Package 'hyperSpec'

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Type Package

Title Work with Hyperspectral Data, i.e. Spectra + Meta Information (Spatial, Time, Concentration, ...)

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Description Comfortable ways to work with hyperspectral data sets. I.e. spatially or time-resolved spectra, or spectra with any other kind of information associated with each of the spectra. The spectra can be data as obtained in XRF, UV/VIS, Fluorescence, AES, NIR, IR, Raman, NMR, MS, etc. More generally, any data that is recorded over a discretized variable, e.g. absorbance = f(wavelength), stored as a vector of absorbance values for discrete wavelengths is suitable.

License GPL (>= 3)

LazyLoad yes

LazyData yes

Depends R (>= 3.6.0), lattice, grid, ggplot2 (>= 2.2.0), xml2

Suggests R.matlab, tripack, deldir, rgl, plotrix, sp, baseline, compiler, inline, Rcpp, MASS, fastcluster, pls, mvtnorm, digest, reshape, devtools, R.rsp, tibble

Imports testthat, methods, utils, latticeExtra, lazyeval, dplyr

URL https://r-hyperspec.github.io/hyperSpec/ (documentation), https://github.com/r-hyperspec/hyperSpec (code)

BugReports https://github.com/r-hyperspec/hyperSpec/issues

VignetteBuilder R.rsp

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R topics documented:

hyperSpec-package *Package hyperSpec*

Description

Interface for hyperspectral data sets This package gives an interface to handle hyperspectral data sets in R. Hyperspectral data are spatially or time-resolved spectra, or spectra with any other kind of information associated with the spectra. E.g. spectral maps or images, time series, calibration series, etc.

Details

The spectra can be data as obtained in XRF, UV/VIS, Fluorescence, AES, NIR, IR, Raman, NMR, MS, etc.

More generally, any data that is recorded over a discretized variable, e.g. absorbance = f (wavelength), stored as a vector of absorbance values for discrete wavelengths is suitable.

Author(s)

C. Beleites

Maintainer: Claudia Beleites <claudia.beleites@chemometrix.eu>

See Also

`citation("hyperSpec")` produces the correct citation.

`package?hyperSpec` for information about the package

`class?hyperSpec` for details on the S4 class provided by this package.

.cluster.wavelengths *Find clusters of approximately equal wavelengths*

Description

Find clusters of approximately equal wavelengths

Usage

```
.cluster.wavelengths(dots, wl.tolerance)
```

Arguments

`dots`	list of hyperSpec objects to collapse
`wl.tolerance`	wavelength difference tolerance

Value

data.frame with information about suitable wavelength bins

.collapse.equal *Try finding groups of hyperSpec objects with (approximately) equal wavelength axes*

Description

... and directly rbind.fill them.

Usage

```
.collapse.equal(dots, wl.tolerance)
```

Arguments

dots	list with hyperSpec object to collapse
wl.tolerance	wavelength difference tolerance

Value

possible shorter list of dots

.DollarNames.hyperSpec *command line completion for $*

Description

command line completion for $

Usage

```
## S3 method for class 'hyperSpec'
.DollarNames(x, pattern = "")
```

Arguments

x	the hyperSpecobject
pattern	pattern to look for

Value

the name of the extra data slot

Author(s)

C. Beleites

See Also

.DollarNames

.fix_spc_colnames *Ensure that the spectra matrix has the wavelengths in column names*

Description

Ensure that the spectra matrix has the wavelengths in column names

Usage

```
.fix_spc_colnames(spc)
```

Arguments

spc	hyperSpec object

Value

hyperSpec object with wavelengths in column names of $spc

.read.spe.xml *Read XML footer from SPE file format version 3.0*

Description

The new SPE file format, introduced in 2012, was designed to be backwards compatible with the previous format 2.5. The most prominent change is the new plain text XML footer holding vast experimental metadata that gets attached at the end of the file. Thus, the file contains 3 blocks: a 4100-bytes long binary header, a chunk with spectral data, and the XML footer. This function retrieves the XML footer converted to R list, and throws error if it is not available. The file format specification is available at Princeton Instruments FTP server under name 'SPE 3.0 File Format Specification'.

Usage

```
.read.spe.xml(filename)
```

Arguments

filename	- SPE filename

Details

This function relies on R package xml2 to work correctly

Value

xml data from the file converted to R list

.read.spe.xml_string *.read.spe.xml_string*

Description

Read XML footer from SPE file format version 3.0 and return it as a long string for subsequent parsing. Basically the purpose of this function is to check that the file format version is 3.0 or above, and to find and read the correct part of this file.

Usage

```
.read.spe.xml_string(filename)
```

Arguments

filename	- SPE filename

Value

string containing XML footer

---

aggregate *aggregate hyperSpec objects*

Description

Compute summary statistics for subsets of a hyperSpec object.

Usage

```
## S4 method for signature 'hyperSpec'
aggregate(
  x,
  by = stop("by is needed"),
  FUN = stop("FUN is needed."),
  ...,
  out.rows = NULL,
  append.rows = NULL,
  by.isindex = FALSE
)
```

Arguments

x	a hyperSpec object
by	grouping for the rows of x@data. Either a list containing an index vector for each of the subgroups or a vector that can be split in such a list.
FUN	function to compute the summary statistics
...	further arguments passed to FUN
out.rows	number of rows in the resulting hyperSpec object, for memory preallocation.
append.rows	If more rows are needed, how many should be appended? Defaults to 100 or an estimate based on the percentage of groups that are still to be done, whatever is larger.
by.isindex	If a list is given in by: does the list already contain the row indices of the groups? If FALSE, the list in by is computed first (as in aggregate).

Details

aggregate applies FUN to each of the subgroups given by by. It combines the functionality of aggregate, tapply, and ave for hyperSpec objects.

aggregate avoids splitting x@data.

FUN does not need to return exactly one value. The number of returned values needs to be the same for all wavelengths (otherwise the result could not be a matrix), see the examples.

If the initially preallocated data.frame turns out to be too small, more rows are appended and a warning is issued.

Value

A hyperSpec object with an additional column @data$.aggregate tracing which group the rows belong to.

Author(s)

C. Beleites

See Also

tapply, aggregate, ave

Examples

```
cluster.means <- aggregate (chondro, chondro$clusters, mean_pm_sd)
plot(cluster.means, stacked = ".aggregate", fill = ".aggregate",
     col = matlab.dark.palette (3))

## make some "spectra"
spc <- new ("hyperSpec", spc = sweep (matrix (rnorm (10*20), ncol = 20), 1, (1:10)*5, "+"))

## 3 groups
```

```
color <- c("red", "blue", "black")
by <- as.factor (c (1, 1, 1, 1, 1, 1, 5, 1, 2, 2))
by
plot (spc, "spc", col = color[by])

## Example 1: plot the mean of the groups
plot (aggregate (spc, by, mean), "spc", col = color, add = TRUE,
      lines.args = list(lwd = 3, lty = 2))

## Example 2: FUN may return more than one value (here: 3)
plot (aggregate (spc, by, mean_pm_sd), "spc",
      col = rep(color, each = 3), lines.args = list(lwd = 3, lty = 2))

## Example 3: aggregate even takes FUN that return different numbers of
##            values for different groups
plot (spc, "spc", col = color[by])

weird.function <- function (x){
   if (length (x) == 1)
      x + 1 : 10
   else if (length (x) == 2)
      NULL
   else
      x [1]
}

agg <- aggregate (spc, by, weird.function)
agg$.aggregate
plot (agg, "spc",  add = TRUE, col = color[agg$.aggregate],
      lines.args = list (lwd = 3, lty = 2))
```

---

apply *apply Computes summary statistics for the spectra of a* hyperSpec *object.*

Description

apply gives the functionality of apply for hyperSpec objects.

Usage

```
## S4 method for signature 'hyperSpec'
apply(
  X,
  MARGIN,
  FUN,
  ...,
  label.wl = NULL,
```

```
  label.spc = NULL,
  new.wavelength = NULL,
  simplify
)
```

Arguments

X, spc	a hyperSpec object
MARGIN	The subscript which the function will be applied over. 1 indicates rows (FUN is applied to each spectrum), 2 indicates columns (FUN is applied to each wavelength), 1 : 2 indicates that FUN should be applied to each single element of the spectra matrix. Note that many basic mathematical functions are already defined for hyperSpec objects (see Math). If MARGIN is missing, the whole spectra matrix is handed to FUN, see also the examples.
FUN	function to compute the summary statistics
...	further arguments passed to FUN
label.wl, label.spc	new labels for wavelength and spectral intensity axes
new.wavelength	for MARGIN = 2: numeric vector or name of the argument in ... that is to be used (character) as wavelength axis of the resulting object.
simplify	ignored: apply for hyperSpec results are always simplified

Details

The generic functions of group Math are not definded for hyperSpec objects. Instead, apply can be used. For functions like log that work on scalars, MARGIN = 1 : 2 gives the appropriate behaviour.

spcapply does the same as apply with MARGIN = 1, but additionally allows to set a new wavelength axis and adjust the labels.

wlapply does the same as apply with MARGIN = 2, but additionally allows to set a new wavelength axis and adjust the labels.

Value

A hyperSpec object

Author(s)

C. Beleites

See Also

apply, for applying FUN to subgroups of the hyperSpec object: aggregate.

Examples

```
plotspc (apply (chondro, 2, range))

avgflu <- apply (flu, 1, mean,
                 label.spc = expression (bar (I)),
                 new.wavelength = mean (wl (flu)))
avgflu

flu[[,,405:407]]
apply (flu, 1:2, "*", -1)[[,,405:407]]

## without MARGIN the whole matrix is handed to FUN
apply (flu [,,405:407], , print) [[]]

## whereas MARGIN = 1 : 2 leads to FUN being called for each element separately
apply (flu [,,405:407], 1 : 2, print) [[]]
```

Arith *Arithmetical Operators for hyperSpec objects*

Description

Arithmetical Operators: +, -, *, /, ^, %%, %/%, %*% for hyperSpec objects

Usage

```
## S4 method for signature 'hyperSpec,hyperSpec'
Arith(e1, e2)

## S4 method for signature 'hyperSpec,numeric'
Arith(e1, e2)

## S4 method for signature 'hyperSpec,matrix'
Arith(e1, e2)

## S4 method for signature 'hyperSpec,missing'
Arith(e1, e2)

## S4 method for signature 'numeric,hyperSpec'
Arith(e1, e2)

## S4 method for signature 'matrix,hyperSpec'
Arith(e1, e2)

## S4 method for signature 'hyperSpec,hyperSpec'
```

```
x %*% y

## S4 method for signature 'hyperSpec,matrix'
x %*% y

## S4 method for signature 'matrix,hyperSpec'
x %*% y
```

Arguments

e1, e2	or
x, y	either two hyperSpec objects or one hyperSpec object and matrix of same size as hyperSpec[[]] or a vector which length equalling either the number of rows or the number of wavelengths of the hyperSpec object, or a scalar (numeric of length 1).

Details

The arithmetical operators +, -, *, /, \^, %%, %/%, and %*% for hyperSpec objects.

You can use these operators in different ways:

```
e1 + e2
`+` (e1, e2)

x %*% y
`%*%`(x, y)

-x
```

The arithmetical operators +, -, *, /, ^, %%, %/%, and %*% work on the spectra matrix of the hyperSpec object. They have their usual meaning (see Arithmetic). The operators work also with one hyperSpec object and a numeric object or a matrices of the same size as the spectra matrix of the hyperSpec object.

With numeric vectors sweep is most probably more appropriate.

If you want to calculate on the extra data as well, use the data.frame hyperSpec@data directly or as.data.frame (x).

Value

hyperSpec object with the new spectra matrix.

Author(s)

C. Beleites

See Also

sweep-methods for calculations involving a vector and the spectral matrix.

S4groupGeneric for group generic methods.

Arithmetic for the base arithmetic functions.

Comparison for comparison operators, Math for mathematical group generic functions (Math and Math2 groups) working on hyperSpec objects.

matmult for matrix multiplications with %*%.

Examples

```
flu + flu
1 / flu
all((flu + flu - 2 * flu)[[]] == 0)
-flu
flu / flu$c
```

---

as.character,hyperSpec-method

Convert a hyperSpec object to character strings for Display print*,* show*, and* summary *show the result of* as.character.

Description

print, show, and summary differ only in the defaults. show displays the range of values instead,

Usage

```
## S4 method for signature 'hyperSpec'
as.character(
  x,
  digits = getOption("digits"),
  range = TRUE,
  max.print = 5,
  shorten.to = c(2, 1)
)

## S4 method for signature 'hyperSpec'
show(object)

## S4 method for signature 'hyperSpec'
print(x, range = FALSE, ...)

## S4 method for signature 'hyperSpec'
summary(object, ...)
```

Arguments

x	a hyperSpec object
digits	number of digits handed over to format
range	should the values be indicated as range rather then first and last elements?
max.print	maximum number of elements to be printed (of a variable)
shorten.to	if a vector is longer than max.print, only the first shorten.to[1] and the last shorten.to[2] elements are printed
object	a hyperSpec object
...	print and summary hand further arguments to as.character

Value

as.character returns a character vector fit to be printed by cat with sep = "\n".

print invisibly returns x after printing, show returns an invisible NULL.

See Also

as.character

show

print

summary

Examples

```
chondro

show (chondro)

summary (chondro)

print (chondro, range = TRUE)
```

---

as.data.frame

Conversion of a hyperSpec object into a data.frame or matrix as.data.frame *returns* x@data *(as data.frame)* as.matrix *returns the spectra matrix* x@data$spc *as matrix*

Description

The data.frame returned by as.long.df is guaranteed to have columns spc and .wavelength. If nwl (x) == 0 these columns will be NA.

Usage

```
## S3 method for class 'hyperSpec'
as.data.frame(x, row.names = TRUE, optional = NULL, ...)

## S3 method for class 'hyperSpec'
as.matrix(x, ...)

as.wide.df(x, wl.prefix = "")

as.long.df(x, rownames = FALSE, wl.factor = FALSE, na.rm = TRUE)

as.t.df(x)
```

Arguments

x	a hyperSpec object
row.names	if TRUE, a column .row is created containing row names or row indices if no rownames are set. If character vector, the rownames are set accordingly.
optional	ignored
...	ignored
wl.prefix	prefix to prepend wavelength column names
rownames	should the rownames be in column .rownames of the long-format data.frame?
wl.factor	should the wavelengths be returned as a factor (instead of numeric)?
na.rm	if TRUE, rows where spc is not NA are deleted.

Value

x@data and x@data$spc (== x$spc == x [[]]), respectively.

as.wide.df returns a data.frame that consists of the extra data and the spectra matrix converted to a data.frame. The spectra matrix is expanded *in place*.

as.long.df returns the stacked or molten version of x@data. The wavelengths are in column .wavelength.

as.t.df returns a data.frame similar to as.long.df, but each spectrum in its own column. This is useful for exporting summary spectra, see the example.

Author(s)

C. Beleites

See Also

as.data.frame

and base::as.matrix()

[[[()] ([[]]) for a shortcut to as.matrix

stack and melt or reshape2::melt() for other functions producing long-format data.frames.

Examples

```
as.data.frame (chondro [1:3,, 600 ~ 620])
as.matrix (chondro [1:3,, 600 ~ 620])
lm (c ~ spc, data = flu [,,450])

as.wide.df (chondro [1:5,, 600 ~ 610])
summary (as.wide.df (chondro [1:5,, 600 ~ 610]))

as.long.df (flu [,, 405 ~ 410])
summary (as.long.df (flu [,, 405 ~ 410]))
summary (as.long.df (flu [,, 405 ~ 410], rownames = TRUE))
summary (as.long.df (flu [,, 405 ~ 410], wl.factor = TRUE))

df <- as.t.df (apply (chondro, 2, mean_pm_sd))
head (df)

if (require (ggplot2)){
  ggplot (df, aes (x = .wavelength)) +
    geom_ribbon (aes (ymin = mean.minus.sd, ymax = mean.plus.sd),
      fill = "#00000040") +
    geom_line (aes (y = mean))
}
```

---

as.hyperSpec *as.hyperSpec: convenience conversion functions*

Description

These functions are shortcuts to convert other objects into hypeSpec objects.

Usage

```
as.hyperSpec(X, ...)

## S4 method for signature 'matrix'
as.hyperSpec(X, wl = guess.wavelength(colnames(X)), ...)

## S4 method for signature 'data.frame'
as.hyperSpec(
  X,
  spc = NULL,
  wl = guess.wavelength(spc),
  labels = attr(X, "labels"),
  ...
)
```

Arguments

X	the object to convert. A matrix is assumed to contain the spectra matrix, a data.frame is assumed to contain extra data.
...	additional parameters that should be handed over to new ("hyperSpec") (initialize)
wl	wavelength vector. Defaults to guessing from the column names in X
spc	spectra matrix
labels	list with labels

Value

hyperSpec object

Note

Note that the behaviour of as.hyperSpec (X) *was changed: it now assumes* X *to be extra data, and returns a hyperSpec object with 0 wavelengths. To get the old behaviour*

See Also

initialize

Examples

```
tmp <- data.frame(flu [[,, 400 ~ 410]])
(wl <- colnames (tmp))
guess.wavelength (wl)
```

---

barbiturates *Barbiturates Spectra from .spc example files A time series of mass spectra in a list of hyperSpec objects.*

Description

Barbiturates Spectra from .spc example files A time series of mass spectra in a list of hyperSpec objects.

