

hyperSpec Introduction

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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`.

Reporting Issues and Suggesting Enhancements

`bug.report` (`package = "hyperSpec"`) will take you to *hyperSpec*'s issue tracking page at <https://github.com/cbeleites/hyperSpec/issues> where you can report issues you encounter, suggest features and comment on issues or suggested features.

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Suggested Packages

To build this vignette, some packages are suggested but not strictly needed:

pls: available
baseline: available
ggplot2: available
compiler: available
inline: available

1. Introduction

hyperSpec is a R package that allows convenient handling of hyperspectral data sets, i. e. data sets combining spectra with further data on a per-spectrum basis. The spectra can be anything that is recorded over a common discretized axis.

This vignette gives an introduction on basic working techniques using the R package *hyperSpec*. This is done mostly from a spectroscopic point of view: rather than going through the functions provided by *hyperSpec*, it is organized in spectroscopic tasks. However, the functions discussed are printed on the margin for a quick overview.

hyperSpec 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 (acetaminophene) ranging from 100 to 3200 cm^{-1} with overlapping wavelength ranges.
barbiturates 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 their own vignettes showing exemplary work flows for the respective data type.

This document describes how to accomplish typical tasks in the analysis of spectra. 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`.

A complete list of the functions available in *hyperSpec* is given in appendix A (p. 41).

1.1. Notation and Terms

Throughout the documentation of the package, the following terms are used:

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

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

extra data: further information/data belonging to each spectrum
spatial information (spectral images, maps, or profiles), temporal information (kinetics, time series), concentrations (calibration series), class membership information, etc.
hyperSpec object may contain arbitrary numbers of extra data columns.

In R, slots of a S4 class are accessed by the `@` operator. In this vignette, the notation `@xxx` will thus mean “slot *xxx* of an object”. Likewise, named elements of a *list* and 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” (the structure of *hyperSpec* objects is discussed in section 4, p. 6).

2. Remarks on R

2.1. Reporting an Issue with a package

R packages include contact information of the package maintainer, which you can access e. g. by:

```
> maintainer ("hyperSpec")  
[1] "Claudia Beleites <Claudia.Beleites@chemometrix.gmbh>"
```

In case you want to report an issue, R provides a function to do so. `bug.report` will either open an email to the package maintainer or the issue tracker URL given in the package DESCRIPTION.

```
> bug.report (package = "hyperSpec")
```

will take you to *hyperSpec*'s issue tracking page at <https://github.com/cbeleites/hyperSpec/issues>. It also displays essential information about your installation which can help in tracking down the bug.

We're always happy about contributions and tag issues that may be tackled immediately by “help wanted”. Please note that I (Claudia, the official maintainer) may be rather slow in answering pull requests: at the moment I'm traveling a lot professionally so it may take several weeks until I can find some calm chunk of time to do more for *hyperSpec* than emergency fixes. However, this does not mean that I won't do so: I can tell quickly if a pull request won't fit at all into *hyperSpec*.

2.2. 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 appendix A (p. 41).

2.3. 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.

The same is true for "normal" variables: You may create changed copies of the example data sets, work with these and then "reset" to *hyperSpec*'s version of the data set by removing the object in your workspace.

This offers the opportunity of easily writing specialized functions that are adapted to specific tasks. *hyperSpec*'s vignettes use this to set up special versions of the lattice graphics functions that are already wrapped in `print` (see also [R FAQ: Why do lattice/trellis graphics not work?](#)) and allow the code in the code chunks of the vignettes to be exactly what one would type during an interactive R session. For the code, check the `vignettes.defs` file accompanying all *hyperSpec* vignettes.

2.4. 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:

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

`validObject,`
`chk.hy`

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.

2.5. Special Function Names

2.5.1. The Names of Operators

Operators such as `+`, `-`, `*`, `%`, etc. are in fact functions in R. Thus they can be handed over as arguments to other functions (particularly to the vectorization functions `*apply`, `sweep`, etc.). In this case the name of the function must be quoted: ``-`` is the recommended style (although `"-"` will often work as well), e. g.:

```
> sweep (flu, 2, mean, `-`)
```

These functions can also be called in a more function-like style (prefix notation):

```
> `+` (3, 5)
```

```
[1] 8
```

name	default (range)	value	description	used by
debuglevel	0 (1L 2L)		amount of debugging information produced	<code>spc.identify</code> , <code>map.identify</code> , <code>spc.rubberband</code> , various file import functions
gc	FALSE		triggers frequent calling of <code>gc ()</code>	<code>read.ENVI</code> , <code>new ("hyperSpec")</code>
tolerance	$\sqrt{.Machine$.double.eps}$		tolerance for numerical comparisons	file import func- tions (removing empty spectra), <code>normalize01</code>
wl.tolerance	$\sqrt{.Machine$.double.eps}$		tolerance for comparisons of the wavelength axis	<code>rbind</code> , <code>rbind2</code> , <code>bind ("r", ...)</code> , <code>all.equal</code> , <code>collapse</code>
file.remove.emptySpec	TRUE		automatic removing of empty spectra	file import func- tions, see <code>vignette ("fileio")</code>
file.keep.name	TRUE		automatic recording of file name in column <code>\$filename</code>	file import func- tions, see <code>vignette ("fileio")</code>
plot.spc.nmax	25		number of spectra to be plotted by default	<code>plotspc</code>
ggplot.spc.nmax	10			<code>qplotspc</code>

Table 1 *hyperSpec* options. Please refer to the documentation of the respective functions for details about the effect of the options.

2.5.2. Assignment Functions

R allows the definition of functions that do an assignment (set some part of the object), such as:

```
> wl (flu) <- new.wavelength.values
```

an assignment to variable `wl`: ``wl<-``.

3. Loading and the package and configuration

To load *hyperSpec*, use

```
> library ("hyperSpec")
```

The global behaviour of *hyperSpec* can be configured via options. The values of the options are retrieved with `hy.getOptions` and `hy.getOption`, and changed with `hy.setOptions`. Table 1 gives an overview.

4. The structure of hyperSpec objects

hyperSpec is a S4 (or new-style) class. Four slots contain the parts of the object:

`@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)

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

Table 2 Get and set functions for the slots of *hyperSpec* objects

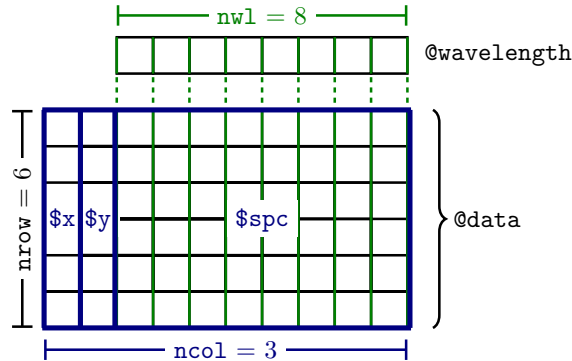


Figure 1 The structure of the data in a *hyperSpec* object.

While the parts of the *hyperSpec* object can be accessed directly, it is good practice to use the functions provided by *hyperSpec* to handle the objects rather than accessing the slots directly (tab. 2). This also ensures that proper (*valid*) objects are returned. In some cases, however, direct access to the slots can considerably speed up calculations, see section 13 (p. 38).

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 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. They are accessed by their names which must be the same for columns of @data and the list elements. 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 e. g. figure 7 on page 29). To get familiar with expressions for axis annotation, see ? plotmath and demo (plotmath).

5. Functions provided by hyperSpec

Table A (p. 41) 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
```

```

5 data columns
300 data points / spectrum
wavelength: Delta * tilde(nu)/cm^-1 [numeric] 602 606 ... 1798
data: (875 rows x 5 columns)
1. y: y [numeric] -4.77 -4.77 ... 19.23
2. x: x [numeric] -11.55 -10.55 ... 22.45
3. filename: filename [character] rawdata/chondro.txt rawdata/chondro.txt ... rawdata/chondro.txt
4. clusters: clusters [factor] matrix matrix ... lacuna + NA
5. spc: I / a.u. [matrix, array300] 501.82 500.46 ... 169.29

```

```
> summary (chondro)
```

```

hyperSpec object
875 spectra
5 data columns
300 data points / spectrum
wavelength: Delta * tilde(nu)/cm^-1 [numeric] 602 606 ... 1798
data: (875 rows x 5 columns)
1. y: y [numeric] -4.77 -4.77 ... 19.23
2. x: x [numeric] -11.55 -10.55 ... 22.45
3. filename: filename [character] rawdata/chondro.txt rawdata/chondro.txt ... rawdata/chondro.txt
4. clusters: clusters [factor] matrix matrix ... lacuna + NA
5. spc: I / a.u. [matrix, array300] 501.82 500.46 ... 169.29

```

The data set `chondro` consists of 875 spectra with 300 data points each, and 5 data columns: two for the spatial information, one factor with the results of a cluster analysis plus `$spc`. These information can be directly obtained by

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

```
> nrow (chondro)
```

```
[1] 875
```

```
> nwl (chondro)
```

```
[1] 300
```

```
> ncol (chondro)
```

```
[1] 5
```

```
> dim (chondro)
```

```

nrow ncol nwl
875    5  300

```

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

```
> colnames (chondro)
```

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

`colnames`,
`rownames`,
`dimnames`, `wl`

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 contain the wavelengths as character, while `wl` (see section 8.5.4, p. 15) yields the numeric vector of wavelengths.

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

`colnames<-`,
`rownames<-`

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 vignette accessible via `vignette ("fileio")`.

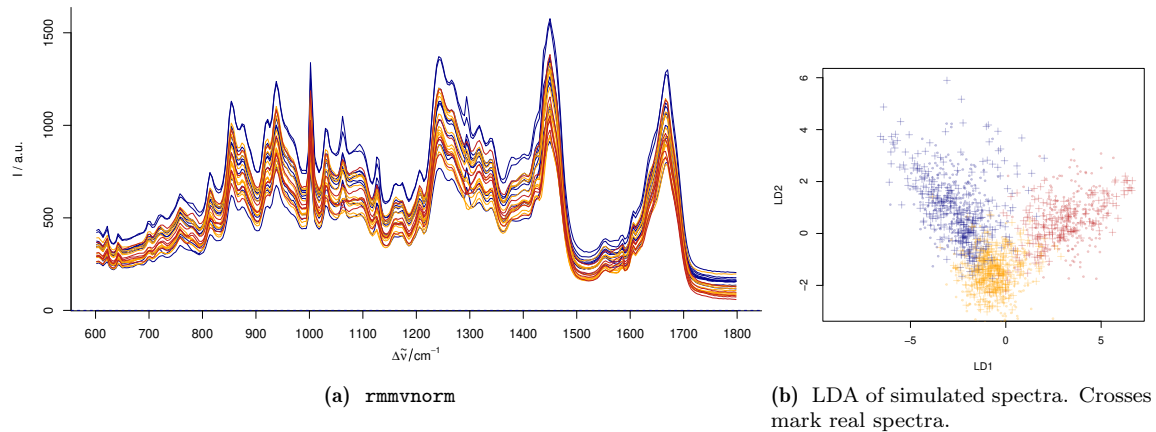


Figure 2 Multivariate normally distributed random spectra.

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)
```

The most frequently needed arguments are:

`spc` the spectra matrix

`wavelength` the wavelength axis vector

`data` the extra data (can already contain 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`.

More information about converting existing data into `hyperSpec` objects can be found in `vignette("fileio")`.

