Abstract

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Random projection for dimensionality reduction - Applied to time-of-flight secondary ion mass spectrometry data

Random projection (RP) is a simple and fast linear method for dimensionality reduction of high-dimensional multivariate data, independent from the data. The method is briefly described and a new memory-saving algorithm is presented for the generation of random projection vectors.

Application of RP to data from scanning experiments with a time-of-flight secondary ion mass spectrometer (TOF-SIMS) showed that data reduced by RP have a satisfying discriminant property for separating target material and minerals without using any knowledge about the composition of the sample. A selection method – based on low dimensional RP data – is described and successfully tested for automatic recognition of characteristic, diverse locations of a sample surface.

RP is demonstrated as an unbiased, powerful method, especially for large data sets, severe hardware restrictions (such as in space experiments) or the need for fast data evaluation of hyperspectral data.