

hyperSpec Introduction

Claudia Beleites <cbeleites@units.it>
CENMAT, DMRN, University of Trieste

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Revision

This document is currently undergoing an extensive revision prior to the next release on CRAN.

Reproducing the Examples in this Vignette

All spectra used in this manual are installed automatically with *hyperSpec*.
Note that some definitions are executed in `vignette.defs`.

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1. Introduction

hyperSpec is a R package that allows convenient handling of (hyper)spectral data sets, i. e. data sets comprising spectra together with further data on a per-spectrum basis. The spectra can be anything that is recorded over a common discretized axis, the *so-called* wavelength axis. Throughout the documentation of the package, the terms intensity and wavelength refer to the spectral ordinate and abscissa, respectively.

However, *hyperSpec* works perfectly fine with any data that fits in that general scheme, so that the three terms may also be used for:

wavelength: frequency, wavenumbers, chemical shift, Raman shift, $\frac{m}{z}$, etc.

intensity: transmission, absorbance, $\frac{e^-}{s}$, ...

extra data: spatial information (spectral images, maps, or profiles), temporal information (kinetics, time series), concentrations (calibration series), class membership information, etc.
Note that there is no restriction on the number of extra data columns.

This vignette gives an introduction on basic working techniques using the R package *hyperSpec*. It comes with five 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
paracetamol a Raman spectrum of paracetamol (acetaminophen) ranging from 100 to 3200 cm⁻¹ with some overlapping wavelength ranges.
It is used mainly in the *plotting* vignette.

barbituates GC-MS spectra with differing wavelength axes as a list of 286 *hyperSpec* objects.

In this vignette, the data sets are used to illustrate appropriate procedures for different tasks and different spectra.

In addition, the first three data sets are accompanied by vignettes that show exemplary work flows for the respective data type.

This document describes how to accomplish spectroscopic tasks. It does not give a complete reference on particular functions. It is therefore recommended to look up the methods in R's help system using `? command`.

After some remarks on the notation used in the document and on the general behaviour of R, section 3 shows how to load the package. Section 4 describes how *hyperSpec* objects are organized internally.

A list of all functions available in *hyperSpec* is given in appendix A (20)

1.1. Notation

This vignette demonstrates working techniques mostly from a spectroscopic point of view: rather than going through the functions provided by *hyperSpec*, it is organized more closely on spectroscopic tasks. However, the functions discussed are printed on the margin for a fast overview.

In R, slots of a S4 class can be accessed directly by the `@` operator. In this vignette, the notation `@xxx` will thus mean “slot *xxx* of an object” see figure 1 on page 5).

Likewise, named elements of a *list*, like the columns of a *data.frame*, are accessed by the `$` operator, and `$xxx` will be used for “column *xxx*”, and as an abbreviation for “column *xxx* of the *data.frame* in slot *data* of the object” see figure 1 on page 5) .

2. Remarks on R

2.1. Generic Functions

Generic Functions are functions that apply to a wide range of data types or classes, e. g. *plot*, *print*, mathematical operators, etc. These functions can be implemented in a specialized way by each class.

hyperSpec implements with a variety of such functions, see table ?? on page ??.

2.2. Functionality Can be Extended at Runtime

R's concept of functions offers much flexibility. Functions may be added or changed by the user in his *workspace* at any time. This is also true for methods belonging to a certain class. Neither restart of R nor reloading of the package or anything the like is needed. If the original function resides in a namespace (as it is the case for all functions in *hyperSpec*), the original function is not deleted. It is just masked by the user's new function but stays accessible via the `::` operator.

This offers the opportunity of easily writing specialized functions that are adapted to specific tasks.

For examples, see the setup of the lattice plotting functions in the `vignettes.defs` file accompanying all *hyperSpec* vignettes.

2.3. Validity Checking

S4 classes have a mechanism to define and enforce that the data actually stored in the object is appropriate for this class. In other words, there is a mechanism of *validity checking*.

The functions provided by *hyperSpec* check the validity of *hyperSpec* objects at the beginning, and — if the validity could be broken by inappropriate arguments — also before leaving the function.

It is highly recommended to use validity checking also for user-defined functions. In addition, non-generic functions should first ensure that the argument actually is a *hyperSpec* object. The two tasks are accomplished by:

```
> .is.hy (object)
> validObject (object)
```

The first line checks whether `object` is a *hyperSpec* object, the second checks its validity. Both functions return TRUE if the checks succeed, otherwise they raise an error and stop.

3. Loading the package

To load *hyperSpec*, use

```
> library (hyperSpec)
```

4. The structure of hyperSpec objects

hyperSpec is a S4 (or new-style) class. It has four so-called *slots* that contain parts of the object:

<code>@wavelength</code>	containing a numeric vector with the wavelength axis of the spectra.
<code>@data</code>	a <i>data.frame</i> with the spectra and all further information belonging to the spectra
<code>@label</code>	a list with appropriate labels (particularly for axis annotations)
<code>@log</code>	a <i>data.frame</i> keeping track of what is done with the object

However, it is good practice to use the functions provided by *hyperSpec* to handle the objects rather than accessing the slots directly (tab). This also ensures that proper (*valid*) objects are retained.

Most of the data is stored in `@data`. This *data.frame* has one special column, `$spc`. It is the column that actually contains the spectra. The spectra are stored in a matrix inside this column, as

slot	get	set
@wavelength	wl	wl<-
@data	[, [[, \$, as.data.frame, as.long.df, ...	[<-, [[<-, \$<-
@label	labels	labels<-
@log	logbook	logentry

Table 1: Get and set functions for the slots of *hyperSpec* objects

Figure 1: The structure of the data in a *hyperSpec* object.

illustrated in figure 1. Even if there are no spectra, `$spc` must still be present. It is then a matrix with zero columns.