7.2. Creating Random Spectra

If `mvtnorm` is available, multivariate normally distributed spectra can be generated from mean and covariance matrix using `rmmvnorm` (fig. 2a). Note that the `hyperSpec` function's name has an additional "m": it already takes care of multiple groups. Mean spectra and pooled covariance matrix can be calculated using `pooled.cov`:

`rmmvnorm`

`pooled.cov`

```
> pcov <- pooled.cov (chondro, chondro$clusters)
> rnd <- rmmvnorm (rep (10, 3), mean = pcov$mean, sigma = pcov$COV)

> cluster.cols <- c ("dark blue", "orange", "#C02020")
> plot (rnd, col = cluster.cols [rnd$.group])
```

fig. 2b shows the linear discriminant analysis (LDA) scores of such simulated spectra in comparison to the real spectra in the `chondro` object:

```
> require ("MASS")
> rnd <- rmmvnorm (rep (200, 3), mean = pcov$mean, sigma = pcov$COV)
> lda <- lda (clusters ~ spc, rnd)
> pred.chondro <- predict (lda, chondro)
> pred.sim <- predict (lda)
```

```

> colors <- c("#00008040", "#FFA50040", "#C0202040")
> plot (pred.chondro$x, col = colors [chondro$clusters], pch = 3)
> points (pred.sim$x, col = colors [rnd$clusters], pch = 20, cex = 0.5)

```

If individual covariance matrices should be used for each group, *sigma* should be an array with the 3rd dimension corresponding to the group.

8. Access to the data

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

`[]`, `[][]`

The difference between these functions is that `[]` returns a *hyperSpec* object, whereas the result of `[][]` is a *data.frame* if extra data columns were selected or otherwise the spectra matrix. Single extra data columns may be retrieved by `$`.

`$`

In order to change data, use `[]<-`, `[][]<-`, and `$<-` (see 8.4 and 8.3).

`[]<-`, `[][]<-`,
`$<-`

8.1. Access Functions and Abbreviations for Parts of the hyperSpec Object's Data

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 wave-
                  length 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). The columns must match exactly
                  in this case.

```

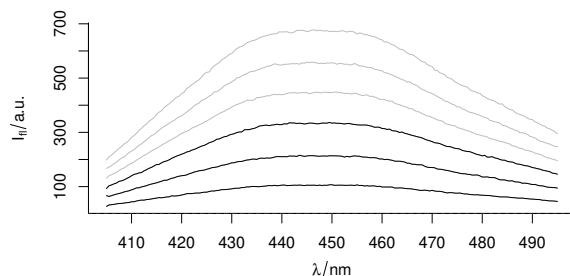
8.2. Selecting and Deleting Spectra

The extraction function `[]` takes the spectra as first argument (For detailed help: see `?`[]``). 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.

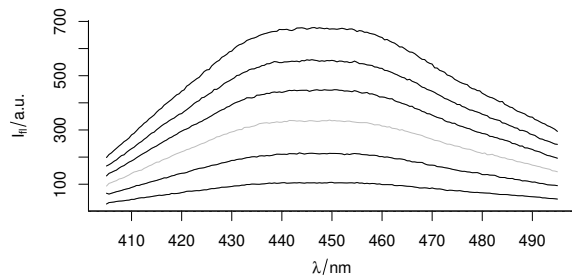
```

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

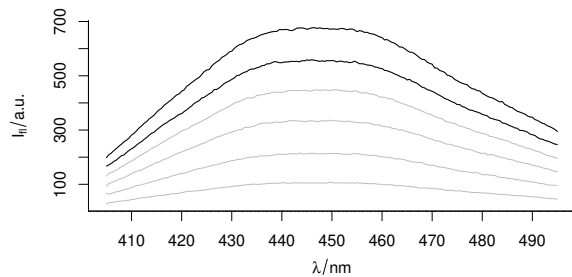
```



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



```
> plot (flu, col = "gray")
> plot (flu [flu$c > 0.2], add = TRUE)
```



8.2.1. Random Samples

A random subset of spectra is conveniently selected by `sample` :

`sample`

```
> sample (chondro, 3)
```

```
hyperSpec object
 3 spectra
 5 data columns
 300 data points / spectrum
wavelength: Delta * tilde(nu)/cm^-1 [numeric] 602 606 ... 1798
data: (3 rows x 5 columns)
 1. y: y [numeric] -0.77 0.23 4.23
 2. x: x [numeric] -0.55 4.45 2.45
 3. filename: filename [character] rawdata/chondro.txt rawdata/chondro.txt rawdata/chondro.txt
 4. clusters: clusters [factor] matrix lacuna lacuna
 5. spc: I / a.u. [matrix, array300] 309.1 281.7 ... 107.92
```

If appropriate indices into the spectra are needed instead, use `isample`:

`isample`

```
> isample (chondro, 3)
```

```
[1] 184 786 716
```

8.2.2. Sequences

Sequences of every n^{th} spectrum or the like can be retrieved with `seq`:

`seq`

```
> seq (chondro, length.out = 3, index = TRUE)
```

```
[1] 1 438 875
```

```

> seq (chondro, by = 100)

hyperSpec object
  9 spectra
  5 data columns
  300 data points / spectrum
wavelength: Delta * tilde(nu)/cm^-1 [numeric] 602 606 ... 1798
data: (9 rows x 5 columns)
  1. y: y [numeric] -4.77 -2.77 ... 17.23
  2. x: x [numeric] -11.55 18.45 ... 18.45
  3. filename: filename [character] rawdata/chondro.txt rawdata/chondro.txt ... rawdata/chondro.txt
  4. clusters: clusters [factor] matrix matrix ... lacuna
  5. spc: I / a.u. [matrix, array300] 501.82 400.94 ... 124.64

```

Here, indices may be requested using `index = TRUE`.

8.3. Selecting Extra Data Columns

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"      "filename" "clusters" "spc"

> chondro [[1 : 3, 1]]

      y
1 -4.77
2 -4.77
3 -4.77

> chondro [[1 : 3, -5]]

      y      x      filename clusters
1 -4.77 -11.55 rawdata/chondro.txt  matrix
2 -4.77 -10.55 rawdata/chondro.txt  matrix
3 -4.77  -9.55 rawdata/chondro.txt  matrix

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

      x
1 -11.55
2 -10.55
3  -9.55

> chondro [[1 : 3, c (FALSE, TRUE)]]      # note the recycling!

      x clusters
1 -11.55  matrix
2 -10.55  matrix
3  -9.55  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

```

hyperSpec supports command line completion for the `$` operator.

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.

8.4. More on the `[[]]` and `[[]]`<- Operators: Accessing Single Elements of the Spectra Matrix

`[[]]` works mostly analogous to `[]`. In addition, however, these two functions also accept index matrices of size $n \times 2$. In this case, a vector of values from the spectra matrix is returned.

```
> 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] 501.82 507.81 456.03
```

```
> diag (chondro [[1 : 3, , min ~ min + 2i]])
```

```
[1] 501.82 507.81 456.03
```

`[[]]`<- also 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] 501.82 507.81 456.03
```

```
> diag (chondro [[1 : 3, , min ~ min + 2i]])
```

```
[1] 501.82 507.81 456.03
```

8.5. Wavelengths

8.5.1. Converting Wavelengths to Indices and vice versa

Spectra in *hyperSpec* have always discretized wavelength axes, they are stored in a matrix with each column corresponding to one wavelength. *hyperSpec* provides two functions to convert the respective column indices into wavelengths and vice versa: `i2wl` and `wl2i`.

`wl2i` `i2wl`

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
> w12i (flu, 405 ~ 410)
[1] 1 2 3 4 5 6 7 8 9 10 11
> w12i (chondro, 1000 : 1010)
[1] 100 101 101 101 101 102 102 102 102 103 103
> w12i (chondro, 1000 ~ 1010)
[1] 100 101 102 103
```

- If the object's wavelength axis is not ordered, the formula approach will give weird results. In that (probably 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:

```
> w12i (flu, min ~ 410)
[1] 1 2 3 4 5 6 7 8 9 10 11
```

Often, specifications like *wavelength ± 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:

```
> w12i (flu, 450 - 2i ~ 450 + 2i)
[1] 89 90 91 92 93
> w12i (flu, max - 2i ~ max)
[1] 179 180 181
```

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

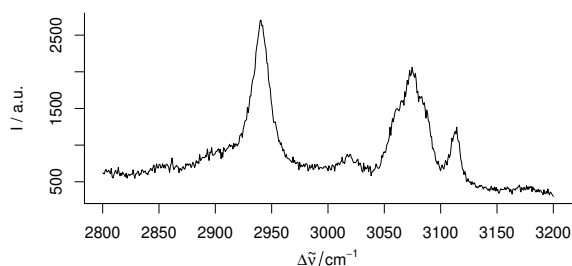
```
> w12i (flu, c (min ~ 406.5, max - 2i ~ max))
[1] 1 2 3 4 179 180 181
```

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

8.5.2. Selecting Wavelength Ranges

Wavelength ranges can easily be selected using `[]`'s third argument:

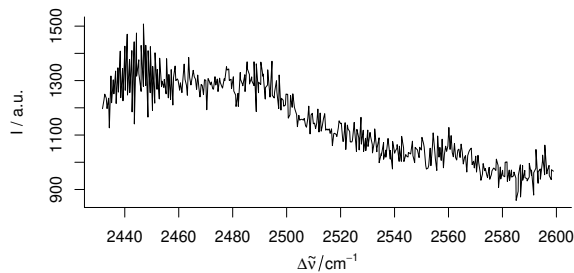
```
> plot (paracetamol [, , 2800 ~ 3200])
```



By default, the values given are treated as wavelengths. If they are indices into the columns of the spectra matrix, use `wl.index = TRUE`:

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

```
> plot (paracetamol [, , 2800 : 3200, w1.index = TRUE])
```

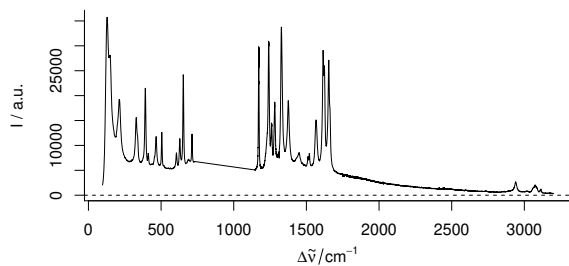


Section 8.5.1 (p. 13) details into the different possibilities of specifying wavelengths.

8.5.3. Deleting Wavelength Ranges

Deleting wavelength ranges may be accomplished using negative index vectors together with `w1.index = TRUE`.

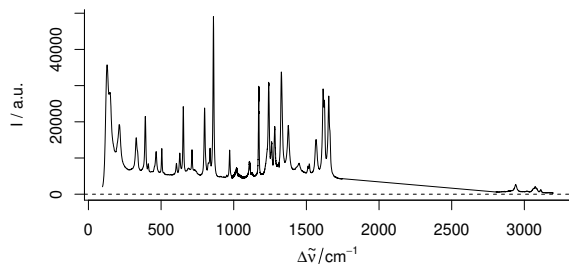
```
> plot (paracetamol [, , -(500 : 1000), w1.index = TRUE])
```



However, this mechanism works only if the proper indices are known.

If the range to be cut out is rather known in the units of the wavelength axis, it is easier to select the remainder of the spectrum instead. To delete the spectral range from 1750 to 2800 cm^{-1} of the paracetamol spectrum one can thus use:

```
> plot (paracetamol [, , c (min ~ 1750, 2800 ~ max)])
```



(It is possible to produce a plot of this data where the cut range is actually omitted and the wavelength axis is optionally cut in order to save space. For details see the “plotting” vignette).

8.5.4. Changing the Wavelength Axis

Sometimes wavelength axes need to be transformed, e. g. converting from wavelengths to frequencies. In this case, retrieve the wavelength axis vector with `w1`, convert each value of the resulting vector

`w1<-`

and assign the result with `wl<-`. Also the label of the wavelength axis may need to be adjusted.

