

L5. Exploration and classification: Applications from archaeometry to spectroscopy

Kurt Varmuza

Vienna Technical University, Vienna, Austria

Evaluation of multivariate data often starts with exploratory data analysis by linear or nonlinear mapping with the aim to obtain a widely unbiased insight into the data structure. Multivariate classification is one of the roots of chemometrics. Applications in some recent projects will be discussed.

An example from archaeometry deals with fatty acid concentration data, measured on tissue samples from human mummies, including the 5000-years old Tyrolean Iceman, as well as 2000-years old corpses found in a permafrost area in Siberia. In another example, PLS mapping of concentration profiles of triterpenoids has been applied to obtain information about the botanical origin of a black glue material found on Neolithic weapons and tools.

Since March 2004 the Rosetta mission of the European Space Agency is cruising towards a comet. One of the instruments on board is a secondary-ion time-of-flight mass spectrometer (TOF-SIMS) dedicated to investigate comet dust particles. Currently available laboratory mass spectra from organic and inorganic reference compounds — presumably relevant for the analysis of comet material - have been evaluated by chemometric methods.