Slot `@label` contains an element for each of the columns in `@data` plus one holding the label for the wavelength axis, `.wavelength`. The elements of the list may be anything suitable for axis annotations, i.e. they should be either character strings or expressions for “pretty” axis annotations (see figure ?? on page ??). To get familiar with expressions for axis annotation, see `? plotmath` and `demo (plotmath)`.

5. Functions provided by hyperSpec

Table A (p. 20) in the appendix gives an overview of the functions implemented by *hyperSpec*.

6. 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:

`print, show,`
`summary`

```
> chondro

hyperSpec object
  875 spectra
  4 data columns
  300 data points / spectrum
wavelength: Delta * tilde(nu)/cm^-1 [numeric] 602 606 ... 1798
data: (875 rows x 4 columns)
  1. y: y/(mu * m) [numeric] -4.77 -4.77 ... 19.23
  2. x: x/(mu * m) [numeric] -11.55 -10.55 ... 22.45
  3. spc: I / a.u. [matrix300] 517.0329 499.7695 ... 168.0361
  4. clusters: clusters [factor] matrix matrix ... lacuna + NA

> summary (chondro)

hyperSpec object
  875 spectra
  4 data columns
  300 data points / spectrum
wavelength: Delta * tilde(nu)/cm^-1 [numeric] 602 606 ... 1798
data: (875 rows x 4 columns)
```

```

1. y: y/(mu * m) [numeric] -4.77 -4.77 ... 19.23
2. x: x/(mu * m) [numeric] -11.55 -10.55 ... 22.45
3. spc: I / a.u. [matrix300] 517.0329 499.7695 ... 168.0361
4. clusters: clusters [factor] matrix matrix ... lacuna + NA
log:
      short      long      date      user
1  scan.txt.Renishaw list(...) 2010-02-24 10:04:06 cb@cb
2      orderwl list(...) 2010-02-24 10:04:06 cb@cb
3      spc.loess list(...) 2010-02-24 10:04:29 cb@cb
4          $<- list(...) 2010-02-24 10:04:47 cb@cb
5          $<- list(...) 2010-02-24 10:04:47 cb@cb

```

```
nrow, ncol,
nwl, dim
```

The data set `chondro` consists of 875 spectra with 300 data points each, and 4 data columns: two for the spatial information plus `$spc`. These informations can be directly obtained by

```

> nrow (chondro)

[1] 875

> nwl (chondro)

[1] 300

> ncol (chondro)

[1] 4

> dim (chondro)

nrow ncol  nwl
 875    4   300

```

```
colnames,
rownames,
dimnames, w1
```

The names of the columns in `@data` are accessed by

```

> colnames (chondro)

[1] "y"      "x"      "spc"    "clusters"

```

Likewise, `rownames` returns the names assigned to the spectra, and `dimnames` yields a list of these three vectors (including also the column names of `$spc`). The column names of the spectra matrix are the wavelengths. They are accessed by `w1`, see section 9.3.2.

```
colnames<-,
rownames<-
```

Extra data column names and rownames of the object may be set by `colnames<-` and `rownames<-`, respectively. `colnames<-` renames the labels as well.

7. Creating a `hyperSpec` Object, Data Import and Export

`hyperSpec` comes with filters for a variety of file formats. These are discussed in detail in a separate document. Use `vignette("file-io")` to read about import and export of spectra into `hyperSpec` objects.

7.1. Creating a hyperSpec Object from Spectra Matrix and Wavelength Vector

If the data is in R's workspace, a *hyperSpec* object is created by:

```
spc <- new ("hyperSpec", spc = spectra.matrix, wavelength = wavelength.vector, data = extra.data)
```

You will usually give the following arguments:

`spc` the spectra matrix

`wavelength` the wavelength axis vector

`data` the extra data (possibly already including the spectra matrix in column `spc`)

`label` a list with the proper labels. Do not forget the wavelength axis label in `$.wavelength` and the spectral intensity axis label in `$spc`.

8. Combining and Decomposing hyperspec Objects

8.1. Binding Objects together

`cbind` `rbind`

hyperSpec Objects can be bound together, either by rows to append a new spectral range or by columns to append new spectra

```
> dim (flu)
nrow ncol nwl
  6    3  181

> dim (cbind (flu, flu))
nrow ncol nwl
  6    3  362

> dim (rbind (flu, flu))
nrow ncol nwl
 12    3  181
```

Thus, you can use `cbind` to add new spectral ranges, and `rbind` to add new spectra to your object.

There is also a more general function, `bind`, taking the direction ("`r`" or "`c`") as first argument and then all objects to bind either in separate arguments or in a list.

As usual for `rbind` and `cbind`, the objects that should be bound together must have the same rows and columns, respectively.

`collapse`

8.2. Binding Objects that do not share the same extra data and/or wavelength axis

`collapse` combines objects that should be bound together by row, but they do not share the columns and/or spectral range. The resulting object has all columns from all input objects, and all wavelengths from the input objects. If an input object does not have a particular column or wavelength, its value in the resulting object is `NA`.

The `barbituates` data is a list of 286 *hyperSpec* objects, each containing one mass spectrum. The spectra have 4 to 101 data points.

```

> barb <- collapse (barbituates)
> barb [[1:3, , min ~ min + 10i]]
      25.95 26.05 26.15 26.95 27.05 27.15 28.05 28.15 29.05 29.15 29.95
[1,]    NA    NA    NA    NA   562    NA    NA 11511  6146    NA    NA
[2,]    NA    NA    NA    NA    NA   618 10151    NA  5040    NA    NA
[3,]    NA    NA    NA    NA   638    NA    NA 10722  5253    NA    NA

```

%%

8.3. Matrix Multiplication

Two *hyperSpec* objects can be matrix multiplied by `%*%`. For an example, see the principal component analysis below (section 12.1 on page 16).

decomposition

8.4. Decomposition

Matrix decompositions are common operations during chemometric data analysis. The results, e. g. of a principal component analysis are two matrices, the so-called scores and loadings. The results can have either the same number of rows as the spectra matrix they were calculated from (scores-like), or they have as many wavelengths as the spectra (loadings-like).