As an example, convert the wavelength axis of `laser` to frequencies. As the wavelengths are in nanometers, and the frequencies are easiest expressed in terahertz, an additional conversion factor of 1000 is needed:

```
> laser
hyperSpec object
  84 spectra
  3 data columns
  36 data points / spectrum
wavelength: lambda/nm [numeric] 404.58 404.62 ... 405.82
data: (84 rows x 3 columns)
  1. t: t / s [numeric] 0 2 ... 5722
  2. spc: I / a.u. [matrix, array36] 164.65 179.72 ... 112.09
  3. filename: filename [character] rawdata/laser.txt.gz rawdata/laser.txt.gz ... rawdata/laser.txt.gz

> wavelengths <- wl (laser)
> frequencies <- 2.998e8 / wavelengths / 1000
> wl (laser) <- frequencies
> labels (laser, ".wavelength") <- "f / THz"
> laser
hyperSpec object
  84 spectra
  3 data columns
  36 data points / spectrum
wavelength: f / THz [numeric] 741.01 740.95 ... 738.76
data: (84 rows x 3 columns)
  1. t: t / s [numeric] 0 2 ... 5722
  2. spc: I / a.u. [matrix, array36] 164.65 179.72 ... 112.09
  3. filename: filename [character] rawdata/laser.txt.gz rawdata/laser.txt.gz ... rawdata/laser.txt.gz

> rm (laser)
```

There are other possibilities of invoking `wl<-` including the new label, e.g.

```
> wl (laser, "f / THz") <- frequencies
```

and

```
> wl (laser) <- list (wl = frequencies, label = "f / THz")
```

see `?`wl<-`` for more information.

8.5.5. Ordering the Wavelength Axis

If the wavelength axis of an object needs reordering (e.g. after `collapse`), `orderwl` can be used:

`orderwl`

```
> barb <- collapse (barbiturates [1 : 3])
> wl (barb)
 [1] 27.05 27.15 28.05 28.15 29.05 30.05 30.15 31.15 32.15 39.00 40.00 40.10 41.10
[14] 43.05 43.85 43.95 44.05 55.00 55.10 56.00 56.10 57.10 68.90 69.00 69.10 70.00
[27] 71.10 71.90 72.00 77.00 82.95 83.05 84.15 85.05 91.00 96.95 98.95 105.10 105.90
[40] 106.00 112.90 113.00 116.95 117.95 118.05 119.05 119.15 119.95 120.05 130.90 131.00 132.95
[53] 133.05 140.90 147.00 158.85 160.90

> barb <- orderwl (barb)
> wl (barb)
 [1] 27.05 27.15 28.05 28.15 29.05 30.05 30.15 31.15 32.15 39.00 40.00 40.10 41.10
[14] 43.05 43.85 43.95 44.05 55.00 55.10 56.00 56.10 57.10 68.90 69.00 69.10 70.00
[27] 71.10 71.90 72.00 77.00 82.95 83.05 84.15 85.05 91.00 96.95 98.95 105.10 105.90
[40] 106.00 112.90 113.00 116.95 117.95 118.05 119.05 119.15 119.95 120.05 130.90 131.00 132.95
[53] 133.05 140.90 147.00 158.85 160.90
```


8.6. Conversion to Long- and Wide-Format data.frames

as.data.frame

as.data.frame extracts the @data slot as a *data.frame*:

```
> flu <- flu [, ,400 ~ 407] # make a small and handy version of the flu data set
> as.data.frame (flu)
```

```
   spc.405 spc.405.5 spc.406 spc.406.5 spc.407      filename    c n .row
1  27.150  32.345  33.379   34.419  36.531 rawdata/flu1.txt 0.05 1   1
2  66.801  63.715  66.712   69.582  72.530 rawdata/flu2.txt 0.10 2   2
3  93.144 103.068 106.194  110.186 113.249 rawdata/flu3.txt 0.15 3   3
4 130.664 139.998 143.798  148.420 152.133 rawdata/flu4.txt 0.20 4   4
5 167.267 171.898 177.471  184.625 189.752 rawdata/flu5.txt 0.25 5   5
6 198.430 209.458 215.785  224.587 232.528 rawdata/flu6.txt 0.30 6   6
```

```
> colnames (as.data.frame (flu))
```

```
[1] "spc"      "filename" "c"        "n"        ".row"
```

```
> as.data.frame (flu) $ spc
```

```
      405  405.5   406  406.5   407
[1,] 27.150 32.345 33.379 34.419 36.531
[2,] 66.801 63.715 66.712 69.582 72.530
[3,] 93.144 103.068 106.194 110.186 113.249
[4,] 130.664 139.998 143.798 148.420 152.133
[5,] 167.267 171.898 177.471 184.625 189.752
[6,] 198.430 209.458 215.785 224.587 232.528
```

Note that the spectra matrix is still a matrix inside column \$spc.

as.data.frame and the abbreviations \$. and \$.. retrieve the usual wide format *data.frames*:

\$., \$..

```
> flu$.
```

```
   spc.405 spc.405.5 spc.406 spc.406.5 spc.407      filename    c n
1  27.150  32.345  33.379   34.419  36.531 rawdata/flu1.txt 0.05 1
2  66.801  63.715  66.712   69.582  72.530 rawdata/flu2.txt 0.10 2
3  93.144 103.068 106.194  110.186 113.249 rawdata/flu3.txt 0.15 3
4 130.664 139.998 143.798  148.420 152.133 rawdata/flu4.txt 0.20 4
5 167.267 171.898 177.471  184.625 189.752 rawdata/flu5.txt 0.25 5
6 198.430 209.458 215.785  224.587 232.528 rawdata/flu6.txt 0.30 6
```

```
> flu$..
```

```
      filename    c n
1 rawdata/flu1.txt 0.05 1
2 rawdata/flu2.txt 0.10 2
3 rawdata/flu3.txt 0.15 3
4 rawdata/flu4.txt 0.20 4
5 rawdata/flu5.txt 0.25 5
6 rawdata/flu6.txt 0.30 6
```

If another subset of columns needs to be extracted, use [[]]:

[[]]

```
> flu [[, c ("c", "spc")]]
```

```
      c spc.405 spc.405.5 spc.406 spc.406.5 spc.407
1 0.05 27.150  32.345  33.379   34.419  36.531
2 0.10 66.801   63.715  66.712   69.582  72.530
3 0.15 93.144  103.068 106.194  110.186 113.249
4 0.20 130.664 139.998 143.798  148.420 152.133
5 0.25 167.267 171.898 177.471  184.625 189.752
6 0.30 198.430 209.458 215.785  224.587 232.528
```

This can be combined with extracting certain spectra and wavelengths, see below in subsection “Conversion to Matrix” on page 18.

The transpose of a wide format *data.frame* can be obtained by `as.t.df`. For further examples, see the discussion of *ggplot2* in vignette (“plotting”).

```
> as.t.df (apply (flu, 2, mean_pm_sd))
```

	.wavelength	mean.minus.sd	mean	mean.plus.sd
spc.405	405.0	49.958	113.91	177.86
spc.405.5	405.5	53.396	120.08	186.77
spc.406	406.0	55.352	123.89	192.43
spc.406.5	406.5	57.310	128.64	199.96
spc.407	407.0	59.513	132.79	206.06

Some functions need the data being an *unstacked* or *long-format data.frame*. `as.long.df` is the appropriate conversion function.

```
> head (as.long.df (flu), 20)
```

	.wavelength	spc	filename	c	n
1	405.0	27.150	rawdata/flu1.txt	0.05	1
2	405.0	66.801	rawdata/flu2.txt	0.10	2
3	405.0	93.144	rawdata/flu3.txt	0.15	3
4	405.0	130.664	rawdata/flu4.txt	0.20	4
5	405.0	167.267	rawdata/flu5.txt	0.25	5
6	405.0	198.430	rawdata/flu6.txt	0.30	6
1.1	405.5	32.345	rawdata/flu1.txt	0.05	1
2.1	405.5	63.715	rawdata/flu2.txt	0.10	2
3.1	405.5	103.068	rawdata/flu3.txt	0.15	3
4.1	405.5	139.998	rawdata/flu4.txt	0.20	4
5.1	405.5	171.898	rawdata/flu5.txt	0.25	5
6.1	405.5	209.458	rawdata/flu6.txt	0.30	6
1.2	406.0	33.379	rawdata/flu1.txt	0.05	1
2.2	406.0	66.712	rawdata/flu2.txt	0.10	2
3.2	406.0	106.194	rawdata/flu3.txt	0.15	3
4.2	406.0	143.798	rawdata/flu4.txt	0.20	4
5.2	406.0	177.471	rawdata/flu5.txt	0.25	5
6.2	406.0	215.785	rawdata/flu6.txt	0.30	6
1.3	406.5	34.419	rawdata/flu1.txt	0.05	1
2.3	406.5	69.582	rawdata/flu2.txt	0.10	2

8.7. Conversion to Matrix

The spectra matrix is extracted by `as.matrix`, the convenient abbreviation is `[[]]`:

```
> flu [[]]
```

	405	405.5	406	406.5	407
[1,]	27.150	32.345	33.379	34.419	36.531
[2,]	66.801	63.715	66.712	69.582	72.530
[3,]	93.144	103.068	106.194	110.186	113.249
[4,]	130.664	139.998	143.798	148.420	152.133
[5,]	167.267	171.898	177.471	184.625	189.752
[6,]	198.430	209.458	215.785	224.587	232.528

```
> class (flu [[]])
```

```
[1] "matrix" "array"
```

`[[]]` takes the same arguments as `[]`, and can be used to extract a matrix containing parts of the spectra matrix:

```
> flu [[1:3,, 406 ~ 407]]
```

`as.matrix,`
`[[]]`

```

      406  406.5  407
[1,] 33.379 34.419 36.531
[2,] 66.712 69.582 72.530
[3,] 106.194 110.186 113.249

```

If indices for the columns to extract are given, a *data.frame* is returned instead of a matrix:

```

> flu [[1:3, c ("filename", "spc"), 406 ~ 407]]

      filename spc.406 spc.406.5 spc.407
1 rawdata/flu1.txt 33.379  34.419  36.531
2 rawdata/flu2.txt 66.712  69.582  72.530
3 rawdata/flu3.txt 106.194 110.186 113.249

> rm (flu)

```

9. Combining and Decomposing hyperSpec Objects

9.1. Binding Objects together

hyperSpec Objects can be bound together, either by columns (`cbind`) to append a new spectral range or by row (`rbind`) to append new spectra: cbind rbind

```

> 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

```

There is also a more general function, `bind`, taking the direction ("**r**" or "**c**") as first argument followed by the 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.

For binding row-wise (`rbind`), `collapse` is more flexible but also faster. collapse

9.2. 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`. collapse

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

```

> barb <- collapse (barbiturates)
> wl (barb) [1 : 25]

 [1] 25.95 26.05 26.15 26.95 27.05 27.15 28.05 28.15 29.05 29.15 29.95 30.05 30.15 30.25 31.05 31.15
[17] 32.05 32.15 36.90 37.00 38.00 38.10 38.90 39.00 39.10

```

The resulting object does not have an ordered wavelength axis. This can be obtained in a second step:

```
> barb <- orderwl (barb)
> 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
```

9.3. Binding Objects that do not Share the Same Spectra

`merge` adds a new spectral range (like `cbind`), but works also if spectra are missing in one of the objects. The arguments *by*, *by.x*, and *by.y* specify which columns should be used to decide which spectra are the same. The arguments *all*, *all.x*, and *all.y* determine whether spectra should be kept for the result set if they appear in only one of the objects. For details, see also the help on the base function *merge*.

