BCS WORKSHOP

Multivariate Curve Resolution (MCR)

May 6, 2011

Venue

Vrije Universiteit Brussel
Dep of Analytical Chemistry and Pharmaceutical Technology
Building H
Laarbeeklaan 103
B-1090 Brussels (Jette)
Belgium

Organisation

The Belgian Chemometrics Society

http://chemometrie.kvcv.be

Introduction

Multivariate Curve Resolution methods aim at providing a scientifically meaningful description of the variation in the data through a small bilinear model of basic and interpretable contributions.

The most prominent feature of MCR methods is the straight-forward scientific interpretation of its results, as a consequence of introducing chemical/scientific information about the properties of the basic contributions sought (instrumental responses, concentration profiles, environmental or biological patterns,…) under the form of constraints.

MCR allows working with multi-set structures that may enclose data coming from different experiments, techniques or, in a more general sense, collected under different conditions or in different scenarios. An integral and more rugged description of the problem is obtained, due to the active use of diverse input information and to particular properties of multi-set structures.

The underlying MCR bilinear model offers certain advantages. The matrices of basic contributions can be used as meaningful compressions of the raw data set for other data analysis purposes, e.g. in the case of hyperspectral images. Also, the simplicity and interpretability of the MCR results make this method an excellent option to explore data sets well beyond the typical analytical field, such as environmental or –omics measurements.

Speakers

Anna de Juan

Anna will give an overview of the main aspects mentioned above, stressing briefly the kind of data sets and information that can be used when applying MCR methods and illustrating the power of the method with examples from diverse scientific fields.

Cyril Ruckebusch

The strengths of MCR will be illustrated by the development of strategies for the analysis of data from femto-second transient absorption spectroscopy, a powerful time-resolved technique used for characterizing the dynamics of photo-switchable molecules, of interest in high-resolution imaging and the design of photonic materials.

Christophe Tistaert

A combination of Iterative Key-Set Factor Analysis (IKSFA) and Multivariate Curve Resolution – Alternating Least Squares (MCR-ALS) with spectral selectivity constraint was shown to be capable of resolving four-way 2D-LC-DAD data of urine samples. However, the spectrally rank deficient peaks could only be quantified when well-resolved chromatographically, and therefore, a new constraint was developed.

Agenda

13.30 Welcome Coffee

14.00 Multivariate Curve Resolution, bringing and extracting scientific knowledge from the data analysis,
Anna de Juan, Chemometrics group. Universitat de Barcelona

15.00 Tailoring MCR for femtosecond spectroscopy data analysis,
Cyril Ruckebusch, LASIR CNRS, Université Lille Nord de France

15.50 Coffee Break

16.10 Resolution of spectrally rank deficient MCR-ALS components in 2D-LC-DAD analysis
Christophe Tistaert, Department of Analytical Chemistry and Pharmaceutical Technology, Vrije Universiteit Brussel

16.50 Reception

Fee

Participation to this workshop is €75, excl. VAT, or €50 for members of the Royal Flemish Chemical Society (KVCV).

Registration

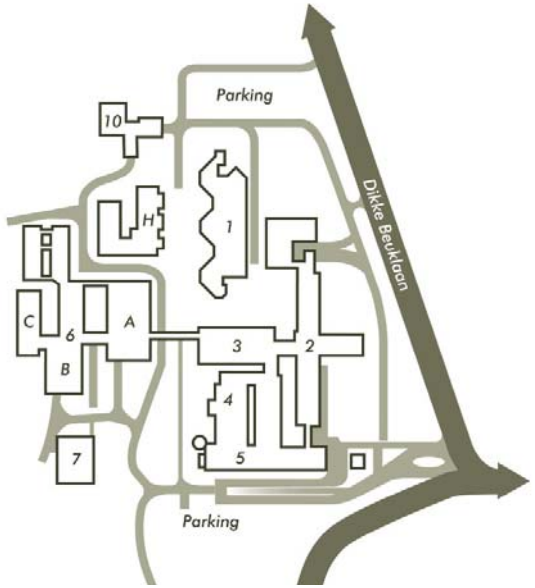
Please register on-line at the BCS website: http://chemometrie.kvcv.be.

How to get to the VUB campus Jette

Car
Exit 9 from Brussels Ring. Follow signs AZ-VUB.

Public transportation to AZ-VUB
Bus 14 from railway station Brussel-Noord, or subway station Simonis.
Bus 221 from Zaventem airport
Bus 13 from subway stations Simonis or Belgica
Bus 84 from subway station Beekkant

Once on campus, you'll have to locate building H, see map below.



The Belgian Chemometrics Society

The Belgian Chemometrics Society (BCS) operates as a section of the Royal Flemish Chemical Society (KVCV) and aims at promoting Chemometrics in Belgium with special attention for the interaction between academia and industry. Its main activity is the organisation of workshops and a bi-annual symposium.

Not a BCS member yet ? You are very welcome to join ! Just drop a line to chemometrie@kvcv.be

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