**Motivation**

We present hyperSpec, a new software that greatly facilitates the analysis of spectra using the statistical software R. [1] [http://r-project.org]. Our needs for spectroscopic data analysis are best met in a programming environment supporting tools for both chemometrics and handling of spectra. Standard and specialized statistical procedures are available in R. This is a big advantage as programming the handling of spectra is far less error prone than programming statistical routines. The correctness of statistical software is a concern, and it has recently been assessed by Keseling and Four[2]. hyperSpec makes R a convenient platform for the analysis of spectral data sets, including spectral images and maps.

**Features**

- Functions to import spectra into R.
- Means to attach any amount of non-spectral data to each of the spectra, such as time, position, concentrations, diagnoses, etc.
- Several plot functions to display spectra, false-colour maps, calibration lines etc., and basic interaction like obtaining the spectrum and wavelength you click at.
- Functions to work with the spectra and do your preferred preprocessing.
- Functions to ease the interaction with statistical data analysis methods – Hand over the spectra matrix e.g. to diat in the dendroide example.
- Hand over the appropriate data frame e.g. to in the calibration example.
- Re-importing the results of e.g. PCA or MSC preprocessing is also possible.

**Requirements**

Our key scenarios for chemometric analysis in biomedical spectroscopy are:

1. We do spectral preprocessing, and use chemometric methods like regression, cluster analysis, classification, etc.
2. We acquire spectral maps of arbitrary shape.
3. The data sets can be large (20,000 spectra and more), so batch processing/scripting should be possible.
4. We combine maps with single spectra (e.g. reference substances).
5. We customize/call standard procedures if our needs are not met.
6. See e.g. the “Centering” in the chondroide example below, or think of developing a test diagram: How to ensure statistical independency at patient level with varying numbers of spectra per patient?
7. We build Graphical User Interfaces (GUIs) for specific tasks.

**Example Work Flow: Raman Map of Chondrocytes in Cartilage**

**Calibration Plot: Quinine Fluorescence**

**Advanced Spectra Plotting: Paracetamol**

**Conclusions**

A software package was developed to ease the analysis of hyperspectral data sets, i.e. spectra together with further information such as spatial coordinates, time series, concentrations etc., in the statistical environment. hyperSpec provides data import and export, convenient plotting functions, and methods to handle and preprocess the spectra. It is easily extensible by the user, and works smoothly with other libraries that provide specialized statistical tools.

**Literature**


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