`merge`

As an example, let's construct a version of the `chondro` data like being taken as two maps with different spectral ranges. In each data set, some spectra are missing.

```
> chondro.low <- sample (chondro [, , 600 ~ 1200], 700)
> nrow (chondro.low)

[1] 700

> chondro.high <- sample (chondro [, , 1400 ~ 1800], 700)
> nrow (chondro.high)

[1] 700
```

As all extra data columns are the same, no special declarations are needed for merging the data:

```
> chondro.merged <- merge (chondro.low, chondro.high)
> nrow (chondro.merged)

[1] 561
```

By default, the result consists of only those spectra, where *both* spectral ranges were available. To keep all spectra replacing missing parts by NA (see fig. 3):

```
> chondro.merged <- merge (chondro.low, chondro.high, all = TRUE)
> nrow (chondro.merged)

[1] 839
```

```
> merged <- merge (chondro [1:7, , 610 ~ 620], chondro [5:10, , 615 ~ 625], all = TRUE)
> merged$.
```

	y	x	filename	clusters	.nx	.ny	spc.1	spc.2	spc.3	spc.4	spc.5	spc.6
1	-4.77	-11.55	rawdata/chondro.txt	matrix	1	NA	488.63	466.18	492.00	NA	NA	NA
2	-4.77	-10.55	rawdata/chondro.txt	matrix	2	NA	489.48	465.05	490.53	NA	NA	NA
3	-4.77	-9.55	rawdata/chondro.txt	matrix	3	NA	456.03	436.62	458.06	NA	NA	NA
4	-4.77	-8.55	rawdata/chondro.txt	matrix	4	NA	464.82	444.85	470.02	NA	NA	NA
5	-4.77	-7.55	rawdata/chondro.txt	matrix	5	1	428.66	410.80	433.12	410.80	433.12	461.19
6	-4.77	-6.55	rawdata/chondro.txt	matrix	6	2	426.07	407.86	431.21	407.86	431.21	458.15
7	-4.77	-5.55	rawdata/chondro.txt	lacuna	7	3	412.37	396.50	421.27	396.50	421.27	445.54
8	-4.77	-4.55	rawdata/chondro.txt	lacuna	NA	4	NA	NA	NA	381.95	406.25	429.67
9	-4.77	-3.55	rawdata/chondro.txt	lacuna	NA	5	NA	NA	NA	397.51	423.30	446.15
10	-4.77	-2.55	rawdata/chondro.txt	lacuna	NA	6	NA	NA	NA	377.39	402.23	424.19
	spc.7											
1	NA											

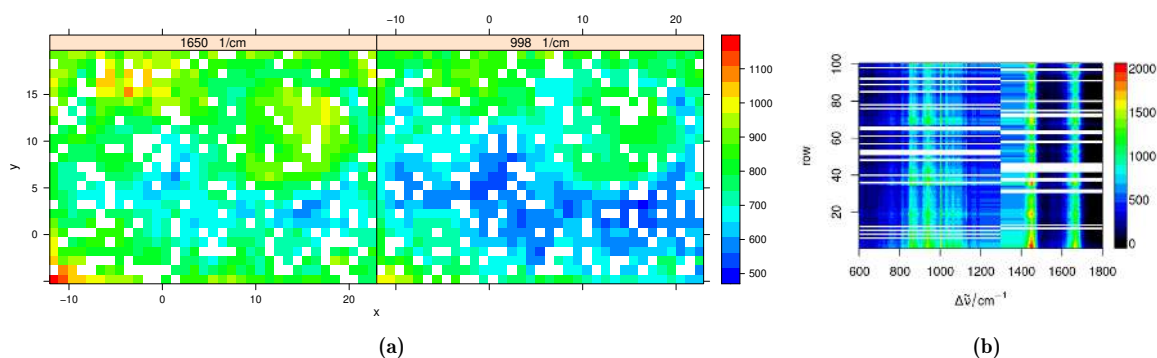


Figure 3 (a) For both spectral ranges some spectra are missing. (b) The missing parts of the spectra are filled with NA.

```

2      NA
3      NA
4      NA
5 397.38
6 394.18
7 382.72
8 368.46
9 381.87
10 362.43

```

If the spectra overlap, the result will have both data points. In the example here one could easily delete duplicate wavelengths. For real data, however, the duplicated wavelength will hardly ever contain the same values. The appropriate method to deal with this situation depends on the data at hand, but it will usually be some kind of spectral interpolation.

One possibility is removing duplicated wavelengths by using the mean intensity. This can conveniently be done by using `approx` using `method = "constant"`. For duplicated wavelengths, the intensities will be combined by the tie function. This already defaults to the mean, but we need `na.rm = TRUE`.

Thus, the function to calculate the new spectral intensities is

```

> approxfun <- function (y, wl, new.wl){
+   approx (wl, y, new.wl, method = "constant",
+         ties = function (x) mean (x, na.rm = TRUE)
+         )$y
+ }

```

which can be applied to the spectra:

```

> merged <- apply (merged, 1, approxfun,
+                 wl = wl (merged), new.wl = unique (wl (merged)),
+                 new.wavelength = "new.wl")
> merged$.

```

	y	x	filename	clusters	.nx	.ny	spc.1	spc.2	spc.3	spc.4	spc.5
1	-4.77	-11.55	rawdata/chondro.txt	matrix	1	NA	488.63	466.18	492.00	NA	NA
2	-4.77	-10.55	rawdata/chondro.txt	matrix	2	NA	489.48	465.05	490.53	NA	NA
3	-4.77	-9.55	rawdata/chondro.txt	matrix	3	NA	456.03	436.62	458.06	NA	NA
4	-4.77	-8.55	rawdata/chondro.txt	matrix	4	NA	464.82	444.85	470.02	NA	NA
5	-4.77	-7.55	rawdata/chondro.txt	matrix	5	1	428.66	410.80	433.12	461.19	397.38
6	-4.77	-6.55	rawdata/chondro.txt	matrix	6	2	426.07	407.86	431.21	458.15	394.18
7	-4.77	-5.55	rawdata/chondro.txt	lacuna	7	3	412.37	396.50	421.27	445.54	382.72

```

8 -4.77 -4.55 rawdata/chondro.txt lacuna NA 4 NA 381.95 406.25 429.67 368.46
9 -4.77 -3.55 rawdata/chondro.txt lacuna NA 5 NA 397.51 423.30 446.15 381.87
10 -4.77 -2.55 rawdata/chondro.txt lacuna NA 6 NA 377.39 402.23 424.19 362.43

```

9.4. Merging extra data to objects that do not (necessarily) share the same spectra

Assume we obtained duplicate reference measurements for some of the concentrations in `flu`:

```

> flu.ref <- data.frame (filename = rep (flu$filename[1:2], each = 2), cref = rep (flu$c [1:2], each = 2) + r
> flu.ref
      filename      cref
1 rawdata/flu1.txt 0.056870
2 rawdata/flu1.txt 0.038592
3 rawdata/flu2.txt 0.071762
4 rawdata/flu2.txt 0.087012

```

This information can be merged into the extra data of `flu` by:

```

> flu.merged <- merge (flu, flu.ref)
> flu.merged$.
      filename      c      cref
1 rawdata/flu1.txt 0.05 0.056870
2 rawdata/flu1.txt 0.05 0.038592
3 rawdata/flu2.txt 0.10 0.071762
4 rawdata/flu2.txt 0.10 0.087012

```

The usual rules for `merge` apply. E. g., if to preserve all spectra of `flu`, use `all.x = TRUE`:

```

> flu.merged <- merge (flu, flu.ref, all.x = TRUE)
> flu.merged$.
      filename      c      cref
1 rawdata/flu1.txt 0.05 0.056870
2 rawdata/flu1.txt 0.05 0.038592
3 rawdata/flu2.txt 0.10 0.071762
4 rawdata/flu2.txt 0.10 0.087012
5 rawdata/flu3.txt 0.15      NA
6 rawdata/flu4.txt 0.20      NA
7 rawdata/flu5.txt 0.25      NA
8 rawdata/flu6.txt 0.30      NA

```

The class of the first object (`x`) determines the resulting class:

```

> merge (flu, flu.ref)
hyperSpec object
 4 spectra
 4 data columns
 181 data points / spectrum
wavelength: lambda/nm [numeric] 405.0 405.5 ... 495
data: (4 rows x 4 columns)
 1. filename: filename [character] rawdata/flu1.txt rawdata/flu1.txt rawdata/flu2.txt rawdata/flu2.txt
 2. spc: I[fl]/"a.u." [matrix, array181] 27.15 27.15 ... 94.61
 3. c: c / (mg / l) [numeric] 0.05 0.05 0.10 0.10
 4. cref: [numeric] 0.056870 0.038592 0.071762 0.087012

> merge (flu.ref, flu)
      filename      cref spc.405 spc.405.5 spc.406 spc.406.5 spc.407 spc.407.5 spc.408 spc.408.5
1 rawdata/flu1.txt 0.056870 27.150 32.345 33.379 34.419 36.531 37.648 38.137 39.177
2 rawdata/flu1.txt 0.038592 27.150 32.345 33.379 34.419 36.531 37.648 38.137 39.177
3 rawdata/flu2.txt 0.071762 66.801 63.715 66.712 69.582 72.530 74.558 77.048 80.260

