Short courses at WSC-13

Prof. Yulia Monakhova. **Independent components analysis (ICA) in practice: tips and tricks**

Independent components analysis (ICA) is a probabilistic method, whose goal is to extract underlying component signals and their concentration ratios, that are maximally independent and non-Gaussian, from mixed observed signals. In this short course, theoretical background of ICA algorithms will first be explained. After that, several practical problems of using different ICA approaches (MILCA, SNICA, JADE, RADICAL, FastICA) will be solved in the Matlab environment. The methods will be applied to quantitative and qualitative analysis of non-trivial mixture types as well as to exploratory analysis using spectroscopic techniques (UV-VIS, NMR, IR). Special attention will be paid on the influence of spectra acquisition parameters, spectra preprocessing, decomposition parameters and the interpretation of ICA outcome. Approaches to absolute analyte quantification will be discussed. The differences to common chemometric approaches – PCA and MCR-ALS – will be highlighted.

Prof. Dmitry Kirsanov. **Multisensor systems' data processing**

Multisensor systems for chemical analysis is a rapidly developing field of research in analytical chemistry. These systems comprise several (typically from 3 to 30) chemical sensors that do not show a sharp selectivity towards a particular substance, but rather have so called cross-sensitivity - a response towards a variety of analytes. In multicomponent samples these multisensor systems produce complex non-resolved analytical signals containing information about several analytes simultaneously. These signals can be effectively treated with chemometric tools to derive qualitative and quantitative information about the samples under study. The lecture will provide the basics of multisensor system for chemical analysis and will demonstrate several examples of multisensor data processing from real experiments using R.

Ivan Krylov**. Basics of PARAFAC decomposition in fluorescence excitation-emission spectroscopy**

The seminar covers the following topics:

- Theoretical basis for the use of canonical tensor decomposition (PARAFAC) in excitation-emission fluorescence spectroscopy
- Deviations of excitation-emission data from the assumptions of PARAFAC and how to counter them with pre-processing: inner filter effects and the scattering signal
- PARAFAC uniqueness and validation of the model: split-half analysis and jack-knifing
- Performing the PARAFAC analysis of the data using the 'albatross' package in the R programming language

Recommended prerequisites: experience in the R programming language or related environments

Software:
- the R programming language <https://r-project.org>
- the "albatross" package <https://CRAN.R-project.org/package=albatross>
- RStudio <https://www.rstudio.com/> or another graphical interface is not required but may be convenient

Please find details and updates at https://files.libs.chem.msu.ru/~ivan/WSC-13/ .