Seminar #4

June 19, 2020, 11:30 am

Signal and Data Processing Workflows for Untargeted Chemical Analysis: Sensor Array and Mass Spectrometry Analysis of Complex Gas Samples

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In diverse sectors such as health, food, environment, complex natural gas samples are analysed. Those samples can contain hundreds or thousands of compounds. In many cases, the question to be answered does not require full separation, quantification, and identification of all compounds. Instead detection of abnormal samples (normal/faulty), assignation of classes to samples (e.g.healthy/disease), or evaluation of global quantitative indexes (e.g odour intensity) is required.

The analysis of gas phase samples can be carried out with high-end lab equipment based on Chromatography-Mass Spectrometry or lower cost systems based on chemical sensors. In all cases, the resulting raw signals/data need substantial efforts to extract the hidden information. In health applications the problem of biomarker discovery becomes like finding a needle in a haystack. Intimate knowledge of the instrumental problems and the sampling conditions is key for the correct interpretation of the results.

These problems are often addressed by building mega-variate predictive models using tools from machine learning. However, in small sample conditions the possibilities to obtain overoptimistic results abound due to the curse of dimensionality. Careful model validation and statement of model validity domains is needed.

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