```

4	rawdata/flu2.txt	0.087012	66.801	63.715	66.712	69.582	72.530	74.558	77.048	80.260
	spc.409	spc.409.5	spc.410	spc.410.5	spc.411	spc.411.5	spc.412	spc.412.5	spc.413	spc.413.5
1	40.736	41.381	44.251	44.126	46.981	49.082	50.274	50.110	52.232	53.040
2	40.736	41.381	44.251	44.126	46.981	49.082	50.274	50.110	52.232	53.040
3	82.539	84.492	88.152	91.085	95.372	95.530	98.995	101.034	103.558	107.027
4	82.539	84.492	88.152	91.085	95.372	95.530	98.995	101.034	103.558	107.027
	spc.414.5	spc.415	spc.415.5	spc.416	spc.416.5	spc.417	spc.417.5	spc.418	spc.418.5	spc.419
1	56.220	57.719	59.514	58.745	60.095	61.841	62.169	66.049	65.245	65.799
2	56.220	57.719	59.514	58.745	60.095	61.841	62.169	66.049	65.245	65.799
3	111.672	113.987	117.033	119.835	123.494	123.324	127.002	130.681	132.358	136.165
4	111.672	113.987	117.033	119.835	123.494	123.324	127.002	130.681	132.358	136.165
	spc.419.5	spc.420	spc.420.5	spc.421	spc.421.5	spc.422	spc.422.5	spc.423	spc.423.5	spc.424
1	66.943	69.136	70.925	73.834	74.386	74.173	75.531	76.430	76.132	77.891
2	66.943	69.136	70.925	73.834	74.386	74.173	75.531	76.430	76.132	77.891
3	138.399	140.224	141.043	143.131	147.180	150.012	153.693	155.728	158.472	159.501
4	138.399	140.224	141.043	143.131	147.180	150.012	153.693	155.728	158.472	159.501
	spc.424.5	spc.425	spc.425.5	spc.426	spc.426.5	spc.427	spc.427.5	spc.428	spc.428.5	spc.429
1	79.369	79.427	82.028	83.878	83.814	85.507	86.502	88.937	88.995	89.515
2	79.369	79.427	82.028	83.878	83.814	85.507	86.502	88.937	88.995	89.515
3	160.816	163.910	166.255	169.592	170.828	172.088	175.211	178.471	179.681	181.829
4	160.816	163.910	166.255	169.592	170.828	172.088	175.211	178.471	179.681	181.829
	spc.429.5	spc.430	spc.430.5	spc.431	spc.431.5	spc.432	spc.432.5	spc.433	spc.433.5	spc.434
1	90.557	91.706	93.579	94.013	94.210	96.442	96.627	98.962	98.848	100.568
2	90.557	91.706	93.579	94.013	94.210	96.442	96.627	98.962	98.848	100.568
3	184.429	187.756	187.938	191.057	192.509	192.801	195.556	197.891	198.782	200.995
4	184.429	187.756	187.938	191.057	192.509	192.801	195.556	197.891	198.782	200.995
	spc.434.5	spc.435	spc.435.5	spc.436	spc.436.5	spc.437	spc.437.5	spc.438	spc.438.5	spc.439
1	100.449	99.916	99.719	100.886	101.445	102.643	104.230	103.111	104.758	103.158
2	100.449	99.916	99.719	100.886	101.445	102.643	104.230	103.111	104.758	103.158
3	201.522	200.206	204.132	204.904	203.988	205.756	204.817	206.091	208.607	210.797
4	201.522	200.206	204.132	204.904	203.988	205.756	204.817	206.091	208.607	210.797
	spc.439.5	spc.440	spc.440.5	spc.441	spc.441.5	spc.442	spc.442.5	spc.443	spc.443.5	spc.444
1	103.943	105.371	105.863	103.680	104.090	104.654	105.226	104.804	105.810	104.758
2	103.943	105.371	105.863	103.680	104.090	104.654	105.226	104.804	105.810	104.758
3	210.584	210.190	210.542	209.859	212.827	212.521	212.420	211.222	215.564	213.425
4	210.584	210.190	210.542	209.859	212.827	212.521	212.420	211.222	215.564	213.425
	spc.444.5	spc.445	spc.445.5	spc.446	spc.446.5	spc.447	spc.447.5	spc.448	spc.448.5	spc.449
1	103.883	105.362	105.015	105.059	105.349	103.987	105.439	104.197	105.098	104.723
2	103.883	105.362	105.015	105.059	105.349	103.987	105.439	104.197	105.098	104.723
3	211.159	212.975	213.989	214.172	213.476	212.489	211.741	212.705	212.940	212.129
4	211.159	212.975	213.989	214.172	213.476	212.489	211.741	212.705	212.940	212.129
	spc.449.5	spc.450	spc.450.5	spc.451	spc.451.5	spc.452	spc.452.5	spc.453	spc.453.5	spc.454
1	106.667	106.950	104.755	105.083	105.300	105.213	104.781	104.539	105.133	105.170
2	106.667	106.950	104.755	105.083	105.300	105.213	104.781	104.539	105.133	105.170
3	213.773	213.497	213.464	213.171	212.836	211.963	208.799	211.506	209.477	211.860
4	213.773	213.497	213.464	213.171	212.836	211.963	208.799	211.506	209.477	211.860
	spc.454.5	spc.455	spc.455.5	spc.456	spc.456.5	spc.457	spc.457.5	spc.458	spc.458.5	spc.459
1	104.057	106.385	104.080	104.401	102.181	103.442	101.797	102.872	102.389	100.419
2	104.057	106.385	104.080	104.401	102.181	103.442	101.797	102.872	102.389	100.419
3	213.262	212.284	211.773	209.391	208.856	208.340	206.506	206.777	206.645	205.255
4	213.262	212.284	211.773	209.391	208.856	208.340	206.506	206.777	206.645	205.255
	spc.459.5	spc.460	spc.460.5	spc.461	spc.461.5	spc.462	spc.462.5	spc.463	spc.463.5	spc.464
1	101.162	98.611	98.429	98.576	98.341	98.467	95.149	94.711	95.274	94.884
2	101.162	98.611	98.429	98.576	98.341	98.467	95.149	94.711	95.274	94.884
3	201.747	201.988	199.570	200.551	198.768	197.033	194.145	193.383	193.665	192.513
4	201.747	201.988	199.570	200.551	198.768	197.033	194.145	193.383	193.665	192.513
	spc.464.5	spc.465	spc.465.5	spc.466	spc.466.5	spc.467	spc.467.5	spc.468	spc.468.5	spc.469
1	93.621	92.466	92.115	91.309	89.539	88.281	86.136	86.162	86.817	85.958
2	93.621	92.466	92.115	91.309	89.539	88.281	86.136	86.162	86.817	85.958
3	190.633	186.456	186.054	182.305	182.334	180.569	180.506	180.213	175.211	171.650
4	190.633	186.456	186.054	182.305	182.334	180.569	180.506	180.213	175.211	171.650
	spc.469.5	spc.470	spc.470.5	spc.471	spc.471.5	spc.472	spc.472.5	spc.473	spc.473.5	spc.474
1	84.067	86.212	83.683	82.569	82.705	81.260	78.752	76.675	77.953	77.507
2	84.067	86.212	83.683	82.569	82.705	81.260	78.752	76.675	77.953	77.507
3	170.417	170.374	169.407	164.890	164.141	163.173	160.989	159.665	157.746	155.135

```

4 170.417 170.374 169.407 164.890 164.141 163.173 160.989 159.665 157.746 155.135
  spc.474.5 spc.475 spc.475.5 spc.476 spc.476.5 spc.477 spc.477.5 spc.478 spc.478.5 spc.479
1 76.164 75.646 76.437 74.570 72.879 72.803 71.052 70.214 69.605 69.990
2 76.164 75.646 76.437 74.570 72.879 72.803 71.052 70.214 69.605 69.990
3 153.239 151.523 149.197 147.495 147.490 145.434 144.819 142.439 142.690 142.881
4 153.239 151.523 149.197 147.495 147.490 145.434 144.819 142.439 142.690 142.881
  spc.479.5 spc.480 spc.480.5 spc.481 spc.481.5 spc.482 spc.482.5 spc.483 spc.483.5 spc.484
1 68.780 68.342 67.685 67.277 67.048 65.313 64.509 63.506 62.184 62.045
2 68.780 68.342 67.685 67.277 67.048 65.313 64.509 63.506 62.184 62.045
3 139.838 135.479 135.253 135.846 133.559 133.318 132.824 128.930 125.203 124.740
4 139.838 135.479 135.253 135.846 133.559 133.318 132.824 128.930 125.203 124.740
  spc.484.5 spc.485 spc.485.5 spc.486 spc.486.5 spc.487 spc.487.5 spc.488 spc.488.5 spc.489
1 62.027 61.799 60.528 59.342 59.125 57.748 57.447 57.743 56.275 55.492
2 62.027 61.799 60.528 59.342 59.125 57.748 57.447 57.743 56.275 55.492
3 124.717 121.678 120.902 121.406 117.668 117.041 115.941 112.229 112.724 111.673
4 124.717 121.678 120.902 121.406 117.668 117.041 115.941 112.229 112.724 111.673
  spc.489.5 spc.490 spc.490.5 spc.491 spc.491.5 spc.492 spc.492.5 spc.493 spc.493.5 spc.494
1 54.409 53.833 53.263 52.457 52.140 49.784 49.623 48.338 47.304 47.163
2 54.409 53.833 53.263 52.457 52.140 49.784 49.623 48.338 47.304 47.163
3 109.698 107.641 108.051 105.220 102.953 102.758 100.628 97.965 97.353 96.602
4 109.698 107.641 108.051 105.220 102.953 102.758 100.628 97.965 97.353 96.602
  spc.494.5 spc.495 c
1 46.412 45.256 0.05
2 46.412 45.256 0.05
3 96.206 94.610 0.10
4 96.206 94.610 0.10

```

9.5. Matrix Multiplication

Two *hyperSpec* objects can be matrix multiplied by `%*%`. For an example, see the principal component analysis below (section 12.1 on page 33).

9.6. 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 33.

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 `flu` and `flu2` 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.

`flu` returns a *hyperSpec* object, `flu2` the spectra matrix `$spc` (or the *data.frame* `@data` if in addition data columns were specified) only.

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

hyperSpec object
 6 spectra
 3 data columns
 8 data points / spectrum
wavelength: lambda/nm [numeric] 405.0 405.5 ... 408.5
data: (6 rows x 3 columns)
 1. spc: I[fl]/"a.u." [matrix, array8] 27.150 66.801 ... 256.89
 2. filename: filename [character] rawdata/flu1.txt rawdata/flu2.txt ... rawdata/flu6.txt
 3. c: c / (mg / l) [numeric] 0.05 0.10 ... 0.3

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

      405  405.5    406    494  494.5    495
[1,] 27.150 32.345 33.379 47.163 46.412 45.256
[2,] 66.801 63.715 66.712 96.602 96.206 94.610
[3,] 93.144 103.068 106.194 149.539 148.527 145.793
[4,] 130.664 139.998 143.798 201.484 198.867 195.867
[5,] 167.267 171.898 177.471 252.066 248.067 246.952
[6,] 198.430 209.458 215.785 307.519 302.325 294.649
```

11.2. Shifting Spectra

Sometimes, spectra need to be aligned along the spectral axis.

In general, two options are available for shifting spectra along the wavelength axis.

1. The wavelength axis can be shifted, while the intensities stay unaffected.
2. the spectra are interpolated onto a new wavelength axis, while the nominal wavelengths stay.

The first method is very straightforward (see fig 4a):

```
> tmp <- chondro
> wl (tmp) <- wl (tmp) - 10
```

but it cannot be used if each spectrum (or groups of spectra) are shifted individually.

In that case, interpolation is needed. R offers many possibilities to interpolate (e.g. `approx` for constant / linear approximation, `spline` for spline interpolation, `loess` can be used to obtain smoothed approximations, etc.). The appropriate interpolation strategy will depend on the spectra, and *hyperSpec* therefore leaves it up to the user to select a sensible interpolation function.

As an example, we will use natural splines to do the interpolation. It is convenient to set it up as a function:

```
> interpolate <- function (spc, shift, wl){
+   spline (wl + shift, spc, xout = wl, method = "natural")$y
+ }
```

This function can now be applied to a set of spectra (see fig 4b):

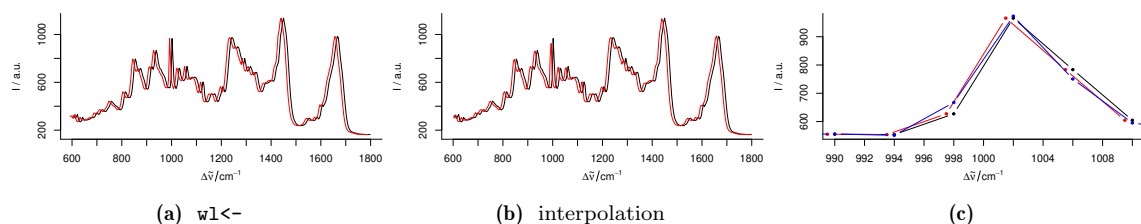


Figure 4 Shifting the Spectra along the Wavelength Axis. (a) Changing the wavelength values. (b) Interpolation. (c) Detail view of the phenylalanine band: shifting by `wl<-` (red) does not affect the intensities, while the spectrum is slightly changed by interpolations (blue).

```
> tmp <- apply (chondro, 1, interpolate, shift = -10, wl = wl (chondro))
```

If different spectra need to be offset by different shift, use a loop²

```
> shifts <- rnorm (nrow (chondro))
> tmp <- chondro [[]]
> for (i in seq_len (nrow (chondro)))
+   tmp [i, ] <- interpolate (tmp [i, ], shifts [i], wl = wl (chondro))
> chondro [[]] <- tmp
```

11.2.1. Calculating the Shift

Often, the shift in the spectra is determined by aligning a particular signal. This strategy works best with spectrally oversampled data that allows accurate determination of the signal position.

For the `chondro` data, let's use the maximum of the phenylalanine band between 990 and 1020 cm^{-1} . As just the very maximum is too coarse, we'll use the maximum of a square polynomial fitted to the maximum and its two neighbours.