Format

The data sets consists of 286 spectra. They are the result of importing the BARBITUATES.SPC example data from Thermo Galactic's spc file format specification.

Author(s)

C. Beleites and Thermo Galactic

References

The raw data is available at http://hyperspec.r-forge.r-project.org/blob/fileio.zip

Examples

```
barbiturates [1:3]
length (barbiturates)

barb <- collapse (barbiturates, collapse.equal = FALSE)
barb <- orderwl (barb)

plot (barb [1:3], lines.args = list (type = "h"),
      col = matlab.dark.palette (3), stacked = TRUE,
      stacked.args = list (add.factor = .2))

if (require (latticeExtra)){
levelplot (spc ~ .wavelength * z, log (barb), panel = panel.levelplot.points,
   cex = 0.3, col = "#00000000", col.regions = matlab.palette (20))
}

plotc (apply (barb [,, 42.9~43.2], 1, sum, na.rm = TRUE), spc ~ z,
       panel = panel.lines, ylab = expression (I[m/z == 43] / "a.u."))
```

---

bind *Binding hyperSpec Objects*

Description

The former difficulties with binding S4 objects are resolved since R version 3.2.0 and `cbind` and `rbind` now work as intended and expected for hyperSpec objects.

`cbind2` binds the spectral matrices of two `hyperSpec` objects by column. All columns besides `spc` with the same name in `x@data` and `y@data` must have the same elements. Rows are ordered before checking.

Usage

```
bind(
  direction = stop("direction ('c' or 'r') required"),
  ...,
  wl.tolerance = hy.getOption("wl.tolerance")
)

## S3 method for class 'hyperSpec'
cbind(...)

## S3 method for class 'hyperSpec'
```

```
rbind(...)

## S4 method for signature 'hyperSpec,hyperSpec'
cbind2(x, y)

## S4 method for signature 'hyperSpec,missing'
cbind2(x, y)

## S4 method for signature 'hyperSpec,hyperSpec'
rbind2(x, y, wl.tolerance = hy.getOption("wl.tolerance"))

## S4 method for signature 'hyperSpec,missing'
rbind2(x, y, wl.tolerance)
```

Arguments

direction	"r" or "c" to bind rows or columns
...	The hyperSpec objects to be combined. Alternatively, *one* list of hyperSpec objects can be given to bind.
wl.tolerance	rbind and rbind2 check for equal wavelengths with this tolerance.
x, y	hyperSpec objects

Details

Therefore, calling rbind.hyperSpec and cbind.hyperSpec is now depecated: cbind and rbind should now be called directly.

However, in consequence it is no longer possible to call cbind or rbind with a list of hyperSpec objects. In that case, use bind or do.call (see example).

bind does the common work for both column- and row-wise binding.

Value

a hyperSpec object, possibly with different row order (for bind ("c", ...{}) and cbind2).

Note

You might have to make sure that the objects either all have or all do not have rownames and/or colnames.

Author(s)

C. Beleites

See Also

rbind2, cbind2 rbind, cbind

merge and collapse for combining objects that do not share spectra or wavelengths, respectively.

Examples

```
chondro
bind ("r", chondro, chondro)
rbind (chondro, chondro)
cbind (chondro, chondro)
bind ("r", list (chondro, chondro, chondro))

x <- chondro[,, 600 : 605]
x$a <- 1
x@data <- x@data[, sample (ncol (x), ncol (x))] # reorder columns

y <- chondro [nrow (chondro) : 1,, 1730 : 1750] # reorder rows
y$b <- 2

cbind2 (x, y) # works

y$y[3] <- 5
try (cbind2 (x, y)) # error

# list of hyperSpec objects

lhy <- list (flu, flu)
do.call ("rbind", lhy)
bind ("r", lhy)
```

---

chk.hy *Validation of hyperSpec objects*

Description

Check whether an object is a hyperSpec object and validate the object

Usage

```
chk.hy(object)
```

Arguments

object	the object to check

Value

TRUE if the check passes, otherwise stop with an error.

Author(s)

C. Beleites

See Also

validObject

Examples

```
chk.hy (chondro)
validObject (chondro)
```

---

chondro *Raman spectra of 2 Chondrocytes in Cartilage A Raman-map (laterally resolved Raman spectra) of chondrocytes in cartilage.*

Description

See the vignette `vignette("chondro",package = "hyperSpec")`.

Usage

```
chondro
```

Format

The data set has 875 Raman spectra measured on a 25 $\times$ 35 grid with 1 micron step size. Spatial information is in `chondro$x` and `chondro$y`. Each spectrum has 300 data points in the range of ca. 600 - 1800 cm^{-1}.

Author(s)

A. Bonifacio and C. Beleites

References

The raw data is available at http://hyperspec.r-forge.r-project.org/blob/chondro.zip

Examples

```
chondro

## do baseline correction
baselines <- spc.fit.poly.below (chondro)
chondro <- chondro - baselines

## area normalization
chondro <- chondro / colMeans (chondro)

## substact common composition
chondro <- chondro - quantile (chondro, 0.05)
```

```
cols <- c ("dark blue", "orange", "#C02020")
plotmap (chondro, clusters ~ x * y, col.regions = cols)

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

## plot nucleic acid bands
plotmap (chondro[, , c( 728, 782, 1098, 1240, 1482, 1577)],
     col.regions = colorRampPalette (c ("white", "gold", "dark green"), space = "Lab") (20))
```

`collapse` *Collapse hyperSpec objects*

Description

collapse/bind several hyperSpec objects into one object

Usage

```
collapse(
  ...,
  wl.tolerance = hy.getOption("wl.tolerance"),
  collapse.equal = TRUE
)
```

Arguments

`...`	hyperSpec objects to be collapsed into one object. Instead of giving several arguments, a list with all objects to be collapsed may be given.
`wl.tolerance`	tolerance to decide which wavelengths are considered equal.
`collapse.equal`	logical indicating whether to try first finding groups of spectra with (approximately) equal wavelength axes. If the data is known to contain few or no such groups, `collapse()` will be faster with this first pass being turned off.

Details

The spectra from all objects will be put into one object. The resulting object has all wavelengths that occur in any of the input objects, `wl.tolerance` is used to determine which difference in the wavelengths is tolerated as equal: clusters of approximately equal wavelengths will span at most `2 * wl.tolerance`. Differences up to +/- `wl.tolerance` are considered equal.

The returned object has wavelengths that are the weighted average (by number of spectra) of the wavelengths within any such cluster of approximately equal wavelengths.

Labels will be taken from the first object where they are encountered. However, the order of processing objects is not necessarily the same as the order of objects in the input: `collapse` first processes groups of input objects that share all wavelengths (within `wl.tolerance`).

Data points corresponding to wavelengths not in the original spectrum will be set to NA. Extra data is combined in the same manner.

If the objects are named, the names will be preserved in extra data column $.name. If the wavelengths are names, names are preserved and taken from the first object where they were encountered, the same applies to possible column names of the spectra matrix.

Value

a hyperSpec object

Author(s)

C. Beleites

See Also

`merge()`, `rbind()`, and `plyr::rbind.fill()`

Examples

```
barbiturates [1:3]
collapse (barbiturates [1:3])

a <- barbiturates [[1]]
b <- barbiturates [[2]]
c <- barbiturates [[3]]

a
b
c
collapse (a, b, c)

collapse (barbiturates [1:3], collapse.equal = FALSE)
```

`colSums` *colSums, colMeans, rowSums and rowMeans functions for hyperSpec objects*

Description

hyperSpec objects can use the base functions `colMeans`, `colSums`, `rowMeans` and `rowSums`.

Usage

```
## S4 method for signature 'hyperSpec'
colMeans(x, na.rm = TRUE, ..., label.spc)

## S4 method for signature 'hyperSpec'
colSums(x, na.rm = TRUE, ..., label.spc)

## S4 method for signature 'hyperSpec'
rowMeans(x, na.rm = TRUE, ..., label.wavelength)

## S4 method for signature 'hyperSpec'
rowSums(x, na.rm = TRUE, ..., label.wavelength)
```

Arguments

x	hyperSpec object
na.rm, ...	further parameters to the base functions na.rm defaults to TRUE for hyperSpec objects.
label.spc	labels for the intensity axis for loadings-like (col) statistics
label.wavelength	labels for the wavelength axis for scores-like (row) statistics

See Also

colSums

Examples

```
colMeans (flu)
colSums (flu)
colSums (flu)
rowSums (flu)
```

Comparison *Comparison of hyperSpec objects*

Description

The comparison operators >, <, >=, <=, ==, and != for hyperSpec objects.

Usage

```
## S4 method for signature 'hyperSpec,hyperSpec'
Compare(e1, e2)

## S4 method for signature 'hyperSpec,numeric'
```

```
Compare(e1, e2)

## S4 method for signature 'hyperSpec,matrix'
Compare(e1, e2)

## S4 method for signature 'numeric,hyperSpec'
Compare(e1, e2)

## S4 method for signature 'matrix,hyperSpec'
Compare(e1, e2)

## S4 method for signature 'hyperSpec,hyperSpec'
all.equal(
  target,
  current,
  ...,
  check.attributes = FALSE,
  check.names = FALSE,
  check.column.order = FALSE,
  check.label = FALSE,
  tolerance = hy.getOption("tolerance"),
  wl.tolerance = hy.getOption("wl.tolerance")
)
```

Arguments

`e1, e2`	Either two `hyperSpec` objects or one `hyperSpec` object and matrix of same size as `hyperSpec[[]]` or a scalar (numeric of length 1). As `hyperSpec` objects must have numeric spectra matrices, the resulting matrix of the comparison is returned directly.
`target, current`	two `hyperSpec` objects that are tested for equality
`...`	handed to `all.equal` when testing the slots of the `hyperSpec` objects
`check.attributes, check.names`	see `all.equal`
`check.column.order`	If two objects have the same data, but the order of the columns (determined by the names) differs, should they be regarded as different?
`check.label`	Should the slot `label` be checked? If the labels differ only in the order of their entries, they are conidered equal.
`tolerance, wl.tolerance`	tolerances for checking wavelengths and data, respectively

Details

`all.equal` checks the equality of two hyperSpec objects.

The comparison operators >, <, >=, <=, ==, and != work on the spectra matrix of the `hyperSpec` object. They have their usual meaning (see `Comparison`). The operators work also with one

hyperSpec object and a numeric (scalar) object or a matrices of the same size as the spectra matrix of the hyperSpec object.

With numeric vectors sweep might be more appropriate.

If you want to calculate on the data.frame hyperSpec@data, you have to do this directly on hyperSpec@data.

Value

a logical matrix for the comparison operators.

all.equal returns either TRUE, or a character vector describing the differences. In conditions, the result must therefore be tested with isTRUE.

Author(s)

C. Beleites

See Also

sweep-methods for calculations involving a vector and the spectral matrix.

S4groupGeneric for group generic methods.

Comparison for the base comparison functions.

Arith for arithmetic operators, Math for mathematical group generic functions (groups Math and Math2) working on hyperSpec objects.

all.equal and isTRUE

Examples

```
flu [,,445 ~ 450] > 300

all (flu == flu[[]])
```

---

count_lines *count lines (of an ASCII file)*

Description

count lines (of an ASCII file)

Usage

```
count_lines(file, chunksize = 10000)
```

Arguments

file	the file name or connection
chunksize	file is read in chunks of chunksize lines.

Value

number of lines in file

Author(s)

C. Beleites

---

cov,hyperSpec,missing-method

Covariance matrices for hyperSpec objects

Description

Covariance matrices for hyperSpec objects

Usage

```
## S4 method for signature 'hyperSpec,missing'
cov(
  x,
  y = NULL,
  use = "everything",
  method = c("pearson", "kendall", "spearman")
)

pooled.cov(x, groups, ..., regularize = 1e-05 * max(abs(COV)))
```

Arguments

x	hyperSpec object
y	not supported
use, method	handed to cov
groups	factor indicating the groups
...	ignored
regularize	regularization of the covariance matrix. Set 0 to switch off pooled.cov calculates pooled covariance like e.g. in LDA.

Value

covariance matrix of size nwl(x) x nwl(x)

Author(s)

C. Beleites

See Also

cov

Examples

```
image (cov (chondro))
pcov <-  pooled.cov (chondro, chondro$clusters)
plot (pcov$means)
image (pcov$COV)
```

---

decomposition — *Convert Principal Component Decomposition or the like into a hyperSpec Object*

Description

Decomposition of the spectra matrix is a common procedure in chemometric data analysis. `scores` and `loadings` convert the result matrices into new `hyperSpec` objects.

Usage

```
decomposition(
  object,
  x,
  wavelength = seq_len(ncol(x)),
  label.wavelength,
  label.spc,
  scores = TRUE,
  retain.columns = FALSE,
  ...
)
```

Arguments

`object`	A `hyperSpec` object.
`x`	matrix with the new content for `object@data$spc`. Its size must correspond to rows (for `scores`) and to either columns or rows (for `loadings`) of `object`.
`wavelength`	for a scores-like `x`: the new `object@wavelength`.
`label.wavelength`	The new label for the wavelength axis (if `x` is scores-like). If not given, the label of `object` is kept.

label.spc	The new label for the spectra matrix. If not given, the label of object is kept.
scores	is x a scores-like matrix?
retain.columns	for loading-like decompostition (i.e. x holds loadings, pure component spectra or the like), the data columns need special attention. Columns with different values across the rows will be set to NA if retain.columns is TRUE, otherwise they will be deleted.
...	ignored.

Details

Multivariate data are frequently decomposed by methods like principal component analysis, partial least squares, linear discriminant analysis, and the like. These methods yield latent spectra (or latent variables, loadings, components, ...) that are linear combination coefficients along the wavelength axis and scores for each spectrum and loading.

The loadings matrix gives a coordinate transformation, and the scores are values in that new coordinate system.

The obtained latent variables are spectra-like objects: a latent variable has a coefficient for each wavelength. If such a matrix (with the same number of columns as object has wavelengths) is given to decomposition (also setting scores = FALSE), the spectra matrix is replaced by x. Moreover, all columns of object@data that did not contain the same value for all spectra are set to NA. Thus, for the resulting hyperSpec object, plotspc and related functions are meaningful. plotmap cannot be applied as the loadings are not laterally resolved.

The scores matrix needs to have the same number of rows as object has spectra. If such a matrix is given, decomposition will replace the spectra matrix is replaced by x and object@wavelength by wavelength. The information related to each of the spectra is retained. For such a hyperSpec object, plotmap and plotc and the like can be applied. It is also possible to use the spectra plotting, but the interpretation is not that of the spectrum any longer.

Value

A hyperSpec object, updated according to x

Author(s)

C. Beleites

See Also

See %*% for matrix multiplication of hyperSpec objects.

See e.g. prcomp and princomp for principal component analysis, and package pls for Partial Least Squares Regression.

Examples

```
pca <- prcomp (flu)

pca.loadings <- decomposition (flu, t (pca$rotation), scores = FALSE)
```

```
pca.center <- decomposition (flu, pca$center, scores = FALSE)
pca.scores <- decomposition (flu, pca$x)

plot (pca.center)
plot (pca.loadings, col = c ("red", "gray50"))
plotc (pca.scores, groups = .wavelength)
```

---

dimnames,hyperSpec-method

dimnames for hyperSpec objects

Description

hyperSpec objects can have row- and column names like data.frames. The "names" of the wavelengths are treated separately: see wl

Usage

```
## S4 method for signature 'hyperSpec'
dimnames(x)

## S4 method for signature 'hyperSpec'
rownames(x, do.NULL = TRUE, prefix = "row")

## S4 replacement method for signature 'hyperSpec'
 rownames(x) <- value

## S4 method for signature 'hyperSpec'
colnames(x, do.NULL = TRUE, prefix = "col")

## S4 replacement method for signature 'hyperSpec'
 colnames(x) <- value
```

Arguments

x	the hyperSpec object
do.NULL	handed to rownames or colnames: logical. Should this create names if they are NULL?
prefix	handed to rownames or colnames
value	the new names

Author(s)

C. Beleites

See Also

wl for the wavelength dimension

dimnames

rownames

colnames

Examples

```
dimnames (flu)
rownames (flu)
colnames (chondro)
```

---

droplevels,hyperSpec-method

droplevels for hyperSpec object

Description

calls base::droplevels() on the data.frame in spc@data.

Usage

```
## S4 method for signature 'hyperSpec'
droplevels(x, ...)
```

Arguments

x	hyperSpec object
...	handed to base::droplevels.data.frame()

Value

hyperSpec object with unused levels of all factors in @data dropped.

See Also

base::droplevels()

Examples

```
chondro[1:3]$clusters
droplevels (chondro [1:3])$clusters
```

empty *Empty hyperSpec object*

Description

Empty produces an hyperSpec object with the same columns and wavelengths as `x`. The new object will either contain no rows at all (default), or the given number of rows with all data initialized to `spc` and `extra`, respectively.