Both types of result objects can be “re-imported” into *hyperSpec* objects with function `decomposition`. A scores-like object retains all per-spectrum information (i. e. the extra data) while the spectra matrix and wavelength vector are replaced. A loadings-like object retains the wavelength information, while extra data is deleted (set to NA) unless the value is constant for all spectra.

A demonstration can be found in the principal component analysis example (section 12.1) on page 16.

9. Access to the data

The main functions to retrieve the data of a *hyperSpec* object are `[]` and `[[[]]`.

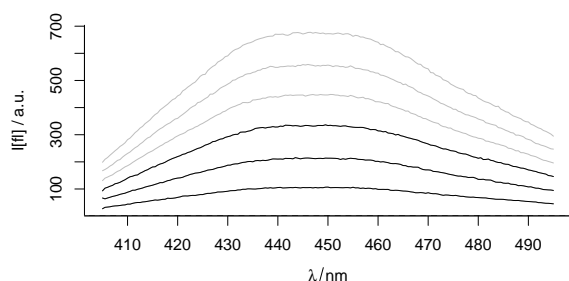
9.1. Selecting and Deleting Spectra

The extraction function `[]` (or `[[[]]`, if the spectra *matrix* or the *data.frame* is needed rather than a *hyperSpec* object) takes the spectra as first argument (For detailed help: `? "[]"`). It may be a vector giving the indices of the spectra to extract (select), a vector with negative indices indicating which spectra should be deleted, or a logical. Note that a matrix given to `[]` will be treated as a vector.

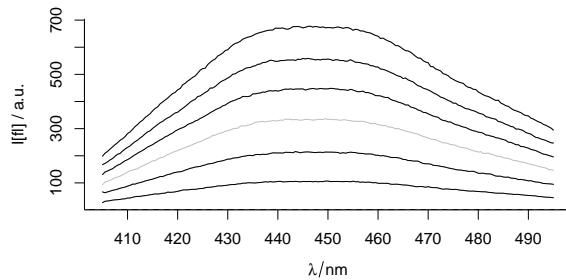
```

> plot (flu, col = "gray")
> plot (flu [1 : 3], add = TRUE)

```




```
> plot (flu, col = "gray")
> plot (flu [-3], add = TRUE)
```



```
> chondro [chondro$y > 10]
```

hyperSpec object

350 spectra

4 data columns

300 data points / spectrum

wavelength: Delta * tilde(nu)/cm⁻¹ [numeric] 602 606 ... 1798

data: (350 rows x 4 columns)

1. y: y/(mu * m) [numeric] 10.23 10.23 ... 19.23

2. x: x/(mu * m) [numeric] -11.55 -10.55 ... 22.45

3. spc: I / a.u. [matrix300] 357.3975 335.9266 ... 168.0361

4. clusters: clusters [factor] lacuna lacuna ... lacuna

9.2. Accessing the Extra Data

The second argument of the extraction functions `[]` and `[[[]]` specifies the (extra) data columns. They can be given like any column specification for a *data.frame*, i. e. numeric, logical, or by a vector of the column names:

```
> colnames (chondro)
```

```
[1] "y"      "x"      "spc"    "clusters"
```

```
> chondro [[1 : 3, 1]]
```

```
      y
1 -4.77
2 -4.77
3 -4.77
```

```
> chondro [[1 : 3, -3]]
```

```
      y      x clusters
1 -4.77 -11.55  matrix
2 -4.77 -10.55  matrix
3 -4.77  -9.55  matrix
```

```
> chondro [[1 : 3, "x"]]
```

```
      x
1 -11.55
2 -10.55
3  -9.55
```

```
> chondro [[1 : 3, c (TRUE, FALSE, FALSE)]]
```

```
      y clusters
1 -4.77  matrix
2 -4.77  matrix
3 -4.77  matrix
```

To select one column, the `$` operator is more convenient:

```
> flu$c
[1] 0.05 0.10 0.15 0.20 0.25 0.30
```

The extra data may also be set this way:

```
> flu$n <- list (1 : 6, label = "sample no.")
```

This function will append new columns, if necessary.

9.3. Wavelengths and Spectral Axis

9.3.1. Wavelength Indices

wl2i i2wl

Spectra in *hyperSpec* have always discretized wavelength axes, they are stored in a matrix with column corresponding to one wavelength. *hyperSpec* provides two conversion functions: `i2wl` returns the wavelength corresponding to the given indices and `wl2i` calculates index vectors from wavelengths.

If the wavelengths are given as a numeric vector, they are each converted to the corresponding wavelength. In addition there is a more sophisticated possibility of specifying wavelength ranges using a *formula*. The basic syntax is *start* ~ *end*. This yields a vector *index of start* : *index of end*.

The result of the formula conversion differs from the numeric vector conversion in three ways:

- The colon operator for constructing vectors accepts only integer numbers, the tilde (for formulas) does not have this restriction.
- If the vector does not take into account the spectral resolution, one may get only every n^{th} point or repetitions of the same index:

```
> wl2i (flu, 405 : 410)
[1] 1 3 5 7 9 11
> wl2i (flu, 405 ~ 410)
[1] 1 2 3 4 5 6 7 8 9 10 11
> wl2i (chondro, 1000 : 1010)
[1] 100 101 101 101 101 102 102 102 102 103 103
> wl2i (chondro, 1000 ~ 1010)
[1] 100 101 102 103
```

- If the object's wavelength axis is not ordered, the formula approach doesn't work. In that (rare) case, use `orderwl` first to obtain an object with ordered wavelength axis.