```
> find.max <- function (y, x){
+   pos <- which.max (y) + (-1:1)
+   X <- x [pos] - x [pos [2]]
+   Y <- y [pos] - y [pos [2]]
+
+   X <- cbind (1, X, X^2)
+   coef <- qr.solve (X, Y)
+
+   - coef [2] / coef [3] / 2 + x [pos [2]]
+ }
> bandpos <- apply (chondro [, 990 ~ 1020], 1, find.max, wl (chondro [, 990 ~ 1020]))
> refpos <- find.max (colMeans (chondro [, 990 ~ 1020]), wl (chondro [, 990 ~ 1020]))
> shift1 <- refpos - bandpos
```

A second possibility is to optimize the shift. For this strategy, the spectra must be sufficiently similar, while low spectral resolution is compensated by using larger spectral windows.

```
> chondro <- chondro - spc.fit.poly.below (chondro [, min+3i ~ max - 3i], chondro)
> chondro <- sweep (chondro, 1, rowMeans (chondro [[]], na.rm = TRUE), "/")
```

²`sweep` cannot be used here, and while there is the possibility to use `sapply` or `mapply`, they are not faster than the for loop in this case. Make sure to work on a copy of the spectra matrix, as that is much faster than row-wise extracting and changing the spectra by `[]` and `[]<-`.

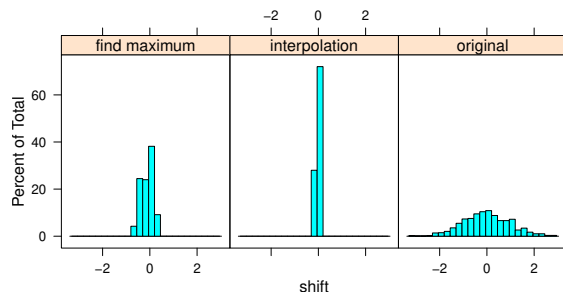


Figure 5 The shifts used to disturb the chondrocyte data (original), and the remaining shift after correction with the two methods discussed here.

```

> targetfn <- function (shift, wl, spc, targetspc){
+   error <- spline (wl + shift, spc, xout = wl)$y - targetspc
+   sum (error^2)
+ }
> shift2 <- numeric (nrow (chondro))
> tmp <- chondro [[]]
> target <- colMeans (chondro [[]])
> for (i in 1 : nrow (chondro))
+   shift2 [i] <- unlist (optimize (targetfn, interval = c (-5, 5), wl = chondro@wavelength,
+                               spc = tmp[i,], targetspc = target)$minimum)

```

Figure 5 shows that the second correction method works better for the chondrocyte data. This was expected, as the spectra are hardly or not oversampled, but are very similar to each other.

11.3. Removing Bad Data

11.3.1. Bad Spectra

Occasionally, one may want to remove spectra because of too low or too high signal.

E.g. for infrared spectra one may state that the absorbance maximum should be, say, between 0.1 and 1. *hyperSpec*'s comparison operators return a logical matrix of the size of the spectra that is suitable for later indexing:

```

> ir.spc <- chondro / 1500 ## fake IR data
> high.int <- apply (ir.spc > 1, 1, any) # any point above 1 is bad
> low.int <- apply (ir.spc, 1, max) < 0.1 # the maximum should be at least 0.1
> ir.spc <- ir.spc [! high.int & ! low.int]

```

11.3.2. Removing Spectra outside mean $\pm n$ sd

```

> mean_sd_filter <- function (x, n = 5) {
+   x <- x - mean (x)
+   s <- n * sd (x)
+   (x <= s) & (x > -s)
+ }
> OK <- apply (chondro [[]], 2, mean_sd_filter, n = 4) # logical matrix
> spc.OK <- chondro [apply (OK, 1, all)]

> plot (chondro [! apply (OK, 1, all)])
> i <- which (! OK, arr.ind = TRUE)
> points (wl (chondro) [i [,2]], chondro[[!OK]], pch = 19, col = "red", cex = 0.5)

```

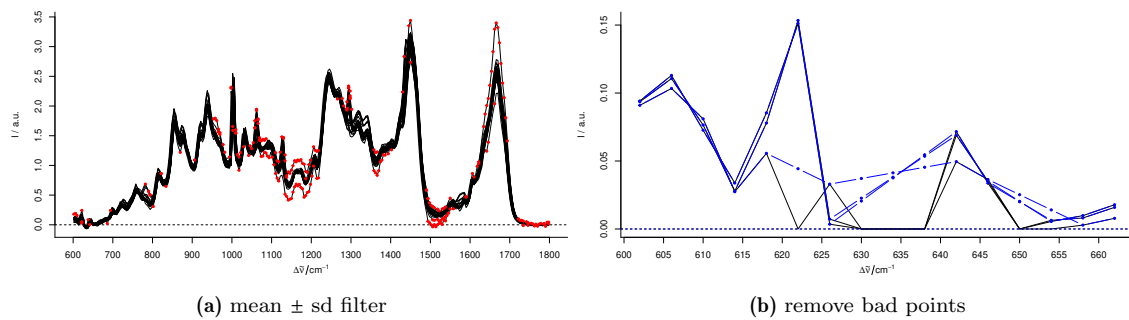


Figure 6 filtering data

11.3.3. Bad Data Points

Assume the data contains once in a while a detector readout of 0:

```
> spc <- chondro [1 : 3, , min ~ min + 15i]
> spc [[cbind (1:3, sample (nwl (spc), 3)), wl.index = TRUE]] <- 0
> spc [[]]

      602      606      610      614      618      622      626      630      634      638
[1,] 0.090953 0.10337 0.080993 0.027388 0.055640 0.00000 0.0329966 -0.051216 -0.059316 -0.045534
[2,] 0.093583 0.11062 0.076464 0.027846 0.077909 0.15340 0.0072395 -0.048685 0.000000 -0.025735
[3,] 0.094160 0.11297 0.072646 0.033798 0.085400 0.15116 0.0035066 -0.050193 -0.057225 0.000000

      642      646      650      654      658      662
[1,] 0.049536 0.036396 -4.9231e-03 -0.0014483 0.0028445 0.0078247
[2,] 0.068929 0.035123 -1.5151e-03 0.0054916 0.0098408 0.0178217
[3,] 0.071607 0.033700 3.4519e-05 0.0063748 0.0081104 0.0158933
```

We can set these points to NA, again using that the comparison returns a suitable logical matrix:

```
> spc [[spc < 1e-4]] <- NA
> spc [[]]

      602      606      610      614      618      622      626 630 634 638      642      646
[1,] 0.090953 0.10337 0.080993 0.027388 0.055640      NA 0.0329966 NA NA NA 0.049536 0.036396
[2,] 0.093583 0.11062 0.076464 0.027846 0.077909 0.15340 0.0072395 NA NA NA 0.068929 0.035123
[3,] 0.094160 0.11297 0.072646 0.033798 0.085400 0.15116 0.0035066 NA NA NA 0.071607 0.033700

      650      654      658      662
[1,] NA      NA 0.0028445 0.0078247
[2,] NA 0.0054916 0.0098408 0.0178217
[3,] NA 0.0063748 0.0081104 0.0158933
```

Depending on the type of analysis, one may want to replace the NAs by interpolating the neighbour values. So far, *hyperSpec* provides three functions that can interpolate the NAs: `spc.NA.approx`, `spc.loess`, and `spc.bin` with `na.rm = TRUE` (the latter two are discussed below).

`spc.NA.approx`,
`spc.loess`,
`spc.bin`

```
> if (!exists("spc.NA.approx")){
+   spc.NA.approx <- spc.NA.linapprox
+ }

> spc.corrected <- spc.NA.approx (spc)
> spc.corrected [[]]

      602      606      610      614      618      622      626      630      634      638
[1,] 0.090953 0.10337 0.080993 0.027388 0.055640 0.044318 0.0329966 0.037131 0.041266 0.045401
[2,] 0.093583 0.11062 0.076464 0.027846 0.077909 0.153402 0.0072395 0.022662 0.038084 0.053507
[3,] 0.094160 0.11297 0.072646 0.033798 0.085400 0.151161 0.0035066 0.020532 0.037557 0.054582
```

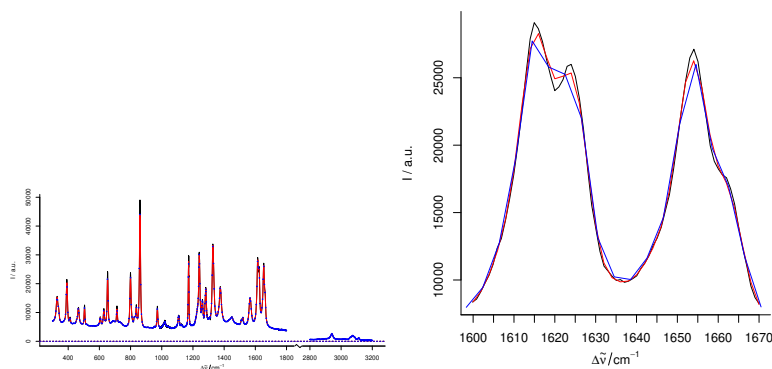


Figure 7 Smoothing interpolation by `spc.loess` with new data point spacing of 2 cm^{-1} (red) and `spc.bin` (blue). The magnification on the right shows how interpolation may cause a loss in signal height.

	642	646	650	654	658	662
[1,]	0.049536	0.036396	0.025212	0.0140282	0.0028445	0.0078247
[2,]	0.068929	0.035123	0.020307	0.0054916	0.0098408	0.0178217
[3,]	0.071607	0.033700	0.020037	0.0063748	0.0081104	0.0158933

11.3.4. Spikes in Raman Spectra

...coming soon...

11.4. Smoothing Interpolation

Spectra acquired by grating instruments are frequently interpolated onto a new wavelength axis, e.g. because the unequal data point spacing should be removed. 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 do so: `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)
> b <- spc.bin (paracetamol, 4)
> plot (b, wl.range = c (300 ~ 1800, 2800 ~ max), xoffset = 850,
+       lines.args = list (pch = 20, cex = .3, type = "p"), col = "blue", add = TRUE)
```

`spc.loess` applies R's `loess` function for spectral interpolation. Figure 7 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.

`spc.bin`
`spc.loess`

11.5. Background Correction

sweep

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

11.6. Offset Correction

apply sweep

Calculate the offsets and sweep them off the spectra:

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

If the offset is calculated by a function, as here with the `min`, *hyperSpec*'s `sweep` method offers a shortcut: `sweep`'s *STATS* argument may be the function instead of a numeric vector:

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

11.7. Baseline Correction

hyperSpec comes with two functions to fit polynomial baselines.

spc.fit.poly
spc.fit.poly.below

`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)
> chondro <- chondro - bl
```

For details, see `vignette (baselinebelow)`.

Package *baseline* [1] offers many more functions for baseline correction. The `baseline` function works on the spectra matrix, which is extracted by `[[[]]`. The result is a *baseline* object, but can easily be re-imported into the *hyperSpec* object:

```
> corrected <- hyperSpec::chondro [1] # start with the unchanged data set
> require ("baseline")
> bl <- baseline (corrected [[[]], method = "modpolyfit", degree = 4)
> corrected [[[]] <- getCorrected (bl)
```

Fig. 8 shows the result for the first spectrum of `chondro`.