Usage

```
empty(x, nrow = 0, spc = NA, extra = NA)
```

Arguments

`x`	hyperSpec object
`nrow`	number of rows the new object should have
`spc`	value to initialize the new spectra matrix with
`extra`	value to initialize the new extra data with

Author(s)

C. Beleites

Examples

```
empty (chondro, nrow = 2, spc = 0)
```

flu *Quinine Fluorescence Spectra Fluorescence spectra of different dilutions of quinine forming a calibration set.*

Description

See the vignette: `vignette ("flu",package = "hyperSpec")`

Format

The data set has 6 fluorescence emission spectra measured on quinine concentrations between 0.05 mg/l and 0.30 mg/l. Each spectrum consists of 181 data points in the range of 405 nm to 495 nm.

Author(s)

M. Kammer and C. Beleites

Examples

```
flu

plot (flu)

plotc (flu)
```

`Future-functions` *Future functions*

Description

These functions will be introduced in **hyperSpec** v1.0 and will replace some current functions. Now they appear here just for compatibility with other packages, which should be released on CRAN. They are not intended to be used by **hyperSpec** v0.100 users directly.

Usage

```
.spc_io_postprocess_optional(...)

wl_convert_units(x, from, to, ref_wl = NULL)

hy_set_options(...)

hy_get_option(...)

hy_set_options(...)

read_txt_long(...)

read_txt_wide(...)

.wl_fix_unit_name(...)

assert_hyperSpec(...)
```

Arguments

`...`	Arguments to functions.
`x, from, to, ref_wl`	Arguments to functions.

guess.wavelength *guess wavelengths from character vector*

Description

character vectors used for names (e.g. colnames for matrices or data.frames) are often treated by `make.names` or similar functions that produce suitable names (e.g. by prepending "X" to numbers.). Such names cannot be directly converted to numeric.

Usage

```
guess.wavelength(X)
```

Arguments

X	character with numbers hidden inside

Details

`guess.wavlength` tries to extract numbers from X which may be surrounded by such "protecting" characters.

Value

numeric

Examples

```
tmp <- data.frame(flu [[,, 400 ~ 410]])
(wl <- colnames (tmp))
guess.wavelength (wl)
```

hy.getOptions *Options for package hyperSpec Functions to access and set hyperSpec's options.*

Description

Currently, the following options are defined:

Name	Default Value (range)	Description	Used by
debuglevel	0 (1L 2L 3L)	amount of debugging information produced	`spc.identify` various file imp `spc.fit.poly`
gc	FALSE	triggers frequent calling of gc ()	`read.ENVI`, ne
file.remove.emptyspc	TRUE	remove empty spectra directly on file import	various file imp

file.keep.name	TRUE	always create filename column	various file imp
tolerance	`sqrt(.Machine$double.eps)`	tolerance for numerical comparisons	`normalize01`,
wl.tolerance	`sqrt(.Machine$double.eps)`	tolerance for comparisons of the wavelength axis	`all.equal`, `co`
plot.spc.nmax	25	number of spectra to be plotted by default	`plotspc`
ggplot.spc.nmax	10		`qplotspc`

Usage

```
hy.getOptions(...)

hy.getOption(name)

hy.setOptions(...)
```

Arguments

`...`	`hy.setOptions`: pairs of argument names and values. `hy.getOptions`: indices (or names) of the options.
`name`	the name of the option

Details

`hy.setOptions` will discard any values that were given without a name.

Value

`hy.getOptions`	returns a list of all options
`hy.setOptions`	invisibly returns a list with the options
`hy.getOption`	returns the value of the requested option

Author(s)

C. Beleites

Examples

```
hy.getOptions()
```

hy.unittest *hyperSpec unit tests*

Description

If testthat is available, run the unit tests and display the results.

Usage

```
hy.unittest(standalone = TRUE, reporter = "progress")
```

Arguments

standalone	run the unit test on their own, e.g. from the console (‘TRUE‘) or within testthat tests (‘FALSE‘), e.g. via ‘devtools::test()‘
reporter	the reporter to use, defaults to [testthat::ProgressReporter]

Value

Invisibly returns a data frame with the test results

Author(s)

Claudia Beleites

Examples

```
hy.unittest ()
```

hyperSpec-class *Class "hyperSpec" This class handles hyperspectral data sets, i.e. spatially or time-resolved spectra, or spectra with any other kind of information associated with the spectra.*

Description

The spectra can be data as obtained in XRF, UV/VIS, Fluorescence, AES, NIR, IR, Raman, NMR, MS, etc.

Details

More generally, any data that is recorded over a discretized variable, e.g. absorbance = f (wavelength), stored as a vector of absorbance values for discrete wavelengths is suitable.

Slots

`wavelength` wavelengths (wavenumbers, frequencies, etc.) for each of the columns of the spectra matrix

`data` the data (extra data and spectra matrix)

`label` expressions for column labels (incl. units). The label of the wavelength axis is in the special element `.wavelength`.

`log` deprecated.

Note

Please note that the logbook is now removed.

Author(s)

C. Beleites

See Also

See the vignette "hyperspec" for an introduction to hyperSpec from a spectroscopic point of view.

Examples

```
showClass("hyperSpec")
## Not run: vignette ("hyperspec")
```

`initialize` *Creating a hyperSpec Object*

Description

Like other S4 objects, a hyperSpec object can be created by `new`. The hyperSpec object is then `initialized` using the given parameters.

Usage

```
## S4 method for signature 'hyperSpec'
initialize(.Object, spc = NULL, data = NULL, wavelength = NULL, labels = NULL)
```

Arguments

`.Object`	the new `hyperSpec` object.
`spc`	the spectra matrix. `spc` does not need to be a matrix, it is converted explicitly by `I(as.matrix(spc))`.

data	data.frame, possibly with the spectra in data$spc, and further variates in more columns. A matrix can be entered as *one* column of a data frame by: data.frame (spc = I (as.matrix (spc))). However, it will usually be more convenient if the spectra are given in spc
wavelength	The wavelengths corresponding to the columns of data. If no wavelengths are given, an appropriate vector is derived from the column names of data$spc. If this is not possible, 1 : ncol (data$spc) is used instead.
labels	A list containing the labels for the columns of the data slot of the hyperSpec object and for the wavelength (in label$.wavelength). The labels should be given in a form ready for the text-drawing functions (see plotmath). If label is not given, a list containing NULL for each of the columns ofdata and wavelength is used.

Details

If option gc is TRUE, the initialization will have frequent calls to gc () which can help to avoid swapping or running out of memory.

Author(s)

C.Beleites

See Also

new for more information on creating and initializing S4 objects.

plotmath on expressions for math annotations as for slot label.

hy.setOptions

Examples

```
new ("hyperSpec")

spc <- matrix (rnorm (12), ncol = 4)
new ("hyperSpec", spc = spc)
new ("hyperSpec", data = data.frame (x = letters[1:3]),
     spc = spc)

colnames (spc) <- 600:603
new ("hyperSpec", spc = spc)  # wavelength taken from colnames (spc)

# given wavelengths precede over colnames of spc
new ("hyperSpec", spc = spc, wavelength = 700:703)

# specifying labels
h <- new ("hyperSpec", spc = spc, data = data.frame (pos = 1 : 3),
          label = list (spc = "I / a.u.",
                        .wavelength = expression (tilde (nu) / cm^-1),
                        pos = expression ("/" (x, mu*m)))
```

```
)

plot (h)
plotc (h, spc ~ pos)
```

`labels<-` *Get and Set Labels of a hyperSpec Object* `value` *may be a list or vector of labels giving the new label for each of the entries specified by* `which`.

Description

The names of the labels are the same as the colnames of the `data.frame`. The label for the wavelength axis has the name `.wavelength`.

Usage

```
labels (object, which = NULL, ...) <- value

## S4 method for signature 'hyperSpec'
labels(object, which = bquote(), drop = TRUE, ..., use.colnames = TRUE)
```

Arguments

`object`	a hyperSpec object
`which`	numeric or character to specify the label(s)
`...`	ignored
`value`	the new label(s)
`drop`	if the result would be a list with only one element, should the element be returned instead?
`use.colnames`	should missing labels be replaced by column names of the extra data?

Details

The labels should be given in a form ready for the text-drawing functions (see `plotmath`), e.g. as `expression` or a `character`.

Value

`labels<-` returns a `hyperSpec` object.

`labels` returns a list of labels. If `drop` is `TRUE` and the list contains only one element, the element is returned instead.

Author(s)

C. Beleites

See Also

labels

Examples

```
labels (flu, "c") <- expression ("/" ("c", "mg / l"))


labels (chondro)
```

---

laser *Laser Emission A time series of an unstable laser emission.*

Description

see the Vignette

Format

The data set consists of 84 laser emission spectra measured during 95 min. Each spectrum has 36 data points in the range of 404.5 nm to 405.8 nm.

Author(s)

C. Beleites

Examples

```
laser

cols <- c ("black", "blue", "darkgreen", "red")
wl <- c (405.0, 405.1, 405.3, 405.4)
plotspc (laser, axis.args=list (x = list (at = seq (404.5, 405.8, .1))))
for (i in seq_along (wl))
   abline (v = wl[i], col = cols[i], lwd = 2, lty = 2)

plotc (laser [,, wl], spc ~ t, groups = .wavelength, type = "b",
       col = cols)

## Not run: vignette ("laser", package="hyperSpec")
```

legendright *Plot multivariate data into colour channels*

Description

plot graph with legend right of it

Usage

```
legendright(p, l, legend.width = 8, legend.unit = "lines")

qmixtile(
  object,
  purecol = stop("pure component colors needed."),
  mapping = aes_string(x = "x", y = "y", fill = "spc"),
  ...,
  map.tileonly = FALSE
)

normalize.colrange(x, na.rm = TRUE, legend = FALSE, n = 100, ...)

normalize.range(x, na.rm = TRUE, legend = FALSE, n = 100, ...)

normalize.null(x, na.rm = TRUE, legend = FALSE, n = 100, ...)

normalize.minmax(x, min = 0, max = 1, legend = FALSE, n = 100, ...)

qmixlegend(
  x,
  purecol,
  dx = 0.33,
  ny = 100,
  labels = names(purecol),
  normalize = normalize.colrange,
  ...
)

colmix.rgb(
  x,
  purecol,
  against = 1,
  sub = TRUE,
  normalize = normalize.colrange,
  ...
)
```

Arguments

p	plot object
l	legend object
legend.width, legend.unit	size of legend part
object	matrix to be plotted with mixed colour channels
purecol	pure component colours, names determine legend labels
mapping	see geom_tile
...	qmixtile: handed to colmix.rgb qmixlegend and colmix.rgb hand further arguments to the normalize function
map.tileonly	if TRUE, mapping will be handed to geom_tile instead of ggplot.
x	matrix with component intensities in columns
na.rm	see link[base]{min}
legend	should a legend be produced instead of normalized values?
n	of colours to produce in legend
min	numeric with value corresponding to "lowest" colour for each column
max	numeric with value corresponding to "hightest" colour for each column
dx	width of label bar
ny	number of colours in legend
labels	component names
normalize	function to normalize the values.
against	value to mix against (for sub = TRUE only, 1 = white, 0 = black)
sub	subtractive color mixing?

Value

invisible NULL

list with components ymin, max and fill to specify value and fill colour value (still numeric!) for the legend, otherwise the normalized values

ggplot object with legend

character with colours

Author(s)

Claudia Beleites

Claudia Beleites

Claudia Beleites

makeraster *makeraster*

Description

find an evenly spaced grid for x

Usage

```
makeraster(x, startx, d, newlevels, tol = 0.1)

fitraster(x, tol = 0.1)
```

Arguments

x	numeric to be fitted with a raster
startx	starting point ("origin") for calculation of the raster
d	step size of the raster
newlevels	levels of the raster
tol	tolerance for rounding to new levels: elements of x within tol of the distance between the levels of the new grid are rounded to the new grid point.

Details

makeraster fits the data to the specified raster.

fitraster tries different raster parameter and returns the raster that covers most of the x values: The differences between the values of x are calculated (possible step sizes). For each of those step sizes, different points are tried (until all points have been covered by a raster) and the parameter combination leading to the best coverage (i.e. most points on the grid) ist used.

Note that only differences between the sorted values of x are considered as step size.

Value

list with elements

x	the values of x, possibly rounded to the raster values
levels	the values of the raster

Author(s)

Claudia Beleites

Examples

```
x <- c (sample (1:20, 10), (0 : 5) + 0.5)
raster <- makeraster (x, x [1], 2)
raster
plot (x)
abline (h = raster$levels, col = "#00000040")

## unoccupied levels
missing <- setdiff (raster$levels, raster$x)
abline (h = missing, col = "red")

## points acutally on the raster
onraster <- raster$x %in% raster$levels
points (which (onraster), raster$x [onraster], col = "blue", pch = 20)


raster <- fitraster (x)
raster
plot (x)
abline (h = raster$levels, col = "#00000040")

## unoccupied levels
missing <- setdiff (raster$levels, raster$x)
abline (h = missing, col = "red")

## points acutally on the raster
onraster <- raster$x %in% raster$levels
points (which (onraster), raster$x [onraster], col = "blue", pch = 20)

x <- c (sample (1:20, 10), (0 : 5) + 0.45)
raster <- fitraster (x)
raster
plot (x)
abline (h = raster$levels, col = "#00000040")

## unoccupied levels
missing <- setdiff (raster$levels, raster$x)
abline (h = missing, col = "red")

## points acutally on the raster
onraster <- raster$x %in% raster$levels
points (which (onraster), raster$x [onraster], col = "blue", pch = 20)
```

`map.sel.poly` *Interactively select a polygon (grid graphics) and highlight points*

Description

Click the points that should be connected as polygon. Input ends with right click (see `grid.locator`). Polygon will be drawn closed.

Usage

```
map.sel.poly(data, pch = 19, size = 0.3, ...)

sel.poly(pch = 19, size = 0.3, ...)
```

Arguments

data	hyperSpec object for plotting map or list returned by plotmap
pch	symbol to display the points of the polygon for sel.poly
size	size for polygon point symbol for sel.poly
...	further arguments for grid.points and grid.lines

Details

map.sel.poly is a convenience wrapper for plotmap, sel.poly, and point.in.polygon. For custiomized plotting, the plot can be produced by plotmap, plotvoronoi or levelplot, and the result of that plot command handed over to map.sel.poly, see the example below.

If even more customized plotting is required,sel.poly should be used (see example).

Value

map.sel.poly: array of indices for points within the selected polygon

sel.poly: n x 2 matrix with the corner points of the polygon

Author(s)

Claudia Beleites, Sebastian Mellor

Claudia Beleites

See Also

grid.locator, map.identify

grid.locator

Examples

```
if (interactive ()){
## convenience wrapper
map.sel.poly (chondro)

## customized version
data <- sample (chondro [,, 1004 - 2i ~ 1004 + 2i], 300)

plotdata <- plotvoronoi (data, clusters ~ y * x, col.regions = alois.palette ())
print (plotdata)
map.sel.poly (plotdata)

## even more customization:
```

```
plotvoronoi (data)

## interactively retrieve polygon
polygon <- sel.poly ()

## find data points within polygon
require ("sp")
i.sel <- which (point.in.polygon (data$x, data$y, polygon [, 1], polygon [, 2]) > 0)

## work with selected points
grid.points (unit (data$x [i.sel], "native"), unit (data$y [i.sel], "native"))
}
```

`mark.dendrogram` *Mark groups in* `hclust` *dendrograms*

Description

Groups are marked by colored rectangles as well as by their levels.

Usage

```
mark.dendrogram(
  dendrogram,
  groups,
  col = seq_along(unique(groups)),
  pos.marker = 0,
  height = 0.025 * max(dendrogram$height),
  pos.text = -2.5 * height,
  border = NA,
  text.col = "black",
  label,
  label.right = TRUE,
  ...
)
```

Arguments

`dendrogram`	the dendrogram
`groups`	factor giving the the groups to mark
`col`	vector with colors for each group
`pos.marker`	top of the marker rectangle
`height`	height of the marker rectangle
`pos.text`	position of the text label
`border`	see `text`
`text.col`	color (vector) giving the color for the text markers

label	side label see example
label.right	should the side labels be at the right side?
...	handed to rect and text

Details

The dendrogram should be plotted separately, see the example.

Author(s)

Claudia Beleites

Examples

```
dend <- hclust (pearson.dist (laser[[]]))
par (xpd = TRUE, mar = c (5.1, 4, 4, 3)) # allows plotting into the margin
plot (dend, hang = -1, labels = FALSE)

## mark clusters
clusters <- as.factor (cutree (dend, k = 4))
levels (clusters) <- LETTERS [1 : 4]
mark.dendrogram (dend, clusters, label = "cluster")

## mark independent factor
mark.dendrogram (dend, as.factor (laser [,,405.36] > 11000),
pos.marker = -0.02, pos.text = - 0.03)

## mark continuous variable: convert it to a factor and omit labels
mark.dendrogram (dend, cut (laser [[,, 405.36]], 100), alois.palette (100),
                 pos.marker = -.015, text.col = NA,
                 label = expression (I [lambda == 405.36~nm]), label.right = FALSE)
```

---

markpeak *Mark peak Marks location of the* first *spectrum at the data point closest to the specified position on the current plot.*

Description

Mark peak

Marks location of the *first* spectrum at the data point closest to the specified position on the current plot.

Usage

```
markpeak(spc, xpos, col = "red")
```

Arguments

spc	the hyperSpec object
xpos	position of the peak(s) in current x-axis units
col	color of the markers and text

Author(s)

R. Kiselev

Examples

```
plot (chondro [7])
markpeak (chondro [7], 1662)
```

Math2,hyperSpec-method

Math Functions for hyperSpec Objects

Description

Mathematical functions for hyperSpec Objects.

