

Workshop on chemometrics for environmental sciences

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In spite of the excellent results obtained in the last 30 years for the analysis of chemical data, chemometrics is still not regarded as a standard tool for the investigation of data obtained from environmental surveys. Techniques such as PCA and PLSR are often perceived as black-box procedures that involve much mathematics and many equations. This perception worsens even more for multi-way data analysis, which often requires a level of abstraction that discourages the non-initiated. The aim of the workshop is to illustrate some applications to the analysis of environmental data of selected basic techniques like PCA and the extensions that are best suited for environmental studies (e.g. Tucker models). The workshop will count for 2 ECTS points.

Organization

The workshop will be held at the Life Sciences Faculty, University of Copenhagen on 28-29th February, 2008. PhD students and post-docs in environmental chemistry who want to familiarise with standard and multi-way chemometric techniques are the targets of the workshop. Attendance will be limited to 20 participants, both PhD's and researchers; the employees of RECETO institutions will be prioritised. Qualified experts have been invited to present recent results on the application of chemometrics to various types of environmental data. The Matlab packages used in the practical exercises are publicly available and additional tools to facilitate the access to more advanced features will be provided at the workshop.

Schedule

Both days will be organised with a theoretical introduction to the models, followed by the presentation of some applications on environmental data and of some basic practical aspects. The strictly necessary Matlab tools will be illustrated. The afternoons will be dedicated to practical exercises: two the first day and one the second, followed by a discussion on the results.

Day 1

8.30 - 8.40	Introduction to the workshop
8.40 - 9.00	Introduction to multivariate data analysis
9.00 - 9.40	Two-way methods for environmental data (PCA) some applications*
9.40 - 10.20	Practical aspects of two-way data analysis (e.g., preprocessing, validation) [†]
10:20 - 10:30	Break
10.30 - 12.00	Introduction to the Matlab tools for the workshop (scripts, graphics)
12.00 - 13.00	Lunch
13.00 - 16.30	Two practical exercises: 1h 30' + 15' explanation each
16.30 - 17.00	Discussion

Day 2

8.30 - 8.35	Introduction
8.35 - 9.20	Multi-way models in chemistry [‡]
9.20 - 10.00	PARAFAC and Tucker as ideal methods for environmental studies [‡]
10.00 - 10.15	Break
10.15 - 11.15	Practical aspects of N-way data analysis (e.g., preprocessing, validation)
11.15 - 12.00	Introduction to the Matlab tools (scripts, graphics)
12.00 - 13.00	Lunch
13.00 - 16.30	One practical exercise: 3h + 30' explanation
16.30 - 17.00	Discussion

* Contribution by M. Bassompierre

[†] Contribution by L. Nørgaard

[‡] Contribution by R. Bro