

hyperSpec Introduction

Claudia Beleites (cbeleites@units.it)
CENMAT, DMRN, University of Trieste

July 7, 2009

1 Introduction

This vignette gives an introduction on basic working techniques using the R package *hyperSpec*. It comes with three data sets,

chondro a Raman map of chondrocytes in cartilage,

flu a set of fluorescence spectra of a calibration series, and

laser a time series of an unstable laser emission

In this vignette, all three data sets are used in an indetmixed way to illustrate appropriate procedures for different tasks.

2 Loading the package

hyperSpec is loaded by

```
> library(hyperSpec)
```

Package hyperSpec, version 0.5

To get started, try

```
help("hyperSpec")
help(package = "hyperSpec")
vignette(package = "hyperSpec")
```

If you use this package please cite it appropriately.

```
citation("hyperSpec")
```

will give you the correct reference.

The project is hosted on <http://r-forge.r-project.org/projects/hyperspec/>

3 The structure of hyperSpec objects

hyperSpec is a S4 (or new-style) class. It has four *slots*,

wavelength containing a numeric vector with the wavelength axis of the spectra

data a **data.frame** with the spectra and all further information belonging to the spectra

label a list with appropriate labels (particularly for axis annotations)

log a **data.frame** keeping track of what is done with the object

In R, slots can be accessed directly by the `@` operator. In this vignette, the notation `@xxx` will thus mean *slot xxx of an object*.

However, it is considered good practice not to access the slots directly but rather to use *hyperSpec*'s more convenient functions to handle the objects. This also helps ensuring, that proper (*valid*) objects are retained.

4 Obtaining Basic Information about hyperSpec objects

As usual, the *print* and *show* methods display information about the object, and *summary* yields some additional details about the data handling done so far:

```
> chondro

hyperSpec object
  875 spectra
  3 data columns
  300 data points / spectrum
wavelength: tilde(nu)/cm^-1 [numeric 300]  602 606 ... 1798
data: (875 rows x 3 columns)
  (1) y: y/(mu * m) [numeric 875] range -4.77 -3.77 ... 19.23
  (2) x: x/(mu * m) [numeric 875] range -11.55 -10.55 ... 22.45
  (3) spc: I / a.u. [matrix 875 x 300] range 80.04420 81.75761 ... 1858.881

> summary(chondro)

hyperSpec object
  875 spectra
  3 data columns
  300 data points / spectrum
wavelength: tilde(nu)/cm^-1 [numeric 300]  602 606 ... 1798
data: (875 rows x 3 columns)
  (1) y: y/(mu * m) [numeric 875] range -4.77 -3.77 ... 19.23
  (2) x: x/(mu * m) [numeric 875] range -11.55 -10.55 ... 22.45
  (3) spc: I / a.u. [matrix 875 x 300] range 80.04420 81.75761 ... 1858.881
log:
      short      long      date      user
1  scan.txt.Renishaw list(...) 2009-07-07 12:02:48 cb@cb
2      orderwl list(...) 2009-07-07 12:02:48 cb@cb
3      spc.loess list(...) 2009-07-07 12:03:13 cb@cb
```

The data set `chondro` consists of 875 spectra with 300 data points each, and 3 data columns (one, `spc`, for the spatial information).

5 Session information

R session information:

```
> toLatex(sessionInfo())

• R version 2.9.1 (2009-06-26), x86_64-pc-linux-gnu
• Locale: LC_CTYPE=en_US.UTF-8;LC_NUMERIC=C;LC_TIME=en_US.UTF-8;LC_COLLATE=en_US.UTF-8;LC_MONETARY=C;LC_MESSAGES=
8;LC_PAPER=en_US.UTF-8;LC_NAME=C;LC_ADDRESS=C;LC_TELEPHONE=C;LC_MEASUREMENT=en_US.UTF-8;LC_IDENTIFICATION=C
• Base packages: base, datasets, graphics, grDevices, methods, stats, utils
• Other packages: hyperSpec 0.5, lattice 0.17-25
• Loaded via a namespace (and not attached): grid 2.9.1
```