Usage

```
## S4 method for signature 'hyperSpec'
Math2(x, digits)

## S4 method for signature 'hyperSpec'
log(x, base = exp(1), ...)

## S4 method for signature 'hyperSpec'
Math(x)
```

Arguments

x	the hyperSpec object
digits	integer stating the rounding precision
base	base of logarithm
...	ignored

Details

The functions abs, sign, sqrt, floor, ceiling, trunc, round, signif, exp, log, expm1, log1p, cos, sin, tan, acos, asin, atan, cosh, sinh, tanh, acosh, asinh, atanh, lgamma, gamma, digamma, trigamma, cumsum, cumprod, cummax, cummin for hyperSpec objects.

Value

a hyperSpec object

Author(s)

C. Beleites

See Also

S4groupGeneric for group generic methods.

Math for the base math functions.

Arith for arithmetic operators, Comparison for comparison operators, and Summary for group generic functions working on hyperSpec objects.

Examples

```
log (flu)
```

`matlab.palette` *Matlab-like Palettes Two palettes going from blue over green to red, approximately as the standard palette of Matlab does. The second one has darker green values and is better suited for plotting lines on white background.*

Description

Matlab-like Palettes Two palettes going from blue over green to red, approximately as the standard palette of Matlab does. The second one has darker green values and is better suited for plotting lines on white background.

Usage

```
matlab.palette(n = 100, ...)

matlab.dark.palette(n = 100, ...)

alois.palette(n = 100, ...)
```

Arguments

n	the number of colors to be in the palette.
...	further arguments are handed to rainbow (alois.palette: colorRampPalette)

Value

A vector containing the color values in the form "\#rrbbggaa".

Author(s)

C. Beleites and A. Bonifacio

See Also

rainbow

Examples

```
plotmap (chondro [,, 778], col.regions = matlab.palette ())


plot (flu, col = matlab.dark.palette (nrow (flu)))

plotmap (chondro, col = alois.palette)
```

---

mean_sd,numeric-method

Mean and Standard Deviation Calculate mean and standard deviation, and mean, mean ± one standard deviation, respectively.

Description

These functions are provided for convenience.

Usage

```
## S4 method for signature 'numeric'
mean_sd(x, na.rm = TRUE, ...)

## S4 method for signature 'matrix'
mean_sd(x, na.rm = TRUE, ...)

## S4 method for signature 'hyperSpec'
mean_sd(x, na.rm = TRUE, ...)

## S4 method for signature 'numeric'
mean_pm_sd(x, na.rm = TRUE, ...)

## S4 method for signature 'matrix'
mean_pm_sd(x, na.rm = TRUE, ...)
```

```
## S4 method for signature 'hyperSpec'
mean_pm_sd(x, na.rm = TRUE, ...)

## S4 method for signature 'hyperSpec'
mean(x, na.rm = TRUE, ...)

## S4 method for signature 'hyperSpec'
quantile(x, probs = seq(0, 1, 0.5), na.rm = TRUE, names = "num", ...)
```

Arguments

x	a numeric vector
na.rm	handed to mean and sd
...	ignored (needed to make function generic)
probs	the quantiles, see quantile
names	"pretty" results in percentages (like quantile's names = TRUE), "num" results in the row names being as.character(probs) (good for ggplot2 getting the order of the quantiles right). Otherwise, no names are assigned.

Value

mean_sd returns a vector with two values (mean and standard deviation) of x.

mean_sd (matrix) returns a matrix with the mean spectrum in the first row and the standard deviation in the 2nd.

mean_sd returns a hyperSpec object with the mean spectrum in the first row and the standard deviation in the 2nd.

mean_pm_sd returns a vector with 3 values: mean - 1 sd, mean, mean + 1 sd

mean_pm_sd (matrix) returns a matrix containing mean - sd, mean, and mean + sd rows.

For hyperSpec objects, mean_pm_sd returns a hyperSpec object containing mean - sd, mean, and mean + sd spectra.

For hyperSpec object, mean returns a hyperSpec object containing the mean spectrum.

For hyperSpec object, quantile returns a hyperSpec object containing the respective quantile spectra.

Author(s)

C. Beleites

See Also

mean, sd

mean, sd

quantile

Examples

```
mean_sd (flu [,, 405 ~ 410])

mean_sd (flu$spc)

mean_sd (flu)

  mean_pm_sd (flu$c)

mean_pm_sd (flu$spc)

mean_pm_sd (flu)

plot (mean (chondro))

plot (quantile (chondro))
```

---

merge,hyperSpec,hyperSpec-method

Merge hyperSpec objects

Description

Merges two hyperSpec objects and cbinds their spectra matrices, or merges additional extra data into a hyperSpec object.

Usage

```
## S4 method for signature 'hyperSpec,hyperSpec'
merge(x, y, ...)

## S4 method for signature 'hyperSpec,data.frame'
merge(x, y, ...)

## S4 method for signature 'data.frame,hyperSpec'
merge(x, y, ...)
```

Arguments

x	a hyperSpec object or data.frame
y	a hyperSpec object or data.frame (including derived classes like tibble)
...	handed to merge.data.frame

Details

After merging, the spectra matrix can contain duplicates, and is not ordered according to the wavelength.

If the wavelength axis should be ordered, use `orderwl`.

If a `hyperSpec` object and a `data.frame` are merged, the result is of the class of the first (`x`) object.

Author(s)

C. Beleites

See Also

`merge`.

`collapse` combines hyperSpec objects that do not share the wavelength axis. `rbind`, and `cbind` for combining hyperSpec objects that.

Examples

```
merge (chondro [1:10,, 600], chondro [5:15,, 600], by = c("x", "y"))$.
tmp <- merge (chondro [1:10,, 610], chondro [5:15,, 610],
              by = c("x", "y"), all = TRUE)
tmp$.
wl (tmp)

## remove duplicated wavelengths:
approxfun <- function (y, wl, new.wl){
  approx (wl, y, new.wl, method = "constant",
          ties = function (x) mean (x, na.rm = TRUE)
          )$y
}

merged <- merge (chondro [1:7,, 610 ~ 620], chondro [5:10,, 615 ~ 625], all = TRUE)
merged$.
merged <- apply (merged, 1, approxfun,
                 wl = wl (merged), new.wl = unique (wl (merged)),
                 new.wavelength = "new.wl")
merged$.

## merging data.frame into hyperSpec object => hyperSpec object
y <- data.frame (filename = sample (flu$filename, 4, replace = TRUE), cpred = 1:4)
y
tmp <- merge (flu, y)
tmp$..

## merging hyperSpec object into data.frame => data.frame
merge (y, flu)
```

ncol,hyperSpec-method *The Number of Rows (Spectra), Columns, and Data Points per Spectrum of an hyperSpec Object)*

Description

ncol returns the number of columns in x@data. I.e. the number of columns with additional information to each spectrum (e.g. "x", "y", ...) + 1 (for column spc containing the spectra).

Usage

```
## S4 method for signature 'hyperSpec'
ncol(x)

## S4 method for signature 'hyperSpec'
nrow(x)

nwl(x)

## S4 method for signature 'hyperSpec'
dim(x)

## S4 method for signature 'hyperSpec'
length(x)
```

Arguments

x	a hyperSpec object

Value

nrow, ncol, nwl, and length, return an integer.

dim returns a vector of length 3.

Author(s)

C. Beleites

See Also

ncol

nrow

dim

length

Examples

```
ncol (chondro)
nrow (chondro)

nwl  (chondro)
dim (chondro)
length (chondro)
```

`normalize01` *normalization for mixed colors*

Description

Normalize numbers -> [0, 1]

Usage

```
normalize01(x, ...)

## S4 method for signature 'matrix'
normalize01(x, tolerance = hy.getOption("tolerance"))

## S4 method for signature 'numeric'
normalize01(x, tolerance = hy.getOption("tolerance"))

## S4 method for signature 'hyperSpec'
normalize01(x, ...)
```

Arguments

`x`	vector with values to transform
`...`	additional parameters such as `tolerance` handed down.
`tolerance`	tolerance level for determining what is 0 and 1

Details

The input `x` is mapped to [0, 1] by subtracting the minimum and subsequently dividing by the maximum. If all elements of `x` are equal, 1 is returned.

Value

vector with `x` values mapped to the interval [0, 1]

Author(s)

C. Beleites

See Also

wl.eval, vanderMonde

---

orderwl — *Sorting the Wavelengths of a hyperSpec Object Rearranges the* hyperSpec *object so that the wavelength vector is in increasing (or decreasing) order.*

Description

The wavelength vector is sorted and the columns of the spectra matrix are rearranged accordingly.

Usage

```
orderwl(x, na.last = TRUE, decreasing = FALSE)
```

Arguments

x	The hyperSpec object.
na.last, decreasing	Handed to order.

Value

A hyperSpec object.

Author(s)

C. Beleites

See Also

order

Examples

```
## Example 1: different drawing order in plotspc
spc <- new ("hyperSpec", spc = matrix (rnorm (5) + 1:5, ncol = 5))
spc <- cbind (spc, spc+.5)

plot (spc, "spc")
text (wl (spc), spc [[]], as.character (1:10))
spc <- orderwl (spc)
plot (spc, "spc")
text (wl (spc), spc [[]], as.character (1:10))

## Example 2
```

```
spc <- new ("hyperSpec", spc = matrix (rnorm (5)*2 + 1:5, ncol = 5))
spc <- cbind (spc, spc)

plot (seq_len(nwl(spc)), spc[[]], type = "b")
spc[[]]

spc <- orderwl (spc)
lines (seq_len(nwl(spc)), spc[[]], type = "l", col = "red")
spc[[]]
```

`paracetamol` *Paracetamol Spectrum A Raman spectrum of a paracetamol tablet.*

Description

Paracetamol Spectrum A Raman spectrum of a paracetamol tablet.

Format

The spectrum was acquired with a Renishaw InVia spectrometer from 100 to 3200 cm^-1 in step scan mode. Thus the spectrum has several overlapping wavelength regions.

Author(s)

C. Beleites

Examples

```
paracetamol

plot (paracetamol)
plotspc (paracetamol, c (min ~ 1750, 2800 ~ max), xoffset = 800,
wl.reverse = TRUE)
```

`pearson.dist` *Distance based on Pearson's $R\hat{}2$*

Description

The calculated distance is $D^2 = \frac{1-COR(\mathtt{x}')}{2}$

Usage

```
pearson.dist(x)
```

Arguments

x	a matrix

Details

The distance between the rows of x is calculated. The possible values range from 0 (prefectly correlated) over 0.5 (uncorrelated) to 1 (perfectly anti-correlated).

Value

distance matrix (distance object)

Author(s)

C. Beleites

References

S. Theodoridis and K. Koutroumbas: Pattern Recognition, 3rd ed., p. 495

See Also

as.dist

Examples

```
pearson.dist (flu [[]])
pearson.dist (flu)
```

---

plot-methods *Plotting hyperSpec Objects*

Description

Plotting hyperSpec objects. The plot method for hyperSpec objects is a switchyard to plotspc, plotmap, and plotc.

Usage

```
## S4 method for signature 'hyperSpec,missing'
plot(x, y, ...)

## S4 method for signature 'hyperSpec,character'
plot(x, y, ...)
```

Arguments

x	the hyperSpec object
y	selects what plot should be produced
...	arguments passed to the respective plot function

Details

It also supplies some convenient abbrevations for much used plots.

If y is missing, plot behaves like plot (x,y = "spc").

Supported values for y are:

"spc" calls plotspc to produce a spectra plot.

"spcmeansd" plots mean spectrum +/- one standard deviation

"spcprctile" plots 16th, 50th, and 84th percentile spectre. If the distributions of the intensities at all wavelengths were normal, this would correspond to "spcmeansd". However, this is frequently not the case. Then "spcprctile" gives a better impression of the spectral data set.

"spcprctl5" like "spcprctile", but additionally the 5th and 95th percentile spectra are plotted.

"map" calls plotmap to produce a map plot.

"voronoi" calls plotvoronoi to produce a Voronoi plot (tesselated plot, like "map" for hyperSpec objects with uneven/non-rectangular grid).

"mat" calls plotmat to produce a plot of the spectra matrix (not to be confused with matplot).

"c" calls plotc to produce a calibration (or time series, depth-profile, or the like)

"ts" plots a time series: abbrevation for plotc (x,use.c = "t")

"depth" plots a depth profile: abbrevation for plotc (x,use.c = "z")

Author(s)

C. Beleites

See Also

plotspc for spectra plots (intensity over wavelength),

plotmap for plotting maps, i.e. color coded summary value on two (usually spatial) dimensions.

plotc

plot

Examples

```
plot (flu)

plot (flu, "c")

plot (laser, "ts")
```

```
spc <- apply (chondro, 2, quantile, probs = 0.05)
spc <- sweep (chondro, 2, spc, "-")
plot (spc, "spcprctl5")
plot (spc, "spcprctile")
plot (spc, "spcmeansd")
```

`plotc` *Calibration- and Timeseries Plots, Depth-Profiles and the like* `plotc` *plots intensities of a* `hyperSpec` *object over another dimension such as concentration, time, or a spatial coordinate.*

Description

If `func` is not `NULL`, the summary characteristic is calculated first by applying `func` with the respective arguments (in `func.args`) to each of the spectra. If `func` returns more than one value (for each spectrum), the different values end up as different wavelengths.

Usage

```
plotc(
  object,
  model = spc ~ c,
  groups = NULL,
  func = NULL,
  func.args = list(),
  ...
)
```

Arguments

`object`	the `hyperSpec` object
`model`	the lattice model specifying the plot
`groups`	grouping variable, e.g. `.wavelength` if intensities of more than one wavelength should be plotted
`func`	function to compute a summary value from the spectra to be plotted instead of single intensities
`func.args`	further arguments to `func`
`...`	further arguments to `xyplot`.

Details

If the wavelength is not used in the model specification nor in `groups`, nor for specifying `subsets`, and neither is `func` given, then only the first wavelength's intensities are plotted and a warning is issued.

The special column names `.rownames` and `.wavelength` may be used.

The actual plotting is done by `xyplot`.

Author(s)

C. Beleites

See Also

xyplot

Examples

```
## example 1: calibration of fluorescence
plotc (flu) ## gives a warning

plotc (flu, func = mean)
plotc (flu, func = range, groups = .wavelength)

plotc (flu[,,450], ylab = expression (I ["450 nm"] / a.u.))


calibration <- lm (spc ~ c, data = flu[,,450]$.)
summary (calibration)
plotc (flu [,, 450], type = c("p", "r"))

conc <- list (c = seq (from = 0.04, to = 0.31, by = 0.01))
ci <- predict (calibration, newdata = conc, interval = "confidence", level = 0.999)

panel.ci <-  function (x, y, ...,
                       conc, ci.lwr, ci.upr, ci.col = "#606060") {
   panel.xyplot (x, y, ...)
   panel.lmline (x, y,...)
   panel.lines (conc, ci.lwr, col = ci.col)
   panel.lines (conc, ci.upr, col = ci.col)
}

plotc (flu [,, 450], panel = panel.ci,
       conc = conc$c, ci.lwr = ci [, 2], ci.upr = ci [, 3])

## example 2: time-trace of laser emission modes
cols <- c ("black", "blue", "#008000", "red")
wl <- i2wl (laser, c(13, 17, 21, 23))

plotspc (laser, axis.args=list (x = list (at = seq (404.5, 405.8, .1))))
for (i in seq_along (wl))
   abline (v = wl[i], col = cols[i], lwd = 2)

plotc (laser [,, wl], spc ~ t, groups = .wavelength, type = "b",
       col = cols)
```

plotmap *Plot a Map and Identify/Select Spectra in the Map* levelplot *functions for hyperSpec objects. An image or map of a summary value of each spectrum is plotted. Spectra may be identified by mouse click.*

Description

The model can contain the special column name .wavelength to specify the wavelength axis.

Usage

```
plotmap(object, model = spc ~ x * y, func = mean, func.args = list(), ...)

## S4 method for signature 'hyperSpec,missing'
levelplot(x, data, ...)

## S4 method for signature 'formula,hyperSpec'
levelplot(
  x,
  data,
  transform.factor = TRUE,
  ...,
  contour = FALSE,
  useRaster = !contour
)

map.identify(
  object,
  model = spc ~ x * y,
  voronoi = FALSE,
  ...,
  tol = 0.02,
  warn = TRUE
)

plotvoronoi(object, model = spc ~ x * y, use.tripack = FALSE, mix = FALSE, ...)
```

Arguments

object, data	the hyperSpec object
model, x	formula specifying the columns of object that are to be displayed by levelplot
func, func.args	Before plotting, plotmap applies function func with the arguments given in the list func.args to each of the spectra. Thus a single summary value is displayed for each of the spectra. This can be suppressed manually by setting func to NULL. It is automatically suppressed if .wavelength appears in the formula.

`...` further arguments are passed down the call chain, and finally to `levelplot`

`transform.factor`
: If the color-coded variable is a factor, should `trellis.factor.key` be used to compute the color coding and legend?

`contour, useRaster`
: see `levelplot`

`voronoi` Should the plot for identifying spectra by mouse click be produced by `plotmap` (default) or `plotvoronoi`?

