



VABILO NA INŠTITUTSKO PREDAVANJE / INVITATION TO THE INSTITUTE LECTURE

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Analysis of complex omics data with chemometric techniques

Povzetek / Abstract

The analysis and information extraction of complex omics data is a major challenge for chemometrics. In this lecture I will give 2 examples how chemometric techniques can be applied in an original way for this.

The first application concerns the analysis of a genomics micro array dataset to learn more on the osteogenesis from stem cells. For this an ANOVA-PCA technique has been developed that has successfully been applied on this dataset and has led to a novel hypothesis for the working mechanism of Vitamin D in bone cell formation.

The second example concerns the analysis of LC-MS proteomics data for biomarker discovery. Whereas the use of multivariate pattern recognition techniques for similar purposes is quite common for two-way data like IR spectra or (non-hyphenated) mass spectra they do not seem to have made their way into the analysis of LC-MS data yet. Instead, most published methods seem to rely on modified versions of univariate tests, like the well-known student's t-test.

We present here an improved alignment technique for these data and an alternative methodology employing Linear Discriminant Analysis (LDA) to pinpoint the differential patterns in LC-MS data. We apply it to a number of simulated data sets as well as to two spike-in LC-MS data sets. We show that it is able to extract the relevant information in all these cases and that it performs better than unfolding or projection in combination with LDA.

Vljudno vabljeni! / Kindly invited!