```
> rm (bl, chondro)
```

11.8. Intensity Calibration

11.8.1. 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
```

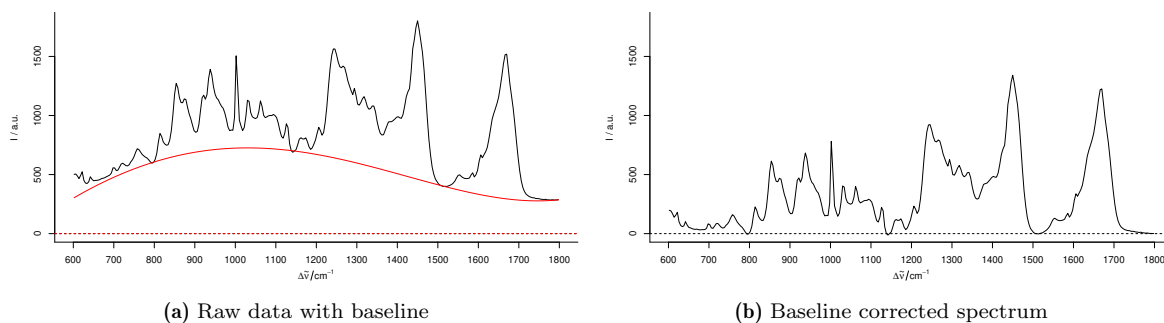


Figure 8 Baseline correction using the *baseline* package: the first spectrum of *chondro* with baseline (left) and after baseline correction (right) with method “modpolyfit”.

11.8.2. Correcting Wavelength Dependence

sweep

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, "/")`

11.8.3. Spectra Dependent Correction

sweep

If the correction depends on the spectra (e.g. due to inhomogeneous illumination while collecting imaging data, differing optical path length, etc.), the *MARGIN* of the *sweep* function needs to be 1 or SPC:

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

11.9. Normalization

apply sweep

Again, *sweep* is the function of choice. E.g. for area normalization, use:

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

(using the mean instead of the sum results in conveniently scaled spectra with intensities around 1.)

If the calculation of the normalization factors is more elaborate, use a two step procedure:

1. Calculate appropriate normalization factors
 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 [, , 1600 ~ 1700], 1, mean)
> chondro <- sweep (chondro, 1, factors, "*")
```

For the special case of area normalization using the mean spectra, the factors can be more conveniently calculated by

```
> factors <- 1 / rowMeans (chondro [, , 1600 ~ 1700])
```

and instead of `sweep` the arithmetic operators (here `*`) can be used directly with the normalization factor:

```
> chondro <- chondro * factors
```

Put together, this results in:

```
> chondro <- chondro / rowMeans (chondro [, , 1600 ~ 1700])
```

For minimum-maximum-normalization, first do an offset- or baseline correction, then normalize using `max`.

11.10. Centering and Variance Scaling the Spectra

scale

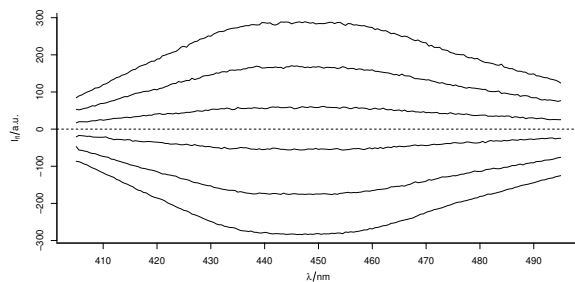
Centering means that the mean spectrum is subtracted from each of the spectra. Many data analysis techniques, like principal component analysis, partial least squares, etc., work much better on centered data. From a spectroscopic point of view it depends on the particular data set whether centering does make sense or not.

Variance scaling is often used in multivariate analysis to adjust the influence and scaling of the variates (that are typically different physical values). However, spectra already do have the same scale of the same physical value. Thus one has to trade off the the expected numeric benefit with the fact that for wavelengths with low signal the noise level will “explode” by variance scaling. Scaling usually makes sense only for centered data.

Both tasks are carried out by the same method in R, `scale`, which will by default both mean center and variance scale the spectra matrix.

To center the `flu` data set, use:

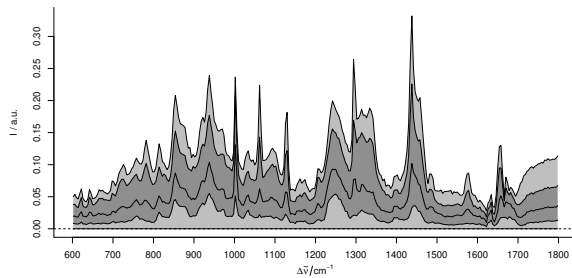
```
> flu.centered <- scale (flu, scale = FALSE)
> plot (flu.centered)
```



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 may be 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 (negative) noise. In order to avoid that, using e. g. the 5th percentile spectrum is more suitable:


```
> chondro <- scale (chondro, center = quantile (chondro, 0.05), scale = FALSE)
> plot (chondro, "spcprct15")
```



See section 13 (p. 13) for some tips to speed up these calculations.

11.11. Multiplicative Scatter Correction (MSC)

pls::msc

MSC can be done using `msc` from package `pls`[2]. It operates on the spectra matrix:

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

11.12. Spectral Arithmetic

+ - * / ^ log
log10

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

```
> 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. `%*%`

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)
```

Many modeling functions call `as.data.frame` on their *data* argument. In that case, the conversion is done automatically:

```
> 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. `decomposition` the loading like spectra, or score maps, see figure 9.

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

hyperSpec object
  875 spectra
  5 data columns
  300 data points / spectrum
wavelength: PC [integer] 1 2 ... 300
data: (875 rows x 5 columns)
  1. y: y [numeric] -4.77 -4.77 ... 19.23
  2. x: x [numeric] -11.55 -10.55 ... 22.45
  3. filename: filename [character] rawdata/chondro.txt rawdata/chondro.txt ... rawdata/chondro.txt
  4. clusters: clusters [factor] matrix matrix ... lacuna + NA
  5. spc: score / a.u. [matrix, array300] -0.43543 -0.92192 ... -2.7756e-17
```

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
  2 data columns
  300 data points / spectrum
wavelength: Delta * tilde(nu)/cm^-1 [numeric] 602 606 ... 1798
data: (300 rows x 2 columns)
  1. filename: filename [character] rawdata/chondro.txt rawdata/chondro.txt ... rawdata/chondro.txt
  2. spc: loading I / a.u. [matrix, array300] -0.0258979 -0.0014762 ... 0.15463
```

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      filename clusters
PC1 NA NA rawdata/chondro.txt <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]$..

      filename measurement
PC1 rawdata/chondro.txt      1
```

12.1.1.1. 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.

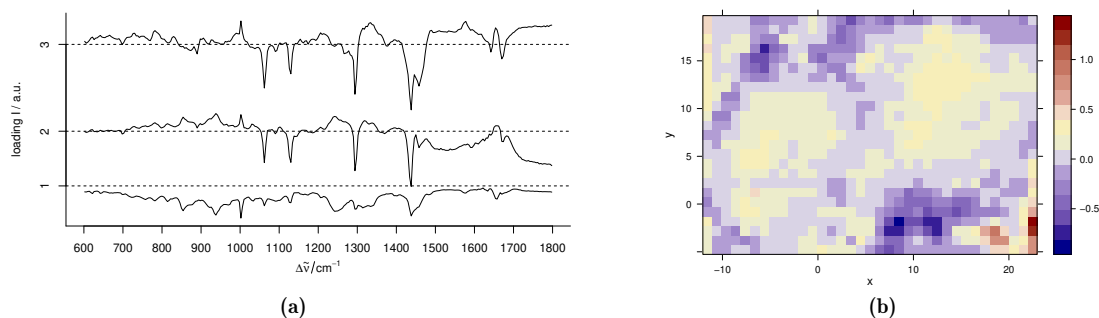


Figure 9 (a) The first three loadings: `plot (loadings [1 : 3], stacked = TRUE)`. (b) The third score map: `plotmap (scores [, , 3])`.

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 new 875×300 spectra matrix is only 10.

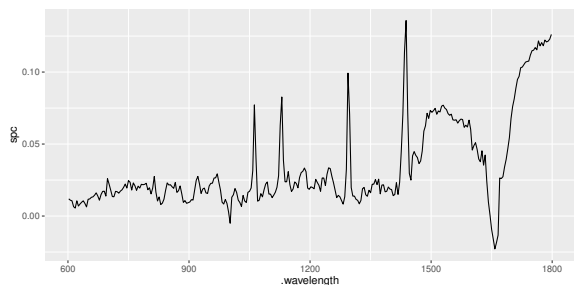
12.2. Data Analysis using long-format data.frame

e. g. plotting with ggplot2

Some functions need the data being an *unstacked* or *long-format data.frame*. `as.long.df` is the appropriate conversion function.

as.long.df

```
> require (ggplot2)
> ggplot (as.long.df (chondro [1]), aes (x = .wavelength, y = spc)) + geom_line ()
```



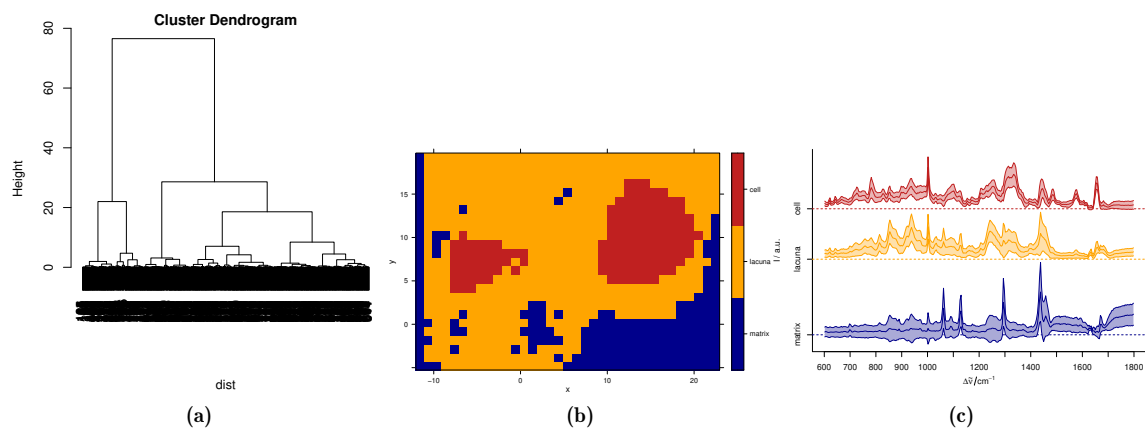


Figure 10 The results of the cluster analysis: (a) the dendrogram (b) the map of the 3 clusters (c) the mean spectra.

12.3. Data Analysis Methods using a matrix e.g. Hierarchical Cluster Analysis

[[]]

Some functions expect their input data in a matrix, so either `as.matrix` (object) or the abbreviation object `[[]]` can be used:

```
> dist <- pearson.dist (chondro [[]])
```

Again, many such functions coerce the data to a matrix automatically, so the *hyperSpec* object can be handed over:

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

```
> 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 10b):

12.4. 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")
```

12.5. Factor columns in hyperSpec Objects: dropping factor levels that are not needed

For subsections of *hyperSpec* objects that do not contain all levels of a factor column, `droplevels` drops the “unpopulated” levels:

```
> tmp <- chondro [1 : 50]
> table (tmp$clusters)
```

```
matrix lacuna cell
      22    28    0
```

```
> tmp <- droplevels (tmp)
> table (tmp$clusters)
```

```
matrix lacuna
      22    28
```

12.6. Splitting an Object, and Binding a List of hyperSpec Objects

split

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

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

```
$matrix
hyperSpec object
  187 spectra
   6 data columns
  300 data points / spectrum
wavelength: Delta * tilde(nu)/cm^-1 [numeric] 602 606 ... 1798
data: (187 rows x 6 columns)
  1. y: y [numeric] -4.77 -4.77 ... 19.23
  2. x: x [numeric] -11.55 -10.55 ... -11.55
  3. filename: filename [character] rawdata/chondro.txt rawdata/chondro.txt ... rawdata/chondro.txt
  4. clusters: clusters [factor] matrix matrix ... matrix
  5. spc: I / a.u. [matrix, array300] 0.011964 0.022204 ... 0.13706
  6. measurement: measurement [numeric] 1 1 ... 1
```