`tol` tolerance for `map.identify` as fraction of the viewport (i.e. in "npc" units)

`warn` should a warning be issued if no point is within the specified tolerance? See also details.

`use.tripack` Whether package tripack should be used for calculating the voronoi polygons. If `FALSE`, package deldir is used instead. See details.

`mix` For Voronoi plots using package tripack, I experienced errors if the data was spatially ordered. Randomly rearrangig the rows of the hyperSpec object circumvents this problem.

Details

`plotmap`, `map.identify`, and the `levelplot` methods internally use the same gateway function to `levelplot`. Thus `transform.factor` can be used with all of them and the panel function defaults to `panel.levelplot.raster` for all three. Two special column names, `.rownames` and `.wavelength` may be used.

`levelplot` plots the spectra matrix.

`plotvoronoi` calls `plotmap` with different default settings, namely the panel function defaults to `panel.voronoi`. `panel.voronoi` depends on either of the packages 'tripack' or 'deldir' being installed. For further information, please consult the help page of `panel.voronoi`. On the `chondro` data set, `plotmap` is roughly 5 times faster than `plotvoronoi` using tripack, and ca. 15 times faster than `plotvoronoi` using deldir. Package tripack, however, is free only for non-commercial use. Also, it seems that tripack version hang (R running at full CPU power, but not responding nor finishing the calculation) for certain data sets. In this case, `mix = TRUE` may help.

`map.identify` calls `plotmap` and `plotvoronoi`, respectively and waits for (left) mouse clicks on points. Other mouse clicks end the input.

Unlike `panel.identify`, the indices returned by `map.identify` are in the same order as the points were clicked. Also, multiple clicks on the same point are returned as multiple entries with the same index.

`map.identify` uses option `debuglevel` similar to `spc.identify`: `debuglevel == 1` will plot the tolerance window if no data point was inside (and additionally labels the point) while `debuglevel == 2` will always plot the tolerance window.

The `map.sel.*` functions offer further interactive selection, see `map.sel.poly`.

Value

`map.identify` returns a vector of row indices into `object` of the clicked points.

The other functions return a lattice object.

Author(s)

C. Beleites

See Also

`vignette (plotting)`, `vignette (hyperspec)`

`plot`

`levelplot`

`trellis.factor.key` for improved color coding of factors

`hyperSpec options` `spc.identify` `map.sel.poly`

`panel.voronoi`

Examples

```
## Not run:
vignette (plotting)
vignette (hyperspec)

## End(Not run)

levelplot (spc ~ y * x, chondro [,,1003]) # properly rotated
plotmap (chondro [,,1003])

# plot spectra matrix
levelplot (spc ~ .wavelength * t, laser, contour = TRUE, col = "#00000080")
# see also plotmat

plotmap (chondro, clusters ~ x * y)

# Voronoi plots
smpl <- sample (chondro, 300)
plotmap (smpl, clusters ~ x * y)
if (require (tripack))
    plotvoronoi (smpl, clusters ~ x * y)
if (require (deldir))
    plotvoronoi (smpl, clusters ~ x * y,
                 use.tripack = FALSE)
```

---

plotmat *Plot spectra matrix*

Description

plots the spectra matrix.

Usage

```
plotmat(
  object,
  y = ".row",
  ylab,
  col = alois.palette(20),
  ...,
  contour = FALSE
)
```

Arguments

object	hyperSpec object
y	character giving the name of the extra data column to label the y axis.
ylab	y axis label, defaults to "row" and the label of the extra data column used for the y axis, respectively.
col	see image
...	further parameters for image
contour	should contour be called instead of image?

Details

If package plotrix is available, a color legend is plotted to the right. The right margin is set to at least 5 lines.

Author(s)

Claudia Beleites

See Also

image, contour, levelplot

Examples

```
plotmat (laser, col = alois.palette (100))

plot (laser, "mat")

plotmat (laser)
plotmat (laser, contour = TRUE, add = TRUE)

## use different y axis labels

plotmat (laser, "t")

plotmat (laser, laser$t / 3600, ylab = "t / h")
```

plotspc *Plotting Spectra Plot the spectra of a* hyperSpec *object, i.e. intensity over wavelength. Instead of the intensity values of the spectra matrix summary values calculated from these may be used.*

Description

This is hyperSpec's main plotting function for spectra plots.

Usually, the stacked argument of plotspc will do fine, but if you need fine control over the stacking, you may calculate the y offsets yourself.

Usage

```
plotspc(
  object,
  wl.range = TRUE,
  wl.index = FALSE,
  wl.reverse = FALSE,
  spc.nmax = hy.getOption("plot.spc.nmax"),
  func = NULL,
  func.args = list(),
  stacked = NULL,
  stacked.args = list(),
  add = FALSE,
  bty = "l",
  plot.args = list(),
  col = "black",
  lines.args = list(),
  xoffset = 0,
  yoffset = 0,
  nxticks = 10,
  axis.args = list(),
  break.args = list(),
  title.args = list(),
  fill = NULL,
  fill.col = NULL,
  border = NA,
  polygon.args = list(),
  zeroline = list(lty = 2, col = col),
  debuglevel = hy.getOption("debuglevel")
)

stacked.offsets(
  x,
  stacked = TRUE,
  min.zero = FALSE,
```

```
  add.factor = 0.05,
  add.sum = 0,
  .spc = NULL,
  debuglevel = hy.getOption("debuglevel")
)
```

Arguments

object	the hyperSpec object
wl.range	the wavelength range to be plotted. Either a numeric vector or a list of vectors with different wavelength ranges to be plotted separately. The values can be either wavelengths or wavelength indices (according to wl.index).
wl.index	if TRUE, wl.range is considered to give column indices into the spectra matrix. Defaults to specifying wavelength values rather than indices.
wl.reverse	if TRUE, the wavelength axis is plotted backwards.
spc.nmax	maximal number of spectra to be plotted (to avoid accidentally plotting of large numbers of spectra).
func	a function to apply to each wavelength in order to calculate summary spectra such as mean, min, max, etc.
func.args	list with furter arguments for func
stacked	if not NULL, a "stacked" plot is produced, see the example. stacked may be TRUE to stack single spectra. A numeric or factor is interpreted as giving the grouping, character is interpreted as the name of the extra data column that holds the groups.
stacked.args	a list with further arguments to stacked.offsets.
add	if TRUE, the output is added to the existing plot
bty	see par
plot.args	list with further arguments to plot
col	see par. col might be a vector giving individual colors for the spectra.
lines.args	list with further arguments to lines. lines.args$type defaults to "l".
xoffset	vector with abscissa offsets for each of the wl.ranges. If it has one element less than there are wl.ranges, 0 is padded at the beginning. The values are interpreted as the distance along the wavelength axis that the following parts of the spectra are shifted towards the origin. E.g. if wl.range = list(600 ~ 1800, 2800 ~ 3200), xoffset = 750 would result in a reasonable plot. See also the examples.
yoffset	ordinate offset values for the spectra. May be offsets to stack the spectra (stacked.offsets). Either one for all spectra, one per spectrum or one per group in stacked.
nxticks	hint how many tick marks the abscissa should have.
axis.args	list with further arguments for axis. axis.args$x should contain arguments for plotting the abscissa, axis.args$y those for the ordinate (again as lists).

break.args	list with arguments for axis.break.
title.args	list with further arguments to title. title.args may contain two lists, $x, and $y to set parameters individually for each axis.
fill	if not NULL, the area between the specified spectra is filled with color col. The grouping can be given as factor or numeric, or as a character with the name of the extra data column to use. If a group contains more than 2 spectra, the first and the last are used. If TRUE spectra n and nrow (spc) - n build a group.
fill.col	character vector with fill color. Defaults to brightened colors from col.
border	character vector with border color. You will need to set the line color col to NA in order see the effect.
polygon.args	list with further arguments to polygon which draws the filled areas.
zeroline	NA or a list with arguments abline, used to plot line (s) marking I = 0. NA suppresses plotting of the line. The line is by default turned off if yoffset is not 0.
debuglevel	if > 0, additional debug output is produced, see options for details
x	a hyperSpec object
min.zero	if TRUE, the lesser of zero and the minimum intensity of the spectrum is used as minimum.
add.factor, add.sum	proportion and absolute amount of space that should be added.
.spc	for internal use. If given, the ranges are evaluated on .spc. However, this may change in future.

Details

New plots are created by plot, but the abscissa and ordinate are drawn separately by axis. Also, title is called explicitly to set up titles and axis labels. This allows fine-grained customization of the plots.

If package plotrix is available, its function axis.break is used to produce break marks for cut wavelength axes.

Empty levels of the stacking factor are dropped (as no stacking offset can be calculated in that case.)

Value

plotspc invisibly returns a list with

x	the abscissa coordinates of the plotted spectral data points
y	a matrix the ordinate coordinates of the plotted spectral data points
wavelengths	the wavelengths of the plotted spectral data points

This can be used together with spc.identify.

a list containing

offsets	numeric with the yoffset for each group in stacked
groups	numeric with the group number for each spectrum
levels	if stacked is a factor, the levels of the groups

Author(s)

C. Beleites

C. Beleites

See Also

plot, axis, title, lines, polygon, par for the description of the respective arguments.

axis.break for cut marks

See plot for some predefined spectra plots such as mean spectrum +/- one standard deviation and the like.

identify and locator about interaction with plots.

plotspc

Examples

```
plotspc (flu)

## artificial example to show wavelength axis cutting
plotspc (chondro [sample (nrow (chondro), 50)],
         wl.range = list (600 ~ 650, 1000 ~ 1100, 1600 ~ 1700),
         xoffset = c (0, 300, 450))

plotspc (chondro [sample (nrow (chondro), 50)],
         wl.range = list (600 ~ 650, 1000 ~ 1100, 1600 ~ 1700),
         xoffset = c (300, 450))

## some journals publish Raman spectra backwards
plotspc (chondro [sample (nrow (chondro), 50)], wl.reverse = TRUE)

plotspc (laser[(0:4)*20+1,,], stacked = TRUE)

plotspc (laser, func = mean_pm_sd,
         col = c(NA, "red", "black"), lines.args = list (lwd = 2),
         fill = c (1, NA, 1),
         fill.col = "yellow", border = "blue",
         polygon.args = list (lty = 2, lwd = 4),
         title.args = list (xlab = expression (lambda[emission] / nm),
                            y = list(line = 3.4),
                            col.lab = "darkgreen"),
         axis.args = list (x = list (col = "magenta"), y = list (las = 1))
        )

mean.pm.sd <- aggregate (chondro, chondro$clusters, mean_pm_sd)
```

```
plot (mean.pm.sd, col = matlab.palette (3), fill = ".aggregate", stacked = ".aggregate")


mean.pm.sd <- aggregate (chondro, chondro$clusters, mean_pm_sd)

offset <- stacked.offsets (mean.pm.sd, ".aggregate")
plot (mean.pm.sd, fill.col = matlab.palette (3), fill = ".aggregate",
      stacked = ".aggregate")

plot (aggregate (chondro, chondro$clusters, mean), yoffset = offset$offsets,
      lines.args = list (lty = 2, lwd = 2), add = TRUE)

barb <- do.call (collapse, barbiturates [1:3])
plot (barb, lines.args = list (type = "h"), stacked = TRUE,
      stacked.args = list (add.factor = .2))
```

`qplotc` *Spectra plotting with ggplot2*

Description

Spectra plotting with ggplot2

Usage

```
qplotc(
  object,
  mapping = aes_string(x = "c", y = "spc"),
  ...,
  func = NULL,
  func.args = list(),
  map.pointonly = FALSE
)
```

Arguments

`object`	hyperSpec object
`mapping`	see `geom_point`
`...`	handed to `geom_point`
`func`	function to summarize the wavelengths, if `NULL`, only the first wavelength is used
`func.args`	arguments to `func`
`map.pointonly`	if `TRUE`, `mapping` will be handed to `geom_point` instead of `ggplot`.

Details

These functions are still experimental and may change substantially in future.

Value

a ggplot object

Author(s)

Claudia Beleites

See Also

plotc

ggplotgeom_point

Examples

```
qplotc (flu)
qplotc (flu) + geom_smooth (method = "lm")
```

---

qplotmap *Spectra plotting with ggplot2*

Description

Spectra plotting with ggplot2

Usage

```
qplotmap(
  object,
  mapping = aes_string(x = "x", y = "y", fill = "spc"),
  ...,
  func = mean,
  func.args = list(),
  map.tileonly = FALSE
)
```

Arguments

object	hyperSpec object
mapping	see geom_tile
...	handed to geom_tile
func	function to summarize the wavelengths
func.args	arguments to func
map.tileonly	if TRUE, mapping will be handed to geom_tile instead of ggplot.

Details

These functions are still experimental and may change substantially in future.

Note that qplotmap will currently produce the wrong scales if x or y are discrete.

Value

a ggplot object

Author(s)

Claudia Beleites

See Also

plotmap

ggplotgeom_tile

Examples

```
qplotmap (chondro)
qplotmap (chondro) + scale_fill_gradientn (colours = alois.palette ())
```

---

qplotmixmap *qplotmap with colour mixing for multivariate overlay*

Description

map plot with colour overlay.

Usage

```
qplotmixmap(object, ...)
```

Arguments

object	hyperSpec object
...	handed over to qmixlegend and qmixtile

Value

invisible list with ggplot2 objects map and legend

Author(s)

Claudia Beleites

See Also

qmixtile

Examples

```
chondro <- chondro - spc.fit.poly.below (chondro)
chondro <- sweep (chondro, 1, apply (chondro, 1, mean), "/")
chondro <- sweep (chondro, 2, apply (chondro, 2, quantile, 0.05), "-")

qplotmixmap (chondro [,,c (940, 1002, 1440)],
             purecol = c (colg = "red", Phe = "green", Lipid = "blue"))
```

---

qplotspc *Spectra plotting with ggplot2*

Description

Spectra plotting with ggplot2

Usage

```
qplotspc(
  x,
  wl.range = TRUE,
  ...,
  mapping = aes_string(x = ".wavelength", y = "spc", group = ".rownames"),
  spc.nmax = hy.getOption("ggplot.spc.nmax"),
  map.lineonly = FALSE,
  debuglevel = hy.getOption("debuglevel")
)
```

Arguments

x	hyperSpec object
wl.range	wavelength ranges to plot
...	handed to geom_line
mapping	see geom_line
spc.nmax	maximum number of spectra to plot
map.lineonly	if TRUE, mapping will be handed to geom_line instead of ggplot.
debuglevel	if > 0, additional debug output is produced

Details

These functions are still experimental and may change substantially in future.

Value

a ggplot object

Author(s)

Claudia Beleites

See Also

plotspc

ggplotgeom_line

Examples

```
qplotspc (chondro)

qplotspc (paracetamol, c (2800 ~ max, min ~ 1800)) + scale_x_reverse (breaks = seq (0, 3200, 400))

qplotspc (aggregate (chondro, chondro$clusters, mean),
          mapping = aes (x = .wavelength, y = spc, colour = clusters)) +
  facet_grid (clusters ~ .)

qplotspc (aggregate (chondro, chondro$clusters, mean_pm_sd),
        mapping = aes (x = .wavelength, y = spc, colour = clusters, group = .rownames)) +
  facet_grid (clusters ~ .)
```

---

rbind.fill.matrix *Bind matrices by row, and fill missing columns with NA*

Description

The matrices are bound together using their column names or the column indices (in that order of precedence.) Numeric columns may be converted to character beforehand, e.g. using format. If a matrix doesn't have colnames, the column number is used (via make.names(unique = TRUE)).

This is an enhancement to rbind which adds in columns that are not present in all inputs, accepts a list of data frames, and operates substantially faster

Usage

```
## S3 method for class 'matrix'
rbind.fill(...)

## S3 method for class 'fill'
rbind(...)
```

Arguments

...	data frames/matrices to row bind together

Details

Note that this means that a column with name `"X1"` is merged with the first column of a matrix without name and so on.

Vectors are converted to 1-column matrices prior to rbind.

Matrices of factors are not supported. (They are anyways quite inconvenient.) You may convert them first to either numeric or character matrices. If a character matrix is merged with a numeric, the result will be character.

Row names are ignored.

The return matrix will always have column names.

Value

a matrix

Author(s)

C. Beleites

See Also

`rbind`, `cbind`, `plyr::rbind.fill()`

Examples

```
A <- matrix (1:4, 2)
B <- matrix (6:11, 2)
A
B
hyperSpec:::rbind.fill.matrix (A, B)

colnames (A) <- c (3, 1)
A
hyperSpec:::rbind.fill.matrix (A, B)

hyperSpec:::rbind.fill.matrix (A, 99)

#' rbind.fill(mtcars[c("mpg", "wt")], mtcars[c("wt", "cyl")])
```

read.asc.PerkinElmer *File import filter PerkinElmer ASCII spectra*

Description

Imports a single spectrum in PerkinElmer's ASCII format. This function is experimental.

Usage

```
read.asc.PerkinElmer(file = stop("filename or connection needed"), ...)
```

Arguments

file	filename (or connection)
...	further parameters are handed to read.txt.long

Value

hyperSpec object

read.cytomat *Import for Cytospec mat files*

Description

These functions allow to import .mat (Matlab V5) files written by Cytospec.

