50 – 11:50 Linear methods for multivariate data analysis: principal component analysis and linear discriminant analysis **Udo Weimar**
12:00 Signal and data pre-processing: experimental design

Evening Session: **Computer Lab**

- 17:30 – 19:30 Exploration of database II using linear methods
20:00 Dinner

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Wednesday 4th February

Non-linear multivariate analysis of chemical sensor data

Morning Session: **Theory**

08:30 – 09:30	Non-linear statistical methods	Krishna Persaud
09:30 – 09:50	Coffee break	
09:50 – 11:50	Introduction to data handling and data formats suitable for data analysis	Krishna Persaud
12:00	Lunch	

Evening Session: **Computer Lab**

17:30 – 19:30	Exploration of database III using non-linear methods	
20:00	Dinner	

Thursday 5th February

Time series analysis of data from chemical sensors

Morning Session: **Theory**

08:30 – 09:30	Problems of sensor drift, time-varying parameters and aging	Julian Gardner
09:30 – 09:50	Coffee break	
09:50 – 10:50	Analysis of time-dependent data-sets: linear models (filters)	Julian Gardner
10:50 – 11:50	Analysis of time-dependent data-sets: non-linear models (with thermally modulated sensors analysed by artificial neural networks and discrete wavelet transforms)	Agustin Gutierrez
12:00	Lunch	

Evening Session: **Computer Lab**

17:30 – 19:30	Exploration of time-varying databases I and IV, sensor data and ion mobility spectra	
20:00	Social Dinner	

Friday 6th February

Large data-sets and bio-inspired techniques

Morning Session: **Theory**

08:30 – 09:30	Feature selection techniques on large sensor arrays	Agustin Gutierrez
09:30 – 09:50	Coffee break	
09:50 – 10:50	Biologically-inspired signal processing	Agustin Gutierrez
10:50 – 11:50	Challenges in the field of chemical and biological sensing: the odour segmentation problem, healthcare and security applications	Julian Gardner
11:50 – 12:00	Concluding remarks and farewell	
12:00	Lunch	

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