`start` and `end` may contain the special variables `min` and `max` that correspond to the lowest and highest wavelengths of the object:

```
> wl2i (flu, min ~ 410)
[1] 1 2 3 4 5 6 7 8 9 10 11
```

Often, specifications like *wavelength $\pm n$ data points* are needed. They can be given using complex numbers in the formula. The imaginary part is added to the index calculated from the wavelength in the real part:

```
> wl2i (flu, 450 - 2i ~ 450 + 2i)
[1] 89 90 91 92 93
> wl2i (flu, max - 2i ~ max)
[1] 179 180 181
```

To specify several wavelength ranges, use a list containing the formulas and vectors¹:

```
> wl2i (flu, 450 - 2i ~ 450 + 2i)
[1] 89 90 91 92 93
> wl2i (flu, c(min ~ 406.5, max - 2i ~ max))
[1] 1 2 3 4 179 180 181
```

This mechanism also works for the wavelength arguments of `[]`, `[[[]]`, and `plotspc`.

9.3.2. Wavelength Axis Conversion

9.4. The Square-Bracket Operators

In addition, `[[[]]` accepts index matrices of size $n \times 2$.

```
> indexmatrix <- matrix (c (1 : 3, 1 : 3), ncol = 2)
> indexmatrix
      [,1] [,2]
[1,]    1    1
[2,]    2    2
[3,]    3    3
> chondro [[indexmatrix, wl.index = TRUE]]
[1] 517.0329 516.3300 436.3566
> diag (chondro [[1 : 3, , min ~ min + 2i]])
[1] 517.0329 516.3300 436.3566
```

9.5. Fast Access to Parts of the hyperSpec Object

[[]] \$. \$..

hyperSpec comes with three abbreviation functions for easy access to the data:

```
x [[]] returns the spectra matrix (x$spc).
x [[i, , l]] the cut spectra matrix is returned if wavelengths are specified in l.
x [[i, j, l]] If data columns are selected (second index), the result is a data.frame.
x [[i, , l]] <- Also, parts of the spectra matrix can be set (only indices for spectra and wavelength are allowed for this function).
x [i, j] <- sets parts of x@data.
x $. returns the complete data.frame x@data, with the spectra in column $spc.
x $.. returns the extra data (x@data without x$spc).
x $.. <- sets the extra data (x@data without x$spc). However, the columns must match exactly in this case.
```

10. Plotting

hyperSpec offers a variety of possibilities to plot spectra, spectral maps, the spectra matrix, time series, depth profiles, etc.. This all is discussed in a separate document: see *vignette* ("plotting").

11. Spectral (Pre)processing

11.1. Cutting the Spectral Range

[] [[]]

The extraction functions `[]` and `[[]]` can be used to cut the spectra: Their third argument takes wavelength specifications as discussed above and also logicals (i.e. vectors specifying with TRUE/FALSE for each column of `$spc` whether it should be included or not).

`[]` returns a *hyperSpec* object, `[[]]` the spectra *matrix*\$`$spc` (or the *data.frame*@`data` if data columns were specified, too) only.

```
> flu[, , min ~ 408.5]

hyperSpec object
  6 spectra
  4 data columns
  8 data points / spectrum
wavelength: lambda/nm [numeric] 405.0 405.5 ... 408.5
data: (6 rows x 4 columns)
  1. file: [factor] rawdata/flu1.txt rawdata/flu2.txt ... rawdata/flu6.txt
  2. spc: I[fl] / a.u. [AsIs matrix x 8] 27.15000 66.80133 ... 256.8913
  3. c: c / (mg / l) [numeric] 0.05 0.10 ... 0.3
  4. n: sample no. [integer] 1 2 ... 6

> flu[[, , c (min ~ min + 2i, max - 2i ~ max)]]
```

¹Formulas are combined to a list by `c`.

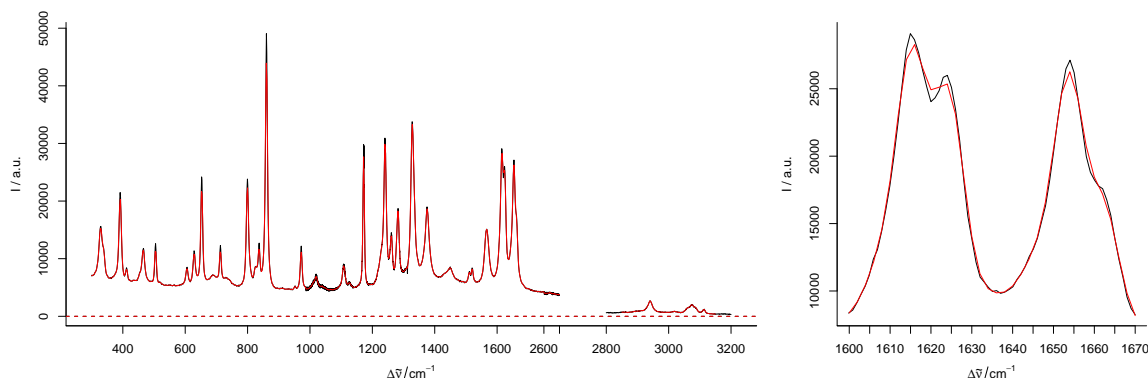


Figure 2: Smoothing interpolation by `spc.loess` with new data point spacing of 2 cm^{-1} . The magnification on the right shows how interpolation may cause a loss in signal.

	405	405.5	406	494	494.5	495
[1,]	27.15000	32.34467	33.37867	47.16267	46.41233	45.25633
[2,]	66.80133	63.71533	66.71200	96.60167	96.20600	94.61033
[3,]	93.14433	103.06767	106.19367	149.53900	148.52667	145.79333
[4,]	130.66367	139.99833	143.79767	201.48433	198.86733	195.86733
[5,]	167.26667	171.89833	177.47067	252.06567	248.06700	246.95200
[6,]	198.43033	209.45800	215.78500	307.51850	302.32550	294.64950

11.2. Spectral Interpolation and Smoothing

Frequently, a *hyperSpec* object needs to be interpolated onto a new wavelength axis. e.g. because measurements resulted in slightly shifted wavelength axes. Or data from a grating spectrometer with unequal data point spacing should be interpolated onto an evenly spaced wavelength axis. Also, the spectra can be smoothed: reducing the spectral resolution allows to increase the signal to noise ratio. For chemometric data analysis reducing the number of data points per spectrum may be crucial as it reduces the dimensionality of the data.

hyperSpec provides two functions to change the wavelength axis of *hyperSpec* objects: `spc.bin` and `spc.loess`.