Usage

```
read.cytomat(...)

read.mat.Cytospec(file, keys2data = FALSE, blocks = TRUE)
```

Arguments

...	read.cytomat for now hands all arguments to read.mat.Cytospec for backwards compatibility.
file	The complete file name (or a connection to) the .mat file.
keys2data	specifies which elements of the Info should be transferred into the extra data
blocks	which blocks should be read? TRUE reads all blocks.

Details

read.cytomat has been renamed to read.mat.Cytospec and is now deprecated. Use read.mat.Cytospec instead.

Value

hyperSpec object if the file contains a single spectra block, otherwise a list with one hyperSpec object for each block.

Note

This function is an ad-hoc implementation and subject to changes.

Author(s)

C. Beleites

See Also

`R.matlab::readMat`

`read.ENVI` *Import of ENVI data as hyperSpec object*

Description

This function allows ENVI data import as `hyperSpec` object.

`read.ENVI.Nicolet` should be a good starting point for writing custom wrappers for `read.ENVI` that take into account your manufacturer's special entries in the header file.

Usage

```
read.ENVI(
  file = stop("read.ENVI: file name needed"),
  headerfile = NULL,
  header = list(),
  keys.hdr2data = FALSE,
  x = 0:1,
  y = x,
  wavelength = NULL,
  label = list(),
  block.lines.skip = 0,
  block.lines.size = NULL,
  ...,
  pull.header.lines = TRUE
)

read.ENVI.HySpex(
  file = stop("read.ENVI.HySpex: file name needed"),
  headerfile = NULL,
  header = list(),
  keys.hdr2data = NULL,
```

```
  ...
)

read.ENVI.Nicolet(
  file = stop("read.ENVI: file name needed"),
  headerfile = NULL,
  header = list(),
  ...,
  x = NA,
  y = NA,
  nicolet.correction = FALSE
)
```

Arguments

`file`	complete name of the binary file
`headerfile`	name of the ASCII header file. If `NULL`, the name of the header file is guessed by looking for a second file with the same basename as `file` but `hdr` or `HDR` suffix.
`header`	list with header information, see details. Overwrites information extracted from the header file.
`keys.hdr2data`	determines which fields of the header file should be put into the extra data. Defaults to none. To specify certain entries, give character vectors containing the lowercase names of the header file entries.
`x, y`	vectors of form c(offset, step size) for the position vectors, see details.
`wavelength, label`	lists that overwrite the respective information from the ENVI header file. These data is then handed to `initialize`
`block.lines.skip, block.lines.size`	BIL and BIP ENVI files may be read in blocks of lines: skip the first `block.lines.skip` lines, then read a block of `block.lines.size` lines. If `block.lines.NULL`, the whole file is read. Blocks are silently truncated at the end of the file (more precisely: to `header$lines`).
`...`	currently unused by `read.ENVI`, `read.ENVI.Nicolet` hands those arguements over to `read.ENVI`
`pull.header.lines`	(internal) flag whether multi-line header entries grouped by curly braces should be pulled into one line each.
`nicolet.correction`	see details

Details

ENVI data usually consists of two files, an ASCII header and a binary data file. The header contains all information necessary for correctly reading the binary file.

I experienced missing header files (or rather: header files without any contents) produced by Bruker Opus' ENVI export.

In this case the necessary information can be given as a list in parameter `header` instead:

header$	values	meaning
samples	integer	no of columns / spectra in x direction
lines	integer	no of lines / spectra in y direction
bands	integer	no of wavelengths / data points per spectrum
'data type'		format of the binary file
	1	1 byte unsigned integer
	2	2 byte signed integer
	3	4 byte signed integer
	4	4 byte float
	5	8 byte double
	9	16 (2 x 8) byte complex double
	12	2 byte unsigned integer
'header offset'	integer	number of bytes to skip before binary data starts
interleave		directions of the data cube
	"BSQ"	band sequential (indexing: [sample, line, band])
	"BIL"	band interleave by line (indexing: [sample, line, band])
	"BIP"	band interleave by pixel (indexing: [band, line, sample])
'byte order'	0 or "little"	little endian
	1 or "big"	big endian
	"swap"	swap byte order

Some more information that is not provided by the ENVI files may be given:

Wavelength axis and axis labels in the respective parameters. For more information, see `initialize`.

The spatial information is by default a sequence from 0 to `header$samples -1` and `header$lines -1`, respectively. `x` and `y` give offset of the first spectrum and step size.

Thus, the object's `$x` colum is: `(0 : header$samples -1) * x [2] + x [1]`. The `$y` colum is calculated analogously.

Nicolet uses some more keywords in their header file. They are interpreted as follows:

description	giving the position of the first spectrum
z plot titles	wavelength and intensity axis units, comma separated
pixel size	interpreted as x and y step size (specify `x = NA` and `y = NA`)

These parameters can be overwritten by giving a list with the respective elements in parameter `header`.

The values in header line description seem to be microns while the pixel size seems to be in microns. If `nicolet.correction` is true, the pixel size values (i.e. the step sizes) are multiplied by 1000.

Value

a `hyperSpec` object

Functions

- `read.ENVI.HySpex`:
- `read.ENVI.Nicolet`:

Author(s)

C. Beleites, testing for the Nicolet files C. Dicko

References

This function was adapted from `caTools::read.ENVI()`:

Jarek Tuszynski (2008). caTools: Tools: moving window statistics, GIF, Base64, ROC AUC, etc.. R package version 1.9.

See Also

`caTools::read.ENVI()`

`textio`

`read.ini` *Read INI files*

Description

`read.ini` reads ini files of the form

Usage

```
read.ini(
  con = stop("Connection con needed."),
  skip = NULL,
  encoding = "unknown"
)
```

Arguments

`con`	connection or file name
`skip`	number of lines to skip before first `[section]` starts
`encoding`	see `readLines`

Details

[section] key = value

into a list.

`read.ini` sanitizes the element names and tries to convert scalars and comma separated numeric vectors to numeric.

Value

a list with one element per section in the .ini file, each containing a list with elements for the key-value-pairs.

Author(s)

C. Beleites

`read.jdx` *JCAMP-DX Import for Shimadzu Library Spectra*

Description

this is a first rough import function for JCAMP-DX spectra.

Usage

```
read.jdx(
  filename = stop("filename is needed"),
  encoding = "",
  header = list(),
  keys.hdr2data = FALSE,
  ...,
  NA.symbols = c("NA", "N/A", "N.A."),
  collapse.multi = TRUE,
  wl.tolerance = hy.getOption("wl.tolerance"),
  collapse.equal = TRUE
)
```

Arguments

`filename`	file name and path of the .jdx file
`encoding`	encoding of the JCAMP-DX file (used by `base::readLines()`)
`header`	list with manually set header values
`keys.hdr2data`	index vector indicating which header entries should be tranfered into the extra data. Usually a character vector of labels (lowercase, without and dashes, blanks, underscores). If `TRUE`, all header entries are read.
`...`	further parameters handed to the data import function, e.g.

parameter	meaning	default
`xtol`	tolerance for checking calculated x values against checkpoints at beginning of line	XFACTOR
`ytol`	tolerance for checking Y values against MINY and MAXY	YFACTOR

`NA.symbols`	character vector of text values that should be converted to `NA`
`collapse.multi`	should hyperSpec objects from multispectra files be collapsed into one hyperSpec object (if `FALSE`, a list of hyperSpec objects is returned).
`wl.tolerance, collapse.equal`	see collapse

Details

So far, AFFN and PAC formats are supported for simple XYDATA, DATA TABLEs and PEAK TABLEs.

NTUPLES / PAGES are not (yet) supported.

DIF, DUF, DIFDUP and SQZ data formats are not (yet) supported.

Value

hyperSpec object

Note

JCAMP-DX support is incomplete and the functions may change without notice. See `vignette("fileio")` and the details section.

Author(s)

C. Beleites with contributions by Bryan Hanson

`read.spc` *Import for Thermo Galactic's spc file format These functions allow to import Thermo Galactic/Grams .spc files.*

Description

Import for Thermo Galactic's spc file format These functions allow to import Thermo Galactic/Grams .spc files.

Usage

```
read.spc(
  filename,
  keys.hdr2data = FALSE,
  keys.log2data = FALSE,
  log.txt = TRUE,
  log.bin = FALSE,
  log.disk = FALSE,
  hdr = list(),
  no.object = FALSE
)
```

Arguments

`filename`	The complete file name of the .spc file.
`keys.hdr2data, keys.log2data`	character vectors with the names of parameters in the .spc file's log block (log2xxx) or header (hdr2xxx) that should go into the extra data (yyy2data) of the returned hyperSpec object. All header fields specified in the .spc file format specification (see below) are imported and can be referred to by their de-capitalized names.
`log.txt`	Should the text part of the .spc file's log block be read?
`log.bin, log.disk`	Should the normal and on-disk binary parts of the .spc file's log block be read? If so, they will be put as raw vectors into the hyperSpec object's log.
`hdr`	A list with fileheader fields that overwrite the settings of actual file's header. Use with care, and look into the source code for detailed insight on the elements of this list.
`no.object`	If `TRUE`, a list with wavelengths, spectra, labels, log and data are returned instead of a hyperSpec object. This parameter will likely be subject to change in future - use with care.

Value

If the file contains multiple spectra with individual wavelength axes, `read.spc` returns a list of hyperSpec objects. Otherwise the result is a hyperSpec object.

`read.spc.KaiserMap` returns a hyperSpec object with data columns x, y, and z containing the stage position as recorded in the .spc files' log.

Note

Only a restricted set of test files was available for development. Particularly, the w-planes feature could not be tested.

If you have .spc files that cannot be read with these function, don't hesitate to contact the package maintainer with your code patch or asking advice.

Author(s)

C. Beleites

References

Source development kit and file format specification of .spc files.

See Also

`textio`

Examples

```
## get the sample .spc files from ftirsearch.com (see above)
## Not run:
# single spectrum
spc <- read.spc ("BENZENE.SPC")
plot (spc)

# multi-spectra .spc file with common wavelength axis
spc <- read.spc ('IG_MULTI.SPC')
spc

# multi-spectra .spc file with individual wavelength axes
spc <- read.spc ("BARBITUATES.SPC")
plot (spc [[1]], lines.args = list (type = "h"))

## End(Not run)
```

`read.spc.Kaiser` *read Kaiser .spc files*

Description

Import functions for Kaiser Optical Systems .spc files

Usage

```
read.spc.Kaiser(files, ..., glob = TRUE)

read.spc.KaiserMap(files, keys.log2data = NULL, ...)

read.spc.KaiserLowHigh(
  files = stop("file names needed"),
  type = c("single", "map"),
  ...,
  glob = TRUE
)
```

Arguments

`files`	If `glob = TRUE`, `filename` can contain wildcards. Thus all files matching the name pattern in `filename` can be specified.
`glob`	If `TRUE` the filename is interpreted as a wildcard containing file name pattern and expanded to all matching file names.
`keys.log2data, ...`	All further arguments are handed over directly to `read.spc`.
`type`	what kind of measurement was done? If `"map"`, `read.spc.KaiserMap` is used instead of `read.spc.Kaiser`.

Details

`read.spc.Kaiser` imports sets of .spc files written by Kaiser Optical Systems' Hologram software. It may also serve as an example how to write wrapper functions for `read.spc` to conveniently import specialized sets of .spc files.

Value

hyperSpec

Examples

```
## for examples, please see `vignette ("fileio", package = "hyperSpec")`.
```

`read.spe` *Import WinSpec SPE file*

Description

Import function for WinSpec SPE files (file version up to 3.0). The calibration data (polynome and calibration data pairs) for x-axis are automatically read and applied to the spectra. Note that the y-calibration data structure is not extracted from the file since it is not saved there by WinSpec and is always empty.

Usage

```
read.spe(
  filename,
  xaxis = "file",
  acc2avg = F,
  cts_sec = F,
  keys.hdr2data = c("exposure_sec", "LaserWavelen", "accumulCount", "numFrames",
    "darkSubtracted")
)

.read.spe.header(filename)

spe.showcalpoints(filename, xaxis = "file", acc2avg = F, cts_sec = F)
```

Arguments

`filename`	Name of the SPE file to read data from
`xaxis`	Units of x-axis, e.g. *"file"*, *"px"*, *"nm"*, *"energy"*, *"raman"*, ... `read.spe` function automatically checks if the x-calibration data are available and uses them (if possible) to reconstruct the xaxis in the selected units.

acc2avg	whether to divide the actual data set by the number of accumulations, thus transforming *accumulated* spectra to *averaged* spectra. WinSpec does not do this automatically, so the spectral intensity is always proportional to the number of accumulations. The flag `@data$averaged` is automatically set to `TRUE`.
cts_sec	whether to divide the actual data set by the exposure time, thus going to count per second unit.
keys.hdr2data	Which metadata from the file header should be saved to the `Data` slot of a newly created hyperSpec object

Value

hyperSpec object

hdr list with `key=value` pairs

Functions

- `.read.spe.header`: Read only header of a WinSpec SPE file (version 2.5)
- `spe.showcalpoints`: Plot the WinSpec SPE file (version 2.5) and show the calibration points stored inside of it (x-axis calibration)

Author(s)

R. Kiselev, C. Beleites

---

read.txt.Horiba *Import Horiba Labspec exported ASCII files*

Description

Read ASCII (.txt) files exported by Horiba's Labspec software (LabRAM spectrometers)

Usage

```
read.txt.Horiba(
  file,
  cols = c(spc = "I / a.u.", .wavelength = expression(Delta * tilde(nu)/cm^-1)),
  header = TRUE,
  sep = "\t",
  row.names = NULL,
  check.names = FALSE,
  ...
)

read.txt.Horiba.xy(file, ...)

read.txt.Horiba.t(
```

```
  file,
  header = TRUE,
  sep = "\t",
  row.names = NULL,
  check.names = FALSE,
  ...
)
```

Arguments

file	connection (file name and path) to the .txt file
cols, header, sep, row.names, check.names, ...	further parameters are handed over to read.txt.wide

Details

read.txt.Horiba.xy reads maps, i.e. .txt files where the first two columns give x and y coordinates.

Value

hyperSpec object

Author(s)

C. Beleites

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read.txt.Shimadzu *Reads Shimadzu GCxGC-qMS - Spectra Files (.txt) as exported by Shimadzu Chrome Solution (v. 2.72) Mass Spectrometer: Shimadzu GCMS-QP 2010 Ultra (www.shimadzu.com)*

Description

Reads Shimadzu GCxGC-qMS - Spectra Files (.txt) as exported by Shimadzu Chrome Solution (v. 2.72) Mass Spectrometer: Shimadzu GCMS-QP 2010 Ultra (www.shimadzu.com)

Usage

```
read.txt.Shimadzu(filename, encoding = "", quiet = TRUE)
```

Arguments

filename	file name and path of the .txt file
encoding	encoding of the txt file (used by readLines)
quiet	suppress printing of progress

Value

list of spectra tables

Note

This is a first rough import function and the functions may change without notice.

Author(s)

Bjoern Egert

`read.txt.wide` *Import/export of hyperSpec objects to/from ASCII files A detailed discussion of hyperSpec's file import and export capabilities is given in vignette "fileio".*

Description

Besides `save` and `load`, two general ways to import and export data into `hyperSpec` objects exist.

Firstly, hyperSpec objects can be imported and exported as ASCII files.

Usage

```
read.txt.wide(
  file = stop("file is required"),
  cols = list(spc = "I / a.u.", .wavelength = expression(lambda/nm)),
  sep = "\t",
  row.names = NULL,
  check.names = FALSE,
  ...
)

read.txt.long(
  file = stop("file is required"),
  cols = list(.wavelength = expression(lambda/nm), spc = "I / a.u."),
  header = TRUE,
  ...
)

write.txt.long(
  object,
  file = "",
  order = c(".rownames", ".wavelength"),
  na.last = TRUE,
  decreasing = FALSE,
  quote = FALSE,
```

```
  sep = "\t",
  row.names = FALSE,
  cols = NULL,
  col.names = TRUE,
  col.labels = FALSE,
  append = FALSE,
  ...
)

write.txt.wide(
  object,
  file = "",
  cols = NULL,
  quote = FALSE,
  sep = "\t",
  row.names = FALSE,
  col.names = TRUE,
  header.lines = 1,
  col.labels = if (header.lines == 1) FALSE else TRUE,
  append = FALSE,
  ...
)
```

Arguments

file	filename or connection
cols	the column names specifying the column order. For data import, a list with elements colname = label; for export a character vector with the colnames. Use wavelength to specify the wavelengths.
check.names	handed to read.table. Make sure this is FALSE, if the column names of the spectra are the wavelength values.
...	arguments handed to read.table and write.table, respectively.
header	the file has (shall have) a header line
object	the hyperSpec object
order	which columns should be ordered? order is used as index vector into a data.frame with columns given by cols.
na.last	handed to order by write.txt.long.
decreasing	logical vector giving the sort order
quote, sep, col.names, row.names	have their usual meaning (see read.table and write.table), but different default values. For file import, row.names should usually be NULL so that the first column becomes a extra data column (as opposed to row names of the extra data).
col.labels	Should the column labels be used rather than the colnames?
append	Should the output be appended to an existing file?
header.lines	Toggle one or two line header (wavelengths in the second header line) for write.txt.wide

Details

Firstly, hyperSpec objects can be imported and exported as ASCII files.

