Module Title:
Curve resolution for multiset and multi-way analysis

Module Code:
DA309

Maximum Number of Students:
20

Total ECTS Credits
2

Notional Learning Hours
(a) Contact Time - 12 h
(b) Private Study - 38 h

Format of Teaching:

Lectures	8 h
Laboratories or Practicals	4 h
Other	0 h

Teaching Strategy:
Formal lectures in 60/90 min timetable and hands-on PC seminars

Convener:

Anna de Juan

University / Department:

University of Barcelona, Department of Analytical Chemistry

Language of Tuition:
English

Module Description - The Purpose or Aims:
1. Introduction of advanced curve resolution techniques for multi-way and multiset data analysis
2. Application of curve resolution techniques to simulated data and real case studies

Specific Learning Outcomes for this module: (contributing to general learning outcomes GLO 1 – GLO 10)

1. Understanding of the principles and fundamentals of the most commonly used curve resolution techniques for multi-way data sets (PARAFAC and related techniques) and for multiset data (Multivariate Curve Resolution-Alternating Least Squares, MCR-ALS).
2. Capacity to apply the algorithms to the practical analysis of simulated and real data sets.
3. Capacity to select the appropriate algorithm according to the structure of the data set and the underlying model of the methods.
4. Capacity to design a data analysis plan according to the chemical problem to be solved, the data available and the correct correspondence data structure-algorithm model.

Summary of Course Content:
This module is focused on providing a general overview of the curve resolution techniques applicable to analyze multi-way and multiset data sets. Although a brief description of the algorithms is mandatory, the module will be more specifically addressed to understand the structure of the chemical multiset and multi-way data and the differences among algorithms in terms of the input information needed, the data structure required and the output provided. The theoretical description will be complemented with practical work on the analysis of simulated and real data sets using specific routines in a MATLAB environment. This practical work will include the use of the algorithms and the planning of the data analysis.

Transferable Skills Taught:
Communication:
Writing data analysis reports.

Information Technology:
Use of standard chemometric software environment (MATLAB)

Assessment Methods:
1. LO1-LO3 – Written exam, including a theoretical part and a practical data analysis problem (60%)
2. LO4. Technical data analysis report based on a case study (40%).

Assessment Criteria:

Threshold

LO1 –basic knowledge of the fundamentals of the different data analysis algorithms
LO2 - basic ability to apply the algorithms when a data analysis protocol is provided
LO4 – capacity to write a systematic report about the results of the data analysis

Good

LO1 – sound knowledge of the fundamentals of the different data analysis algorithms
LO2 – ability to apply the algorithms without a data analysis protocol
LO3 – understanding of the selection criteria of the different algorithms available.
LO4 – capacity to report the results of a data analysis and to extract conclusions linked to the chemical problem under study.

Excellent

LO1 – advanced knowledge of the fundamentals of the different data analysis algorithms.
LO2 – advanced skills in application of the algorithms to practical data analysis.
LO3 – capacity to perform a correct selection of the suitable algorithm according to the data structure.
LO4 – capacity to design a whole data analysis protocol based on the chemical problem, the available chemical information and data sets. Capacity to redefine the data analysis plan from the results obtained.

Resource Implications of Proposal and Proposed Solutions:

Lecture notes and free downloadable MATLAB routines will be available for students.

Recommended literature:

[1] A. Smilde, R. Bro and P. Geladi. *Multi-way analysis. Applications in the chemical sciences.* John Wiley & Sons (2004)
[2] R. Tauler and A. de Juan. 'Multivariate Curve Resolution (and references therein)' in *Practical Guide to Chemometric*', ed. P. Gemperline. CRC (2006).

Pre-Requisites:

Fundamentals of Multivariate Analysis (module DA0306) would be required.
Curve resolution for two-way data sets (module DA0308) is recommended, but not indispensable.