`spc.bin` bins the spectral axis by averaging every *by* data points.

```
> plot (paracetamol, wl.range = c (300 ~ 1800, 2800 ~ max), xoffset = 850)
> p <- spc.loess (paracetamol, c(seq (300, 1800, 2), seq (2850, 3150, 2)))
> plot (p, wl.range = c (300 ~ 1800, 2800 ~ max), xoffset = 850, col = "red", add = TRUE)
```

`spc.loess` applies R's `loess` function for spectral interpolation. Figure 2 shows the result of interpolating from 300 to 1800 and 2850 to 3150 cm^{-1} with 2 cm^{-1} data point distance. This corresponds to a spectral resolution of about 4 cm^{-1} , and the decrease in spectral resolution can be seen at the sharp bands where the maxima are not reached (due to the fact that the interpolation wavelength axis does not necessarily hit the maxima). The original spectrum had 4064 data points with unequal data point spacing (between 0 and 1.4 cm^{-1}). The interpolated spectrum has 902 data points.

11.3. Background Correction

To subtract a background spectrum of each of the spectra in an object, use `sweep (spectra, 2, background.spectrum, "-")`.

`spc.bin`
`spc.loess`

11.4. Offset Correction

Calculate the offsets and sweep them off the spectra:

```
> offsets <- apply (chondro, 1, min)
> chondro.offset.corrected <- sweep (chondro, 1, offsets, "-")
```

11.5. Baseline Correction

hyperSpec comes with two functions to fit polynomial baselines.

`spc.fit.poly` fits a polynomial baseline of the given order. A least-squares fit is done so that the function may be used on rather noisy spectra. However, the user must supply an object that is cut appropriately. Particularly, the supplied wavelength ranges are not weighted.

`spc.fit.poly.below` tries to find appropriate support points for the baseline iteratively.

Both functions return a *hyperSpec* object containing the fitted baselines. They need to be subtracted afterwards:

```
> bl <- spc.fit.poly.below (chondro)
Fitting with npts.min = 15
> chondro <- chondro - bl
```

For details, see vignette (baselinebelow).

11.6. Intensity Calibration

11.6.1. Correcting by a constant, e. g. Readout Bias

CCD cameras often operate with a bias, causing a constant value for each pixel. Such a constant can be immediately subtracted:

```
spectra - constant
```

11.6.2. Correcting Wavelength Dependence

This means that for each of the wavelengths the same correction needs to be applied to all spectra.

1. There might be wavelength dependent offsets (background or dark spectra). They are subtracted:
`sweep (spectra, 2, offset.spectrum, "-")`
2. A multiplicative dependency such as a CCD's photon efficiency:
`sweep (spectra, 2, photon.efficiency, "/")`

11.6.3. Spectra Dependent Correction

If the correction depends on the spectra (e.g. due to inhomogeneous illumination while collecting imaging data²), the *MARGIN* of the `sweep` function needs to be 1:

1. Pixel dependent offsets are subtracted:
`sweep (spectra, 2, pixel.offsets, "-")`
2. A multiplicative dependency:
`sweep (spectra, 2, illumination.factors, "*")`

11.7. Normalization

1. Calculate appropriate normalization factors:
`factors <- 1 / apply (spectra, 1, sum)` for area normalization. `mean` gives equal results, just that the Intensities are on the same scale as before.
For minimum-maximum-normalization, first do an offset- or baseline correction, then calculate the *factors* using `max`.
You may calculate the factors using only a certain wavelength range, thereby normalizing on a particular band or peak.
2. Again, sweep the factor off the spectra:
`normalized <- sweep (spectra, 1, factors, "*")`

```
> factors <- 1 / apply (chondro, 1, mean)
> chondro <- sweep (chondro, 1, factors, "*")
```

11.8. Centering the Data

Centering means that the mean spectrum is subtracted from each of the spectra. Many data analysis techniques, like principal component analysis, partial least squares, etc., work much better on centered data.

However, from a spectroscopic point of view it depends on the particular data set whether centering does make sense or not.

It is perfectly fine to centre the `flu` data set: the interpretation is that centering the data cancels the offset (background spectrum etc.) of the calibration:

```
> flu.centered <- sweep (flu, 2, apply (flu, 2, mean), "-")

> plot (flu.centered)
```

On the other hand, the `chondro` data set consists of Raman spectra, so the spectroscopic interpretation of centering is getting rid of the the average chemical composition of the sample. But: what is the meaning of the “average spectrum” of an inhomogeneous sample? In this case it is better to subtract the minimum spectrum (which will hopefully have almost the same benefit on the data analysis) as it is the spectrum of that chemical composition that is underlying the whole sample.

One more point to consider is that the actual minimum spectrum will pick up lots of the negative noise. In order to avoid that, using e. g. the 5th percentile spectrum is more suitable:

²imaging (as opposed to mapping) refers to simultaneously collecting spatially resolved spectra, either 2d images or line imaging.

```
> chondro <- sweep (chondro, 2, apply (chondro, 2, quantile, 0.05), "-")

> plot (chondro, "spcprct15")
```

11.9. Variance Scaling

Variance scaling is often used in multivariate analysis to adjust the influence and scaling of the variates (that are typically different physical values). However, it is hardly appropriate for spectra that do have the same scale of the same physical value.