A second option is using the package R.matlab which provides the functions readMat and writeMat.

hyperSpec comes with a number of pre-defined functions to import manufacturer specific file formats. For details, see vignette("fileio").

read.spc imports Thermo Galactic's .spc file format, and ENVI files may be read using read.ENVI.

These functions are very flexible and provide lots of arguments.

If you use them to read or write manufacturer specific ASCII formats, please consider writing a wrapper function and contributing this function to **hyperSpec**. An example is in the "flu" vignette (see vignette("flu",package = "hyperSpec").

Note that R accepts many packed formats for ASCII files, see connections. For .zip files, see unzip.

For further information, see the examples below, vignette("fileio") and the documentation of R.matlab.

A second option is using the package R.matlab which provides the functions readMat and writeMat.

hyperSpec comes with a number of pre-defined functions to import manufacturer specific file formats. For details, see vignette("file-io").

read.spc imports Thermo Galactic's .spc file format, and ENVI files may be read using read.ENVI.

These functions are very flexible and provide lots of arguments.

If you use them to read or write manufacturer specific ASCII formats, please consider writing a wrapper function and contributing this function to **hyperSpec**. An example is in the "flu" vignette (see vignette("flu",package = "hyperSpec").

Note that R accepts many packed formats for ASCII files, see connections. For .zip files, see unzip.

For further information, see the examples below and the documentation of R.matlab.

Author(s)

C. Beleites

See Also

vignette("fileio") and http://hyperspec.r-forge.r-project.org/blob/fileio.pdf, respectively

read.table and write.table

R.matlab for .mat files

read.ENVI for ENVI data

read.spc for .spc files

Manufacturer specific file formats: read.txt.Renishaw

Examples

```
## Not run: vignette  ("file-io")

## export & import matlab files
if (require (R.matlab)) {
   # export to matlab file
   writeMat (paste0 (tempdir(), "/test.mat"),
             x = flu[[]], wavelength = flu@wavelength,
             label = lapply (flu@label, as.character))

   # reading a matlab file
   data <- readMat (paste0 (tempdir(), "/test.mat"))
   print (data)
   mat <- new ("hyperSpec", spc = data$x,
               wavelength = as.numeric(data$wavelength),
               label = data$label[,,1])
}

## ascii export & import


write.txt.long (flu,
    file = paste0 (tempdir(), "/flu.txt"),
    cols = c(".wavelength", "spc", "c"),
order = c("c", ".wavelength"),
decreasing = c(FALSE, TRUE))

read.txt.long (file = paste0 (tempdir(), "/flu.txt"),
      cols = list (.wavelength = expression (lambda / nm),
      spc = "I / a.u", c = expression ("/" (c, (mg/l)))))

write.txt.wide (flu,  file = paste0 (tempdir(), "/flu.txt"),
    cols = c("c", "spc"),
col.labels = TRUE, header.lines = 2, row.names = TRUE)

write.txt.wide (flu,  file = paste0 (tempdir(), "/flu.txt"),
                col.labels = FALSE, row.names = FALSE)

read.txt.wide (file = paste0 (tempdir(), "/flu.txt"),
    # give columns in same order as they are in the file
    cols = list (spc = "I / a.u",
                 c = expression ("/"("c", "mg/l")),
                 filename = "filename",
                 # plus wavelength label last
                 .wavelength = "lambda / nm"),
header = TRUE)
```

rmmvnorm *Multivariate normal random numbers*

Description

Interface functions to use rmvnorm for hyperSpec-class objects.

Usage

```
rmmvnorm(n, mean, sigma)

## S4 method for signature 'numeric,hyperSpec,matrix'
rmmvnorm(n, mean, sigma)

## S4 method for signature 'numeric,hyperSpec,array'
rmmvnorm(n, mean, sigma)

## S4 method for signature 'numeric,matrix,matrix'
rmmvnorm(n, mean, sigma)

## S4 method for signature 'numeric,matrix,array'
rmmvnorm(n, mean, sigma)
```

Arguments

n	vector giving the numer of cases to generate for each group
mean	matrix with mean cases in rows
sigma	common covariance matrix or array (ncol (mean) x ncol (mean) x nrow (mean)) with individual covariance matrices for the groups.

Details

The mvtnorm method for hyperSpec objects supports producing multivariate normal data for groups with different mean but common covariance matrix, see the examples.

See Also

rmvnorm

cov and pooled.cov about calculating covariance of hyperSpec objects.

Examples

```
## multiple groups, common covariance matrix

if (require ("mvtnorm")){
   pcov <- pooled.cov (chondro, chondro$clusters)
   rnd <- rmmvnorm (rep (10, 3), mean = pcov$mean, sigma = pcov$COV)
```

```
   plot (rnd, col = rnd$.group)
}
```

`sample,hyperSpec-method`

Random Samples and Permutations Take a sample of the specified size from the elements of x with or without replacement.

Description

Random Samples and Permutations Take a sample of the specified size from the elements of x with or without replacement.

`isample` returns an vector of indices, `sample` returns the corresponding hyperSpec object.

Usage

```
## S4 method for signature 'hyperSpec'
sample(x, size, replace = FALSE, prob = NULL)

isample(x, size = nrow(x), replace = FALSE, prob = NULL)

## S4 method for signature 'data.frame'
sample(x, size, replace = FALSE, prob = NULL, drop = FALSE)

## S4 method for signature 'matrix'
sample(x, size, replace = FALSE, prob = NULL, drop = FALSE)
```

Arguments

`x`	The hyperSpec object, data.frame or matrix to sample fromto sample from
`size`	positive integer giving the number of spectra (rows) to choose.
`replace`	Should sampling be with replacement?
`prob`	A vector of probability weights for obtaining the elements of the vector being sampled.
`drop`	see `drop`: by default, do not drop dimensions of the result

Value

a hyperSpec object, data.frame or matrix with `size` rows for `sample`, and an integer vector for `isample` that is suitable for indexing (into the spectra) of x.

vector with indices suitable for row-indexing x

Author(s)

C. Beleites

See Also

sample

Examples

```
sample (flu, 3)

plot (flu, col = "darkgray")
plot (sample (flu, 3), col = "red", add = TRUE)

plot (flu, col = "darkgray")
plot (sample (flu, 3, replace = TRUE), col = "#0000FF80", add = TRUE,
      lines.args = list (lwd = 2));

isample (flu, 3)
isample (flu, 3, replace = TRUE)
isample (flu, 8, replace = TRUE)
sample (cars, 2)
sample (matrix (1:24, 6), 2)
```

---

scale,hyperSpec-method

Center and scale hyperSpec object

Description

link[base]{scale}s the spectra matrix. scale (x,scale = FALSE) centers the data.

Usage

```
## S4 method for signature 'hyperSpec'
scale(x, center = TRUE, scale = TRUE)
```

Arguments

x	the hyperSpec object
center	if TRUE, the data is centered to colMeans (x), FALSE suppresses centering. Alternatively, an object that can be converted to numeric of length nwl (x) by as.matrix (e.g. hyperSpec object containing 1 spectrum) can specify the center spectrum.
scale	if TRUE, the data is scaled to have unit variance at each wavelength, FALSE suppresses scaling. Alternatively, an object that can be converted to numeric of length nwl (x) by as.matrix (e.g. hyperSpec object containing 1 spectrum) can specify the center spectrum.

Details

Package scale provides a fast alternative for base::scale

Value

the centered & scaled hyperSpec object

Author(s)

C. Beleites

See Also

scale

package scale.

Examples

```
## mean center & variance scale
tmp <- scale (chondro)
plot (tmp, "spcmeansd")
plot (sample (tmp, 5), add = TRUE, col = 2)

## mean center only
tmp <- scale (chondro, scale = FALSE)
plot (tmp, "spcmeansd")
plot (sample (tmp, 5), add = TRUE, col = 2)

## custom center
tmp <- sweep (chondro, 1, mean, `/`)
plot (tmp, "spcmeansd")
tmp <- scale (tmp, center = quantile (tmp, .05), scale = FALSE)
```

---

seq.hyperSpec *Sequence generation along spectra or wavelengths This function generates sequences along the spectra (rows) or wavelengths of hyperSpec objects.*

Description

Note that wl2i generates sequences of indices along the wavelength axis.

Usage

```
## S3 method for class 'hyperSpec'
seq(x, from = 1, to = nrow(x), ..., index = FALSE)
```

Arguments

x	the hyperSpec object
from, to	arguments handed to seq.int
...	arguments for seq, namely by, length.out
index	should a vector with indices be returned rather than a hyperSpec object?

Details

seq had to be implemented as S3 method as the generic has only ... arguments (on which no dispatch with differing types is possible).

seq_along is not generic, but returns a sequence of the length of the object. As hyperSpec provides a Method length, it can be used. The result is a sequence of indices for the spectra.

Value

a numeric or hyperSpec object, depending on index.

Author(s)

C. Beleites

See Also

wl2i to construct sequences of wavelength indices.

seq

Examples

```
seq (flu, index = TRUE)
seq_along (flu)
seq (flu, length.out = 3, index = TRUE) # return value is numeric, not integer!
seq (flu, by = 2, index = TRUE)      # return value is numeric, not integer!

plot (flu, col = "darkgray")
plot (seq (flu, by = 2), add = TRUE, col= "red")
plot (seq (flu, length.out = 2), add = TRUE, col= "blue")
```

spc.bin *Wavelength Binning In order to reduce the spectral resolution and thus gain signal to noise ratio or to reduce the dimensionality of the spectral data set, the spectral resolution can be reduced.*

Description

The mean of every by data points in the spectra is calculated.

Usage

```
spc.bin(spc, by = stop("reduction factor needed"), na.rm = TRUE, ...)
```

Arguments

spc	the hyperSpec object
by	reduction factor
na.rm	decides about the treatment of NAs: if FALSE or 0, the binning is done using na.rm = FALSE if TRUE or 1, the binning is done using na.rm = TRUE if 2, the binning is done using na.rm = FALSE, and resulting NAs are corrected with mean(...{},na.rm = TRUE).
...	ignored

Details

Using na.rm = TRUE always takes about twice as long as na.rm = FALSE.

If the spectra matrix does not contain too many NAs, na.rm = 2 is faster than na.rm = TRUE.

Value

A hyperSpec object with ceiling (nwl (spc) / by) data points per spectrum.

Author(s)

C. Beleites

Examples

```
spc <- spc.bin (flu, 5)

plot (flu[1,,425:475])
plot (spc[1,,425:475], add = TRUE, col = "blue")

nwl (flu)
nwl (spc)
```

spc.fit.poly *Polynomial Baseline Fitting These functions fit polynomal baselines.*

Description

Both functions fit polynomials to be used as baselines. If `apply.to` is `NULL`, a `hyperSpec` object with the polynomial coefficients is returned, otherwise the polynomials are evaluated on the spectral range of `apply.to`.

Usage

```
spc.fit.poly(
  fit.to,
  apply.to = NULL,
  poly.order = 1,
  offset.wl = !(is.null(apply.to))
)

spc.fit.poly.below(
  fit.to,
  apply.to = fit.to,
  poly.order = 1,
  npts.min = max(round(nwl(fit.to) * 0.05), 3 * (poly.order + 1)),
  noise = 0,
  offset.wl = FALSE,
  max.iter = nwl(fit.to),
  stop.on.increase = FALSE,
  debuglevel = hy.getOption("debuglevel")
)
```

Arguments

`fit.to`	`hyperSpec` object on which the baselines are fitted
`apply.to`	`hyperSpec` object on which the baselines are evaluted If `NULL`, a `hyperSpec` object containing the polynomial coefficients rather than evaluted baselines is returned.
`poly.order`	order of the polynomial to be used
`offset.wl`	should the wavelength range be mapped to -> [0, delta wl]? This enhances numerical stability.
`npts.min`	minimal number of points used for fitting the polynomial
`noise`	noise level to be considered during the fit. It may be given as one value for all the spectra, or for each spectrum separately.
`max.iter`	stop at the latest after so many iterations.
`stop.on.increase`	additional stopping rule: stop if the number of support points would increase, regardless whether npts.min was reached or not.

debuglevel — additional output: 1 shows npts.min, 2 plots support points for the final baseline of 1st spectrum, 3 plots support points for 1st spectrum, 4 plots support points for all spectra.

Details

spc.fit.poly calculates the least squares fit of order poly.order to the *complete* spectra given in fit.to. Thus fit.to needs to be cut appropriately.

Value

hyperspec object containing the baselines in the spectra matrix, either as polynomial coefficients or as polynomials evaluted on the spectral range of apply.to

Author(s)

C. Beleites

See Also

vignette ("baseline",package = "hyperSpec")

see options for more on debuglevel

Examples

```
## Not run: vignette ("baseline", package = "hyperSpec")

spc <- chondro [1 : 10]
baselines <- spc.fit.poly(spc [,, c (625 ~ 640, 1785 ~ 1800)], spc)
plot(spc - baselines)


baselines <- spc.fit.poly.below (spc)
plot (spc - baselines)

spc.fit.poly.below(chondro [1:3], debuglevel = 1)
spc.fit.poly.below(chondro [1:3], debuglevel = 2)
spc.fit.poly.below(chondro [1:3], debuglevel = 3, noise = sqrt (rowMeans (chondro [[1:3]])))
```

---

spc.identify — *Identifying Spectra and Spectral Data Points This function allows to identify the spectrum and the wavelength of a point in a plot produced by* plotspc.

Description

This function first finds the spectrum with a point closest to the clicked position (see locator). The distance to the clicked point is evaluated relative to the size of the tolerance window.

Usage

```
spc.identify(
  x,
  y = NULL,
  wavelengths = NULL,
  ispc = NULL,
  tol.wl = diff(range(x))/200,
  tol.spc = diff(range(y))/50,
  point.fn = spc.point.max,
  formatter = spc.label.default,
  ...,
  cex = 0.7,
  adj = c(0, 0.5),
  srt = 90,
  warn = TRUE
)

spc.point.max(wl, spc, wlclick)

spc.point.default(wl, spc, wlclick)

spc.point.min(wl, spc, wlclick)

spc.point.sqr(wl, spc, wlclick, delta = 1L)

spc.label.default(ispc, wl, spc, digits = 3)

spc.label.wlonly(ispc, wl, spc, digits = 3)
```

Arguments

x	either the abscissa coordinates or the list returned by plotspc
y	the ordinate values. Giving y will override any values from x$y.
wavelengths	the wavelengths for the data points. Giving wavelengths will override any values from x$wavelengths.
ispc	if a selection of spectra was plotted, their indices can be given in ispc. In this case ispc [i] is returned rather than i.
tol.wl, tol.spc	tolerance in wavelength and spectral intensity to search around the clicked point. See details.
point.fn	function (wl,spc,wlclick) to determine the actual point to label, see details.
formatter	function (i,wl,spc) that produces the labels. If NULL, no labels are displayed.
...	passed to text in order to produce the labels
cex, adj, srt	see par
warn	Should the user be warned if no point is in the considered window? In addition, see the discussion of option debuglevel in the details.

	If FALSE, the resulting data.frame will have a row of NAs instead.
wl	the wavelength to label
spc	the intensity to label
wlclick	the clicked wavelength
delta	spc.point.sqr fits the parabola in the window wlclick ± delta points.
digits	how many digits of the wavelength should be displayed?

Details

In a second step, max.fn searches for the actual point to label within the specified wavelength window of that spectrum. This allows to label maxima (or minima) without demanding too precise clicks. Currently, the following functions to determine the precise point:

spc.point.default	uses the clicked wavelength together with its spectral intensity
spc.point.max	the point with the highest intensity in the wavelength window
spc.point.min	the point with the lowest intensity in the wavelength window
spc.point.sqr	maximum of a parabola fit throug the point with highest intensity and the two surrounding points

point.fn is called with the arguments wl containing the considered wavelength window, spc the respective intensities of the closest spectrum, and wlclick the wavelength that was clicked. They return a vector of two elements (wavelength and intensity).

As a last step, a label for the point produced by formatter and plotted using text. Currently, the following formatters are available:

spc.label.default	spectrum number, wavelength
spc.label.wlonly	wavelength

formatter functions receive the number of the spectrum ispc, the wavelength wl, and the spectral intensity spc and produce a character variable suitable for labelling. The predefined formatters surround the label text by spaces in order to easily have an appropriate offset from the point of the spectrum.

The warning issued if no spectral point is inside the tolerance window may be switched of by warn = FALSE. In that case, the click will produce a row of NAs in the resulting data.frame.

spc.identify uses option debuglevel to determine whether debugging output should be produced. debuglevel == 2 will plot the tolerance window for every clicked point, debuglevel == 1 will plot the tolerance window only if no data point was inside. See hyperSpec options for details about retrieving and setting options.

You may want to adjust the plot's ylim to ensure that the labels are not clipped. As a dirty shortcut, xpd = NA may help.

