Infrared characterisation of cultural heritage objects: standard approach and going beyond diffraction limit

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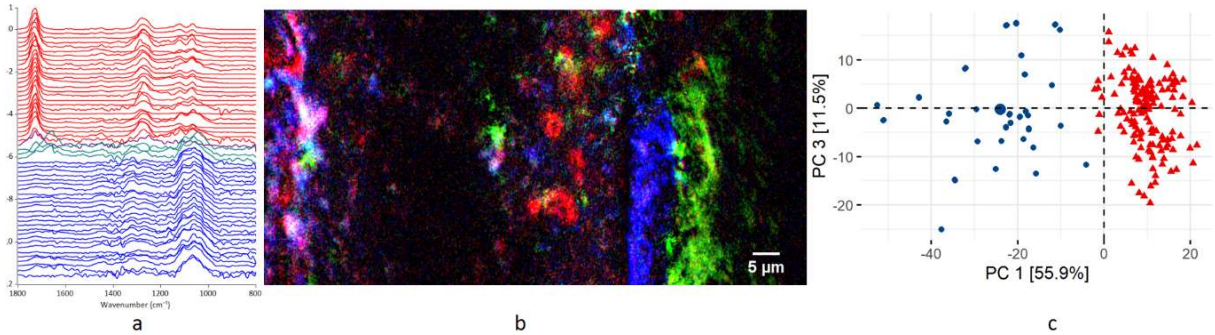
Infrared spectroscopy has been used for analysis of the numerous objects that may be attributed to cultural heritage. Verifying the authenticity of documents, paintings, or musical instruments are just a few examples of this type of analysis. Another vital aspect is evaluating the status of the cultural heritage artefacts, namely checking how environmental conditions of the storage or display influence the safety and integrity of the objects. This issue is critical in the case of paintings, as various ingredients used in the creation process (in canvass, ground, paint, varnish and other layers) may go into interaction and produce potentially irreversible changes.

Innovative techniques based on photothermal effect were recently added to the well-established in laboratories methods as FTIR (Fourier Transform Infrared) spectroscopy and microscopy. They allow to break the diffraction limit of the classic infrared spectroscopy, improve the measurements' spatial resolution, and access the information unavailable before.

In contemporary science, the key to understanding obtained experimental results is proper data processing and evaluation regardless of method that was selected for the samples characterization.

In this contribution detailed data analysis of huge hyperspectral objects collected during experiments (FTIR and novel photothermal effect based spectroscopies) on cultural heritage samples will be presented. Special attention will be paid to proper pre-processing (baseline correction, experimental atrifacts removal, normalization) and the selection of adequate statistical methods. Any spectroscopic results of the experiments (spectra and hyperspectral objects) are highly correlated data-sets with many redundant variables. In order to visualise the results and extract the essential information, dimension reduction methods are required. To find the similarities and differences between spectra it is necessary to evaluate the spectral distance and to cluster the results into groups.

All examples presented here are prepared in open-source R Environment and are freely available at the Github repository. R is recommended by many data sciencists as a versatile platform for spectral data evaluation and it is available for all modern operating systems. It promotes code-driven analysis that enables reproducible and repeatable research.



a b c

(a) Infrared spectra measured for selected points on paint cross-section,
(b) RGB composite image of the spatial distribution for three selected bands
(c) Result of Principal Component Analysis on selected spectra (scatterplot of PC1 versus PC3)