11.10. Multiplicative Scatter Correction (MSC)

MSC can be done using `msc` from package *pls*[1]. It operates on the spectra matrix:

```
> library (pls)
> chondro.msc <- chondro
> chondro.msc [[]] <- msc (chondro [[]])
```

11.11. Spectral Arithmetic

Basic mathematical functions are defined for *hyperSpec* objects. You may convert spectra:
`absorbance.spectra = - log10 (transmission.spectra)`

In this case, do not forget to adapt the label:

```
> labels (absorbance.spectra)$spc <- "A"
```

Be careful: R's `log` function calculates the natural logarithm if no base is given.

The basic arithmetic operators work element-wise in R. Thus they all need either a scalar, or a matrix (or *hyperSpec* object) of the correct size.

Matrix multiplication is done by `%*%`, again each of the operands may be a matrix or a *hyperSpec* object, and must have the correct dimensions.

+ - * / ^ log
log10

labels

12. Data Analysis

12.1. Data Analysis Methods using a data.frame

e. g. Principal Component Analysis with `prcomp`

The `$.` notation is handy, if a data analysis function expects a *data.frame*. The column names can then be used in the formula:

```
> pca <- prcomp (~ spc, data = chondro$. , center = FALSE)
```

Results of such a decomposition can be put again into *hyperSpec* objects. This allows to plot e. g. the loading like spectra, or score maps, see figure 3.


```
> scores <- decomposition (chondro, pca$x, label.wavelength = "PC",
+                           label.spc = "score / a.u.")
> scores

hyperSpec object
  875 spectra
  4 data columns
  300 data points / spectrum
wavelength: PC [integer] 1 2 ... 300
data: (875 rows x 4 columns)
  1. y: y/(mu * m) [numeric] -4.77 -4.77 ... 19.23
  2. x: x/(mu * m) [numeric] -11.55 -10.55 ... 22.45
  3. spc: score / a.u. [AsIs matrix x 300] 1.519974 1.482294 ... 0.0005919229
  4. clusters: clusters [factor] matrix matrix ... lacuna + NA
```

The loadings can be similarly re-imported:

```
> loadings <- decomposition (chondro, t(pca$rotation), scores = FALSE,
+                             label.spc = "loading I / a.u.")
> loadings

hyperSpec object
  300 spectra
  1 data columns
  300 data points / spectrum
wavelength: Delta * tilde(nu)/cm^-1 [numeric] 602 606 ... 1798
data: (300 rows x 1 columns)
  1. spc: loading I / a.u. [AsIs matrix x 300] 0.048952872 0.005090892 ... 0.1876058
```

There is, however, one important difference. The loadings are thought of as values computed from all spectra together. Thus no meaningful extra data can be assigned for the loadings object (at least not if the column consists of different values). Therefore, the loadings object lost all extra data (see above).

retain.columns triggers whether columns that contain different values should be dropped. If it is set to `TRUE`, the columns are retained, but contain NAs:

```
> loadings <- decomposition (chondro, t(pca$rotation), scores = FALSE,
+                             retain.columns = TRUE, label.spc = "loading I / a.u.")
> loadings[1]$..

  y  x clusters
1 NA NA      <NA>
```

If an extra data column does contain only one unique value, it is retained anyways:

```
> chondro$measurement <- 1
> loadings <- decomposition (chondro, t(pca$rotation), scores = FALSE,
+                             label.spc = "loading I / a.u.")
> loadings[1]$..

  measurement
1           1
```

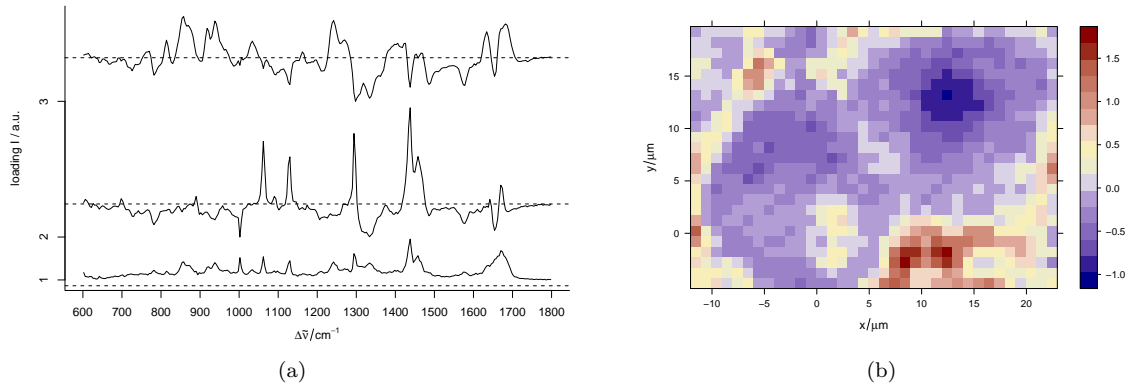


Figure 3: (a) The first three loadings: `plot (loadings [1 : 3], stacked = TRUE)`. (b) The second score map: `plotmap (scores [, , 2])`

12.1.1. PCA as Noise Filter

Principal component analysis is sometimes used as a noise filtering technique. The idea is that the relevant differences are captured in the first components while the higher components contain noise only. Thus the spectra are reconstructed using only the first p components.

This reconstruction is in fact a matrix multiplication:

$$spectra^{(nrow \times nwl)} = scores^{(nrow \times p)} loadings^{(p \times nwl)}$$

Note that this corresponds to a model based on the Beer-Lambert law:

$$A_n(\lambda) = c_{n,i} \epsilon(i, \lambda) + error$$

The matrix formulation puts the n spectra into the rows of A and c , while the i pure components appear in the columns of c and rows of the absorbance coefficients ϵ .

For an ideal data set (constituents varying independently, sufficient signal to noise ratio) one would expect the principal component analysis to extract something like the concentrations and pure component spectra.

If we decide that only the first 10 components actually carry spectroscopic information, we can reconstruct spectra with better signal to noise ratio:

```
> smoothed <- scores [, , 1:10] %*% loadings [1:10]
```

Keep in mind, though, that we cannot be sure how much *useful* information was discarded with the higher components. This kind of noise reduction may influence further modeling of the data. Mathematically speaking, the rank of the 875×300 spectra matrix was reduced to 10.

