ChemoSpec: an R Package for the Chemometric Analysis of Spectroscopic Data

Bryan A. Hanson[1,2*]

1. Dept. of Chemistry & Biochemistry, DePauw University, Greencastle IN USA
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*Contact author: hanson@depauw.edu

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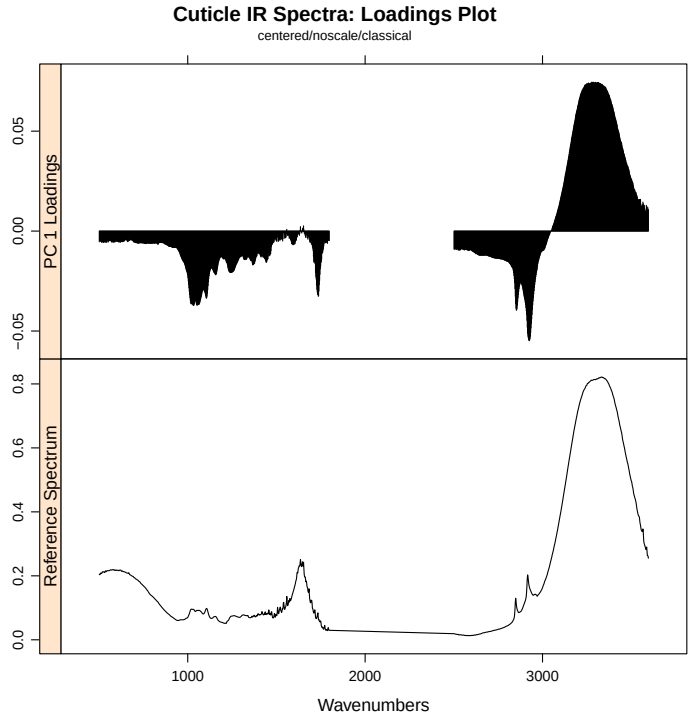
ChemoSpec is a collection of functions for plotting spectra (such as NMR & IR spectra) and carrying out various forms of top-down exploratory data analysis, including hierarchical cluster analysis (HCA), principal components analysis (PCA) and model-based clustering (from **mclust**). S3 classes are used and the data is stored in a `Spectra` object created during data import. Two-dimensional and several 3-dimensional methods are provided for visualizing score plots, including interactive plots and graphical MANOVA methods. Robust methods appropriate for this type of high-dimensional data are employed and diagnostics plots are available. These functions rely heavily on methods and functions discussed in Varmuza & Filzmoser, as well as ideas from the **ggobi** group. **ChemoSpec** is designed to facilitate comparison of samples from treatment and control groups such as typically found in ecological or medical investigations. It is designed to be user friendly and suitable for people with limited background in R, as it was written to support undergraduate research projects. **ChemoSpec** functions will be demonstrated using data from the author's research on plant stress using metabolomics.



References

Bryan A. Hanson (2009) ChemoSpec, `http://github.com/bryanhanson/ChemoSpec`.

K. Varmuza & P. Filzmoser, *Introduction to Multivariate Statistical Analysis in Chemometrics*, CRC Press (2009).