```
$lacuna
hyperSpec object
  546 spectra
   6 data columns
  300 data points / spectrum
wavelength: Delta * tilde(nu)/cm^-1 [numeric] 602 606 ... 1798
data: (546 rows x 6 columns)
  1. y: y [numeric] -4.77 -4.77 ... 19.23
  2. x: x [numeric] -8.55 -7.55 ... 22.45
  3. filename: filename [character] rawdata/chondro.txt rawdata/chondro.txt ... rawdata/chondro.txt
  4. clusters: clusters [factor] lacuna lacuna ... lacuna
  5. spc: I / a.u. [matrix, array300] 0.038900 0.031386 ... 0.049803
  6. measurement: measurement [numeric] 1 1 ... 1
```

```
$cell
hyperSpec object
  142 spectra
   6 data columns
  300 data points / spectrum
wavelength: Delta * tilde(nu)/cm^-1 [numeric] 602 606 ... 1798
data: (142 rows x 6 columns)
  1. y: y [numeric] 4.23 4.23 ... 16.23
  2. x: x [numeric] -7.55 -6.55 ... 14.45
  3. filename: filename [character] rawdata/chondro.txt rawdata/chondro.txt ... rawdata/chondro.txt
  4. clusters: clusters [factor] cell cell ... cell
```

```

5. spc: I / a.u. [matrix, array300] 0.024574 0.027541 ... 0.017377
6. measurement: measurement [numeric] 1 1 ... 1

```

Splitting can be reversed by `rbind` (see section 9.1, page 19). Another, similar way to combine a number of *hyperSpec* objects with different wavelength axes or extra data columns is `collapse` (see section 9.2, page 19). `rbind`
`collapse`

Both `rbind` and `collapse` take care that factor levels are expanded as necessary:

```

> lacunae <- droplevels (chondro [chondro$clusters == "lacuna" & ! is.na (chondro$clusters)])
> summary (lacunae$clusters)

lacuna
 546

> cells <- droplevels (chondro [chondro$clusters == "cell" & ! is.na (chondro$clusters)])
> summary (cells$clusters)

cell
 142

> summary (rbind (cells, lacunae)$clusters)

cell lacuna
 142   546

> summary (collapse (cells, lacunae)$clusters)

cell lacuna
 142   546

```

13. Speed and Memory Considerations

While most of *hyperSpec*'s functions work at a decent speed for interactive sessions (of course depending on the size of the object), iterated (repeated) calculations as for bootstrapping or iterated cross validation may ask for special speed considerations.

As an example, let's again consider the code for shifting the spectra:

```

> tmp <- chondro [1 : 50]
> shifts <- rnorm (nrow (tmp))
> system.time ({
+   for (i in seq_len (nrow (tmp)))
+     tmp [[i]] <- interpolate (tmp [[i]], shifts [i], wl = wl (tmp))
+ })

   user system elapsed
0.028  0.000  0.029

```

Calculations that involve a lot of subsetting (i.e. extracting or changing the spectra matrix or extra data) can be sped up considerably if the required parts of the *hyperSpec* object are extracted beforehand. This is somewhat similar to model fitting in R in general: many model fitting functions in R are much faster if the formula interface is avoided and the appropriate *data.frames* or matrices are handed over directly.

```

> tmp <- chondro [1 : 50]
> system.time ({
+   tmp.matrix <- tmp [[]]
+   wl <- wl (tmp)
+   for (i in seq_len (nrow (tmp)))
+     tmp.matrix [i, ] <- interpolate (tmp.matrix [i, ], shifts [i], wl = wl)
+   tmp [[]] <- tmp.matrix
+ })

```

```
user system elapsed
0.006 0.000 0.006
```

Additional packages.

matrixStats implements fast functions to calculate summary statistics for each row or each column of a matrix. This functionality can be enabled for *hyperSpec* by installing package *hyperSpec.matrixStats* which is available in *hyperSpec*'s development repository at <http://hyperSpec.r-forge.r-project.org/>

Compiled code. R provides interfaces to Fortran and C code, see the manual "Writing R Extensions". *Rcpp*[3, 4, 5] allows to conveniently integrate C++ code. *inline*[6] adds another layer of convenience: inline definition of functions in C, C++, or Fortran.

An intermediate level is byte compilation of R code, which is done by *compiler*[7].

Memory use. In general, it is recommended not to work with variables that are more than approximately a third of the available RAM in size. Particularly the import of raw spectroscopic data can consume large amounts of memory. At certain points, *hyperSpec* provides switches that allow working with data sets that are actually close to this memory limit.

The initialization method `new ("hyperSpec", ...)` takes particular care to avoid unnecessary copies of the spectra matrix. In addition, frequent calls to `gc ()` can be requested by `hy.setOption (gc = TRUE)`. The same behaviour is triggered in `read.ENVI` and its derivatives (`read.ENVI`, `read.ENVI.HySpec`, and `read.ENVI.Nicolet`). The memory consumption of `read.txt.Renishaw` can be lowered by importing the data in chunks (argument *nlines*).

```
new
("hyperSpec"),
read.ENVI*,
read.txt.Renishaw
```

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A. Overview of the functions provided by hyperSpec

Function	Explanation
<i>Access parts of the object</i>	
[Select / extract / delete spectra, wavelength ranges or extra data
[<-	Set parts of spectra or extra data
[[Select / extract / delete spectra, wavelength ranges or extra data, get the result as matrix or data.frame
[[<-	Set parts of spectra matrix
\$	extract a data column (including \$spc)
\$<-	replace a data column (including \$spc)
i2wl	convert spectra matrix column indices to wavelengths
isample	get a random sample of the spectra as index vector
labels	get column labels
labels<-	set column labels
logbook	logging the data treatment
logentry	make a logbook entry
rownames<-	
sample	generate random sample of the spectra
seq.hyperSpec	sequence along the spectra, either as <i>hyperSpec</i> object or index vector

Function	Explanation
<code>wl</code>	extract the wavelengths
<code>wl<-</code>	replace the wavelengths
<code>wl2i</code>	convert wavelengths to spectra matrix column indices
<i>Maths</i>	
<code>%*%</code>	matrix multiplication
<i>Vectorization</i>	
<code>aggregate</code>	
<code>apply</code>	
<code>sweep</code>	
<i>Comparison</i>	
<code>all.equal</code>	
<i>Plotting</i>	
<code>alois.palette</code>	another palette
<code>levelplot</code>	
<code>map.identify</code>	identify spectra in map plot
<code>map.sel.poly</code>	identify spectra in map plot: select polygon
<code>mark.dendrogram</code>	mark samples in hclust dendrogram
<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>sel.poly</code>	polygon selection in lattice plot
<code>spc.identify</code>	identify spectra and wavelengths in spectra plot
<code>spc.label.default</code>	helper for <code>spc.identify</code>
<code>spc.label.wlonly</code>	helper for <code>spc.identify</code>
<code>spc.point.default</code>	helper for <code>spc.identify</code>
<code>spc.point.max</code>	helper for <code>spc.identify</code>
<code>spc.point.min</code>	helper for <code>spc.identify</code>
<code>spc.point.sqr</code>	helper for <code>spc.identify</code>
<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

Function	Explanation
<i>Type conversion</i>	
<code>as.data.frame</code>	
<code>as.long.df</code>	convert to a long-format data.frame.
<code>as.matrix</code>	
<code>as.t.df</code>	convert to a transposed data.frame (spectra in columns)
<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>Combine/split</i>	
<code>bind</code>	commom interface for <code>rbind</code> and <code>cbind</code>
<code>cbind.hyperSpec</code>	
<code>collapse</code>	combine objects by adding columns if necessary. See <code>plyr::rbind.fill</code> .
<code>merge</code>	combines spectral ranges. works if spectra are in only one of the data sets
<code>rbind.hyperSpec</code>	bind objects by row, i. e. add wavelength ranges or extra data
<code>split</code>	
<i>Basic information</i>	
<code>chk.hy</code>	checks whether the object is a <i>hyperSpec</i> object
<code>colnames</code>	
<code>colnames<-</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>summary</code>	summary information including the log
<i>Create and initialize an object</i>	
<code>empty</code>	creates an <i>hyperSpec</i> object with 0 rows, but the same wavelengths as another object
<i>Options</i>	
<code>hy.getOption</code>	get an option
<code>hy.getOptions</code>	get more options
<code>hy.setOptions</code>	set options
<i>Tests</i>	
<code>hy.unittest</code>	run all unit tests
<i>Utility functions</i>	

Function	Explanation
<code>mean</code>	mean spectrum
<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
<code>quantile</code>	quantile spectra
<code>rbind.fill.matrix</code>	transitional until <code>plyr::rbind.fill.matrix</code> is out
<code>wc</code>	word count using <code>wc</code> if available on the system
<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>	loess smoothing interpolation
<i>File import/export</i>	
<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>scan.txt.Witec</code>	import ASCII files produced by Witec Raman spectrometers
<code>scan.zip.Renishaw</code>	directly read zip packed ASCII files produced by Renishaw spectrometers
<code>write.txt.long</code>	export as long-type ASCII file
<code>write.txt.wide</code>	export as wide-type ASCII file

Session Info

```

[,1]
sysname      "Linux"
release     "5.11.0-27-generic"
version     "#29~20.04.1-Ubuntu SMP Wed Aug 11 15:58:17 UTC 2021"
nodename    "cx17007"
machine     "x86_64"
login       "unknown"
user        "cb"
effective_user "cb"

R version 4.1.1 (2021-08-10)
Platform: x86_64-pc-linux-gnu (64-bit)

```

Running under: Ubuntu 20.04.3 LTS

Matrix products: default

BLAS: /usr/lib/x86_64-linux-gnu/openblas-pthread/libblas.so.3

LAPACK: /usr/lib/x86_64-linux-gnu/openblas-pthread/liblapack.so.3

locale:

[1] LC_CTYPE=en_US.UTF-8	LC_NUMERIC=C	LC_TIME=de_DE.UTF-8
[4] LC_COLLATE=C	LC_MONETARY=de_DE.UTF-8	LC_MESSAGES=en_US.UTF-8
[7] LC_PAPER=de_DE.UTF-8	LC_NAME=C	LC_ADDRESS=C
[10] LC_TELEPHONE=C	LC_MEASUREMENT=de_DE.UTF-8	LC_IDENTIFICATION=C

attached base packages:

[1] tools grid stats graphics grDevices utils datasets methods base

other attached packages:

[1] baseline_1.3-1 MASS_7.3-54 hyperSpec_0.100.0 xml2_1.3.2 ggplot2_3.3.5
[6] lattice_0.20-44

loaded via a namespace (and not attached):

[1] pillar_1.6.1	compiler_4.1.1	RColorBrewer_1.1-2	R.methodsS3_1.8.1
[5] R.utils_2.10.1	testthat_3.0.4	digest_0.6.27	lifecycle_1.0.0
[9] tibble_3.1.3	gtable_0.3.0	R.cache_0.15.0	pkgconfig_2.0.3
[13] png_0.1-7	rlang_0.4.11	SparseM_1.81	mvtnorm_1.1-2
[17] R.rsp_0.44.0	withr_2.4.2	dplyr_1.0.7	generics_0.1.0
[21] vctrs_0.3.8	tidyselect_1.1.1	limSolve_1.5.6	glue_1.4.2
[25] R6_2.5.0	jpeg_0.1-9	plotrix_3.8-1	fansi_0.5.0
[29] latticeExtra_0.6-29	farver_2.1.0	purrr_0.3.4	magrittr_2.0.1
[33] scales_1.1.1	ellipsis_0.3.2	lpSolve_5.6.15	colorspace_2.0-2
[37] labeling_0.4.2	quadprog_1.5-8	utf8_1.2.2	lazyeval_0.2.2
[41] munsell_0.5.0	crayon_1.4.1	R.oo_1.24.0	