12.2. Data Analysis Methods using a matrix

e. g. Hierarchical Cluster Analysis

```
> dist <- pearson.dist (chondro [[]])
> dendrogram <- hclust (dist, method = "ward")
```

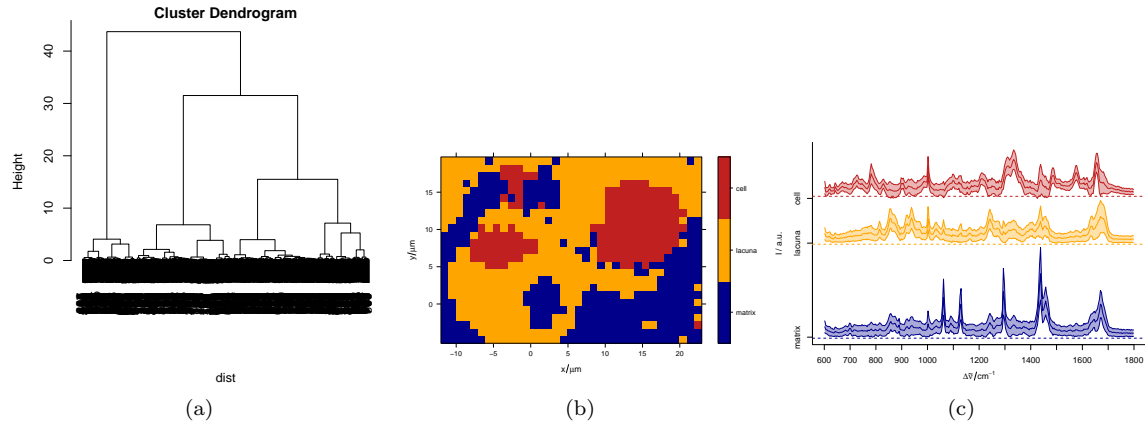


Figure 4: The results of the cluster analysis: (a) the dendrogram (b) the map of the 3 clusters (c) the mean spectra.

```
> plot (dendrogram)
```

In order to plot a cluster map, the cluster membership needs to be calculated from the dendrogram. First, cut the dendrogram so that three clusters result:

```
> chondro$clusters <- as.factor (cutree (dendrogram, k = 3))
```

As the cluster membership was stored as factor, the levels can be meaningful names, which are displayed in the color legend.

```
> levels (chondro$clusters) <- c ("matrix", "lacuna", "cell")
```

Then the result may be plotted (figure 4b):

12.3. Calculating group-wise Sum Characteristics e. g. Cluster Mean Spectra

`aggregate` applies the function given in *FUN* to each of the groups of spectra specified in *by*.

`aggregate`

So we may plot the cluster mean spectra:

```
> means <- aggregate (chondro, by = chondro$clusters, mean_pm_sd)
> plot (means, col = cluster.cols, stacked = ".aggregate", fill = ".aggregate")
```

12.4. Splitting an Object

A *hyperSpec* object may also be split into a list of *hyperSpec* objects:

```
> clusters <- split (chondro, chondro$clusters)
> clusters
```

```

$matrix
hyperSpec object
  292 spectra
  5 data columns
  300 data points / spectrum
wavelength: Delta * tilde(nu)/cm^-1 [numeric] 602 606 ... 1798
data: (292 rows x 5 columns)
  1. y: y/(mu * m) [numeric] -4.77 -4.77 ... 19.23
  2. x: x/(mu * m) [numeric] -11.55 -10.55 ... 21.45
  3. spc: I / a.u. [matrix300] 0.10834684 0.08162965 ... 0.01434837
  4. clusters: clusters [factor] matrix matrix ... matrix
  5. measurement: measurement [numeric] 1 1 ... 1

$lacuna
hyperSpec object
  417 spectra
  5 data columns
  300 data points / spectrum
wavelength: Delta * tilde(nu)/cm^-1 [numeric] 602 606 ... 1798
data: (417 rows x 5 columns)
  1. y: y/(mu * m) [numeric] -4.77 -4.77 ... 19.23
  2. x: x/(mu * m) [numeric] -5.55 -4.55 ... 22.45
  3. spc: I / a.u. [matrix300] 0.05266207 0.05704105 ... 0.02574641
  4. clusters: clusters [factor] lacuna lacuna ... lacuna
  5. measurement: measurement [numeric] 1 1 ... 1

$cell
hyperSpec object
  166 spectra
  5 data columns
  300 data points / spectrum
wavelength: Delta * tilde(nu)/cm^-1 [numeric] 602 606 ... 1798
data: (166 rows x 5 columns)
  1. y: y/(mu * m) [numeric] -2.77 5.23 ... 18.23
  2. x: x/(mu * m) [numeric] 22.45 -5.55 ... -1.55
  3. spc: I / a.u. [matrix300] 0.125600985 -0.009449245 ... 0.02353212
  4. clusters: clusters [factor] cell cell ... cell
  5. measurement: measurement [numeric] 1 1 ... 1

```

Splitting can be reversed by `rbind` (see section 8.1, page 7).

References

- [1] Ron Wehrens and Bjørn-Helge Mevik. *pls: Partial Least Squares Regression (PLSR) and Principal Component Regression (PCR)*, 2007. URL <http://mevik.net/work/software/pls.html>. R package version 2.1-0.

A. Overview of the functions provided by hyperSpec

Function	Explanation
<i>Create and initialize an object</i>	

Function	Explanation
<code>initialize</code>	
<i>Basic information</i>	
<code>colnames</code>	
<code>colnames<-</code>	
<code>dim</code>	
<code>dimnames</code>	
<code>length</code>	
<code>ncol</code>	number of data columns (extra data plus spectra matrix)
<code>nrow</code>	number of spectra
<code>nwl</code>	number of data points per spectrum
<code>print</code>	summary information
<code>rownames</code>	
<code>show</code>	
<code>summary</code>	summary information including the log
<i>Access parts of the object</i>	
<code>[</code>	Select / extract / delete spectra, wavelength ranges or extra data
<code>[<-</code>	Set parts of spectra or extra data
<code>[[</code>	Select / extract / delete spectra, wavelength ranges or extra data, get the result as matrix or data.frame
<code>[[<-</code>	Set parts of spectra matrix
<code>\$</code>	extract a data column (including <code>\$spc</code>)
<code>\$<-</code>	replace a data column (including <code>\$spc</code>)
<code>i2wl</code>	convert spectra matrix column indices to wavelengths
<code>isample</code>	get a random sample of the spectra as index vector
<code>labels</code>	get column labels
<code>labels<-</code>	set column labels
<code>logbook</code>	logging the data treatment
<code>logentry</code>	make a logbook entry
<code>rownames<-</code>	
<code>sample</code>	generate random sample of the spectra
<code>seq.hyperSpec</code>	sequence along the spectra, either as <i>hyperSpec</i> object or index vector
<code>wl</code>	extract the wavelengths
<code>wl<-</code>	replace the wavelengths
<code>wl2i</code>	convert wavelengths to spectra matrix column indices
<i>Type conversion</i>	
<code>as.character</code>	

Function	Explanation
<code>as.data.frame</code>	
<code>as.long.df</code>	convert to a long-format data.frame.
<code>as.matrix</code>	
<code>as.wide.df</code>	convert to a wide-format data.frame with each wavelength one column
<code>decomposition</code>	re-import results of spectral matrix decomposition (or the like) into <i>hyperSpec</i> object
<i>File import/export</i>	
<code>\emph{R.matlab::readMat}</code>	import matlab file
<code>\emph{R.matlab::writeMat}</code>	export as matlab file
<code>read.ENVI</code>	import ENVI file
<code>read.ENVI.Nicolet</code>	import ENVI files written by Nicolet spectrometers
<code>read.spc</code>	import .spc file
<code>read.spc.KaiserMap</code>	import a Raman map saved by Kaiser Optical Systems' Hologram software as multiple .spc files
<code>read.txt.long</code>	import long-type ASCII file
<code>read.txt.wide</code>	import wide-type ASCII file
<code>scan.txt.Renishaw</code>	import ASCII files produced by Renishaw (InVia) spectrometers
<code>write.txt.long</code>	export as long-type ASCII file
<code>write.txt.wide</code>	export as wide-type ASCII file
<i>Combine/split</i>	
<code>bind</code>	common interface for <code>rbind</code> and <code>cbind</code>
<code>cbind2</code>	bind two <i>hyperSpec</i> objects by column
<code>cbind.hyperSpec</code>	
<code>collapse</code>	combine objects by adding columns if necessary. See <code>plyr::rbind.fill</code> .
<code>rbind2</code>	bind two <i>hyperSpec</i> objects by row, i. e. add wavelength ranges or extra data
<code>rbind.hyperSpec</code>	bind objects by row, i. e. add wavelength ranges or extra data
<code>split</code>	
<i>Vectorization</i>	
<code>aggregate</code>	
<code>apply</code>	
<code>sweep</code>	
<i>Maths</i>	
<code>%*%</code>	matrix multiplication
<code>Arith</code>	
<code>log</code>	

Function	Explanation
<code>Math</code>	mathematical functions. See (<code>help (■Math■)</code>)
<code>Math2</code>	rounding
<code>Summary</code>	summary measures such as <code>min</code> , <code>max</code> , etc.
<i>Comparison</i>	
<code>all.equal</code>	
<code>Compare</code>	<code>> < == >= <=</code> return a logical matrix
<code>is.na</code>	
<i>Plotting</i>	
<code>levelplot</code>	
<code>map.identify</code>	identify spectra in map plot
<code>matlab.dark.palette</code>	darker version of <code>matlab.palette</code>
<code>matlab.palette</code>	palette resembling Matlab's jet colors
<code>plot</code>	main switchyard for plotting
<code>plotc</code>	intensity over one other dimension: calibration plots, time series, depth series, etc.
<code>plotmap</code>	false-colour intensity over two other dimensions: spectral images, maps, etc. (rectangular tessellation)
<code>plotspc</code>	spectra plots: intensity over wavelength
<code>plotvoronoi</code>	false-colour intensity over two other dimensions: spectral images, maps, etc. (Voronoi tessellation)
<code>spc.identify</code>	identify spectra and wavelengths in spectra plot
<code>stacked.offsets</code>	calculate intensity axis offsets for stacked spectral plots
<code>trellis.factor.key</code>	modify list of <code>levelplot</code> arguments according to factor levels
<i>Spectra-specific transformations</i>	
<code>orderwl</code>	sort columns of spectra matrix according to the wavelengths
<code>spc.bin</code>	spectral binning
<code>spc.fit.poly</code>	least squares fit of a polynomial
<code>spc.fit.poly.below</code>	least squares fit of a polynomial with automatic support point determination
<code>spc.loess</code>	<code>loess</code> smoothing interpolation
<i>Utility functions</i>	
<code>array2df</code>	convert array into a matrix or data.frame
<code>array2vec</code>	convert array indices (n element vector) into vector indices
<code>factor2num</code>	convert a factor with numeric levels into the numeric
<code>mean_pm_sd</code>	mean \pm one standard deviation of a vector
<code>mean_sd</code>	mean and standard deviation of a vector
<code>pearson.dist</code>	distance measure based on Pearson's R^2

Function	Explanation
<code>rbind.fill</code>	transitional patch of <code>plyr::rbind.fill</code> working with matrices
<code>rbind.fill.matrix</code>	transitional until <code>plyr::rbind.fill.matrix</code> is out
<code>vec2array</code>	convert vector (one element) index into an array into an n element array index
<code>wc</code>	word count using <code>wc</code> if available on the system