Value

a data.frame with columns

ispc	spectra indices of the identified points, i.e. the rows of the hyperSpec object that was plotted. If ispc is given, ispc [i] is returned rather than i.
wavelengths	the wavelengths of the identified points
spc	the intensities of the identified points

Author(s)

C. Beleites

See Also

locator, plotspc, hyperSpec options

map.identify map.sel.poly

Examples

```
if (interactive ()){
ispc <- sample (nrow (laser), 10)
ispc

identified <- spc.identify (plotspc (laser[ispc]))

## convert to the "real" spectra indices
ispc [identified$ispc]
identified$wl
identified$spc

## allow the labels to be plotted into the plot margin
spc.identify (plotspc (laser[ispc]), ispc = ispc, xpd = NA)

spc.identify (plotspc (paracetamol, xoffset = 1100,
              wl.range = c (600 ~ 1700, 2900 ~ 3150)),
              formatter = spc.label.wlonly)

## looking for minima
spc.identify (plot (-paracetamol, wl.reverse = TRUE),
              point.fn = spc.point.min, adj = c (1, 0.5))

}
```

---

spc.loess *loess smoothing interpolation for spectra Spectra can be smoothed and interpolated on a new wavelength axis using* loess.

Description

Applying loess to each of the spectra, an interpolation onto a new wavelength axis is performed. At the same time, the specta are smoothed in order to increase the signal : noise ratio. See loess and loess.control on the parameters that control the amount of smoothing.

Usage

```
spc.loess(spc, newx, enp.target = nwl(spc)/4, surface = "direct", ...)
```

Arguments

spc	the hyperSpec object
newx	wavelengh axis to interpolate on
enp.target, surface, ...	parameters for loess and loess.control.

Value

a new hyperspec object.

Author(s)

C. Beleites

See Also

loess, loess.control

Examples

```
plot (flu, col = "darkgray")
plot (spc.loess(flu, seq (420, 470, 5)), add = TRUE, col = "red")

flu [[3, ]] <- NA_real_
smooth <- spc.loess(flu, seq (420, 470, 5))
smooth [[, ]]
plot (smooth, add = TRUE, col = "blue")
```

spc.NA.approx *Impute missing data points*

Description

Replace NAs in the spectra matrix by interpolation. With less than 4 points available linear interpolation of the 2 neighbour points is used. For larger numbers of neighbour points, smoothing interpolation is performed by smooth.spline.

Usage

```
spc.NA.approx(
  spc,
  neighbours = 1,
  w = rep(1, 2 * neighbours),
  df = 1 + .Machine$double.eps,
  spar = NULL,
  debuglevel = hy.getOption("debuglevel")
)

spc.NA.linapprox(...)
```

Arguments

spc	hyperSpec object with spectra matrix containing NAs
neighbours	how many neighbour data points should be used to fit the line
w, df, spar	see smooth.spline
debuglevel	see options
...	ignored

Value

hyperSpec object

Note

The function has been renamed from spc.NA.linapprox to spc.NA.approx

Author(s)

Claudia Beleites

Examples

```
fluNA <- hyperSpec:::fluNA
spc.NA.approx (fluNA [,, min ~ 410], debuglevel = 1)
spc.NA.approx (fluNA [1,, min ~ 410], debuglevel = 2)
spc.NA.approx (fluNA [4,, min ~ 410], neighbours = 3, df = 4, debuglevel = 2)
```

spc.rubberband *Rubberband baseline correction*

Description

Rubberband baseline

Usage

```
spc.rubberband(spc, ..., upper = FALSE, noise = 0, spline = TRUE)
```

Arguments

spc	hyperSpec object
...	further parameters handed to smooth.spline
upper	logical indicating whether the lower or upper part of the hull should be used
noise	noise level to be taken into account
spline	logical indicating whether the baseline should be an interpolating spline through the support points or piecewise linear.

Details

Baseline with support points determined from a convex hull of the spectrum.

Use `debuglevel >= 1` to obtain debug plots, either directly via function argument or by setting hyperSpec's `debuglevel` option.

Value

hyperSpec object containing the baselines

Note

This function is still experimental

Author(s)

Claudia Beleites

See Also

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

`vignette("baseline")`

hy.setOptions

Examples

```
plot (paracetamol [,, 175 ~ 1800])
bl <- spc.rubberband (paracetamol [,, 175 ~ 1800], noise = 300, df = 20)
plot (bl, add = TRUE, col = 2)

plot (paracetamol [,, 175 ~ 1800] - bl)
```

---

spc.smooth.spline *Spectral smoothing by splines*

Description

Smoothing splines

Usage

```
spc.smooth.spline(spc, newx = wl(spc), ...)
```

Arguments

spc	hyperSpec object
newx	wavelengh axis to interpolate on
...	further parameters handed to smooth.spline

Details

Spectral smoothing by splines

Value

hyperSpec object containing smoothed spectra

Note

This function is still experimental

Author(s)

Claudia Beleites

See Also

spc.loess

smooth.spline

Examples

```
p <- paracetamol [,,2200 ~ max]
plot (p, col = "gray")
smooth <- spc.smooth.spline (p [,, c (2200 ~ 2400, 2500 ~ 2825, 3150 ~ max)],
                             wl (paracetamol [,, 2200 ~ max]),
                             df = 4, spar = 1)
plot (smooth, col = "red", add = TRUE)

plot (p - smooth)
```

`split` *Split a hyperSpec object according to groups* `split` *divides the* `hyperSpec` *object into a list of* `hyperSpec` *objects according to the groups given by* `f`.

Description

The `hyperSpec` objects in the list may be bound together again by `bind ("r",list_of_hyperSpec_objects)`.

Usage

```
## S4 method for signature 'hyperSpec'
split(x, f, drop = TRUE)
```

Arguments

`x`	the `hyperSpec` object
`f`	a factor giving the grouping (or a variable that can be converted into a factor by `as.factor`)
`drop`	if `TRUE`, levels off that do not occur are dropped.

Value

A list of `hyperSpec` objects.

Author(s)

C. Beleites

See Also

`split`

Examples

```
dist <- pearson.dist (chondro[[]])
dend <- hclust (dist, method = "ward")
z <- cutree (dend, h = 0.15)

clusters <- split (chondro, z)
length (clusters)

# difference in cluster mean spectra
plot (apply (clusters[[2]], 2, mean) - apply (clusters[[1]], 2, mean))
```

`subset` *subset*

Description

subset for hyperSpec object

Usage

```
## S4 method for signature 'hyperSpec'
subset(x, ...)
```

Arguments

`x`	hyperSpec object
`...`	handed to `subset` (data.frame method)

Value

hyperSpec object containing the respective subset of spectra.

Author(s)

Claudia Beleites

See Also

`subset`

`Summary` *The functions*

Description

`all`, `any`,

Usage

```
## S4 method for signature 'hyperSpec'
Summary(x, ..., na.rm = FALSE)

## S4 method for signature 'hyperSpec'
is.na(x)

all_wl(expression, na.rm = FALSE)

any_wl(expression, na.rm = FALSE)
```

Arguments

`x`	hyperSpec object
`...`	further objects
`na.rm`	logical indicating whether missing values should be removed
`expression`	expression that evaluates to a logical matrix of the same size as the spectra matrix

Details

`sum`, `prod`,

`min`, `max`,

`range`, and

`is.na`

for `hyperSpec` objects.

All these functions work on the spectra matrix.

Value

`sum`, `prod`, `min`, `max`, and `range` return a numeric, `all`, `any`, and `is.na` a logical.

See Also

`Summary` for the base summary functions.

`all.equal` and `isTRUE`

Examples

```
range (flu)


is.na (flu [,, 405 ~ 410]);

all_wl (flu > 100)

any_wl (flu > 300)
! any_wl (is.na (flu))
```

---

sweep — *Sweep Summary Statistic out of an hyperSpec Object* sweep *for* hyperSpec *objects.*

Description

Calls sweep for the spectra matrix.

Usage

```
## S4 method for signature 'hyperSpec'
sweep(x, MARGIN, STATS, FUN = "-", check.margin = TRUE, ...)
```

Arguments

x	a hyperSpec object.
MARGIN	direction of the spectra matrix that STATS goees along.
STATS	the summary statistic to sweep out. Either a vector or a hyperSpec object. hyperSpec offers a non-standard convenience function: if STATS is a function, this function is applied first (with the same MARGIN) to compute the statistic. However, no further arguments to the apply function can be given. See the examples.
FUN	the function to do the sweeping, e.g. '-' or '/'.
check.margin	If TRUE (the default), warn if the length or dimensions of STATS do not match the specified dimensions of x. Set to FALSE for a small speed gain when you *know* that dimensions match.
...	further arguments for FUN

Details

sweep is useful for some spectra preprocessing, like offset correction, substraction of background spectra, and normalization of the spectra.

Value

A hyperSpec object.

Author(s)

C. Beleites

See Also

sweep

Examples

```
## Substract the background / slide / blank spectrum
# the example data does not have spectra of the empty slide,
# so instead the overall composition of the sample is substracted
background <- apply (chondro, 2, quantile, probs = 0.05)
corrected <- sweep (chondro, 2, background, "-")
plot (corrected, "spcprctl5")

## Offset correction
offsets <- apply (chondro, 1, min)
corrected <- sweep (chondro, 1, offsets, "-")
plot (corrected, "spcprctl5")

## Min-max normalization (on max amide I)
# the minimum is set to zero by the offset correction.
factor <- apply (corrected, 1, max)
mm.corrected <- sweep (corrected, 1, factor, "/")
plot (mm.corrected, "spcprctl5")

## convenience: give function to compute STATS:
mm.corrected2 <- sweep (corrected, 1, max, "/")
plot (mm.corrected2)

## checking
stopifnot (all (mm.corrected2 == mm.corrected))
```

---

trellis.factor.key *Color coding legend for factors Modifies a list of lattice arguments (as for levelplot, etc.) according to the factor levels. The colorkey will shows all levels (including unused), and the drawing colors will be set accordingly.*

Description

trellis.factor.key is used during levelplot-based plotting of factors (for hyperSpec objects) unless transform.factor = FALSE is specified.

Usage

```
trellis.factor.key(f, levelplot.args = list())
```

Arguments

f	the factor that will be color-coded
levelplot.args	a list with levelplot arguments

Value

the modified list with levelplot arguments.

Author(s)

C. Beleites

See Also

levelplot

Examples

```
chondro$z <- factor (rep (c("a", "a", "d", "c"),
                          length.out = nrow (chondro)),
                     levels = letters [1 : 4])

str (trellis.factor.key (chondro$z))

plotmap (chondro, z ~ x * y)

## switch off using trellis.factor.key:
## note that the factor levels are collapsed to c(1, 2, 3) rather than
## c (1, 3, 4)
plotmap (chondro, z ~ x * y, transform.factor = FALSE)

plotmap (chondro, z ~ x * y,
         col.regions = c ("gray", "red", "blue", "dark green"))
```

---

vanderMonde *Function evaluation on hyperSpec objects*

Description

vandermonde generates van der Monde matrices, the hyperSpec method generates a hyperSpec object containing the van der Monde matrix of the wavelengths of a hyperSpec object.

Usage

```
vanderMonde(x, order, ...)

## S4 method for signature 'hyperSpec'
vanderMonde(x, order, ..., normalize.wl = normalize01)
```

Arguments

x	object to evaluate the polynomial on
order	of the polynomial
...	hyperSpec method: further arguments to decomposition
normalize.wl	function to transorm the wavelengths before evaluating the polynomial (or other function). normalize01 maps the wavelength range to the interval [0, 1]. Use I to turn off.

Details

It is often numerically preferrable to map `wl (x)` to [0, 1], see the example.

Value

van der Monde matrix

hyperSpec method: hyperSpec object containing van der Monde matrix as spectra and an additional column ".vdm.order" giving the order of each spectrum (term).

Author(s)

C. Beleites

See Also

wl.eval for calculating arbitrary functions of the wavelength,

normalize01

Examples

```
plot (vanderMonde (flu, 2))
plot (vanderMonde (flu, 2, normalize.wl = I))
```

wc *line/word/character count of ASCII files*

Description

'wc()' uses the system command 'wc'. Use at your own risk.

Usage

```
wc(file, flags = c("lines", "words", "bytes"))
```

Arguments

file	the file name or pattern
flags	the parameters to count, character vector with the long form of the parameters

Value

data.frame with the counts and file names, or 'NULL' if wc is not available on the system.

Note

'wc()' now is deprecated and will be removed from hyperSpec in future. Consider using [count_lines()] instead for line counting.

Author(s)

C. Beleites

See Also

[count_lines()]

wl *Getting and Setting the Wavelength Axis* wl *returns the wavelength axis,* wl<- *sets it.*

Description

The wavelength axis of a hyperSpec object can be retrieved and replaced with wl and wl<-, respectively.

Usage

```
wl(x)

wl (x, label=NULL, digits=6) <- value
```

Arguments

x	a hyperSpec object
label	The label for the new wavelength axis. See initialize for details.
digits	handed to signif. See details.
value	either a numeric containing the new wavelength vector, or a list with value$wl containing the new wavelength vector and value$label holding the corresponding label.

Details

When the wavelength axis is replaced, the colnames of x@data$spc are replaced by the rounded new wavelengths. digits specifies the how many significant digits should be used.

There are two ways to set the label of the new wavelength axis, see the examples. If no label is given, a warning will be issued.

Value

a numeric vector

hyperSpec object

Note

wl<- always sets the complete wavelength axis, without changing the columns of the spectra matrix. If you rather want to cut the spectral range, use [, for interpolation along the spectral axis see spc.loess and for spectral binning spc.bin.

Author(s)

C. Beleites

See Also

signif

cutting the spectral range: [

interpolation along the spectral axis: spc.loess

spectral binning: spc.bin

Examples

```
wl (laser)

# convert from wavelength to frequency
plot (laser)
wl (laser, "f / Hz") <- 2.998e8 * wl (laser) * 1e9
plot (laser)
```

```
# convert from Raman shift to wavelength
# excitation was at 785 nm
plot (chondro [1])
wl (chondro) <- list (wl = 1e7 / (1e7/785 - wl (chondro)), label = expression (lambda / nm))
plot (chondro [1])
```

`wl.eval` *Evaluate function on wavelengths of hyperSpec object*

Description

This is useful for generating certain types of baseline "reference spectra".

Usage

```
wl.eval(x, ..., normalize.wl = I)
```

Arguments

`x`	hyperSpec object
`...`	hyperSpec method: expressions to be evaluated
`normalize.wl`	function to transorm the wavelengths before evaluating the polynomial (or other function). Use `normalize01` to map the wavelength range to the interval [0, 1].

Value

hyperSpec object containing one spectrum for each expression

Author(s)

C. Beleites

See Also

`vanderMonde` for polynomials,

`normalize01` to normalize the wavenumbers before evaluating the function

Examples

```
plot (wl.eval (laser, exp = function (x) exp (-x)))
```

wl2i *Conversion between Wavelength and Spectra Matrix Column Index* wl2i *returns the column indices for the spectra matrix for the given wavelengths.* i2wl *converts column indices into wavelengths.*

Description

If wavelength is numeric, each of its elements is converted to the respective index. Values outside the range of x@wavelength become NA.

Usage

```
wl2i(x, wavelength = stop("wavelengths are required."), unlist = TRUE)

i2wl(x, i)
```

Arguments

x	a hyperSpec object
wavelength	the wavelengths to be converted into column indices, either numeric or a formula, see details.
unlist	if multiple wavelength ranges are given, should the indices be unlisted or kept in a list?
i	the column indices into the spectra matrix for which the wavelength is to be computed

Details

If the range is given as a formula (i.e. start ~ end, a sequence

index corresponding to start : index corresponding to end

is returned. If the wavelengths are not ordered, that may lead to chaos. In this case, call orderwl first.

Two special variables can be used: min and max, corresponding to the lowest and highest wavelength of x, respectively.

start and end may be complex numbers. The resulting index for a complex x is then

index (Re (x)) + Im (x)

Value

A numeric containing the resulting indices for wl2i

i2wl returns a numeric with the wavelengths

Author(s)

C. Beleites

Examples

```
flu
wl2i (flu, 405 : 407)
wl2i (flu, 405 ~ 407)

## beginning of the spectrum to 407 nm
wl2i (flu, min ~ 407)

## 2 data points from the beginning of the spectrum to 407 nm
wl2i (flu, min + 2i ~ 407)

## the first 3 data points
wl2i (flu, min ~ min + 2i)

## from 490 nm to end of the spectrum
wl2i (flu, 490 ~ max)

## the last 8 data points
wl2i (flu, max - 7i ~ max)

## get 450 nm +- 3 data points
wl2i (flu, 450 - 3i ~ 450 + 3i)

wl2i (flu, 300 : 400) ## all NA:
wl2i (flu, 600 ~ 700) ## NULL: completely outside flu's wavelength range


i2wl (chondro, 17:20)
```

---

wlconv *Convert different wavelength units*

Description

The following units can be converted into each other: *nm*, cm^{-1}, *eV*, *THz* and *Raman shift*

Usage

```
wlconv(points, src, dst, laser = NULL)

nm2raman(x, laser)

nm2invcm(x, ...)

nm2ev(x, ...)

nm2freq(x, ...)
```

```
invcm2raman(x, laser)

invcm2nm(x, ...)

invcm2ev(x, ...)

invcm2freq(x, ...)

raman2invcm(x, laser)

raman2nm(x, laser)

raman2ev(x, laser)

raman2freq(x, laser)

ev2raman(x, laser)

ev2invcm(x, ...)

ev2nm(x, ...)

ev2freq(x, ...)

freq2nm(x, ...)

freq2invcm(x, ...)

freq2ev(x, ...)

freq2raman(x, laser)
```

Arguments

points	data for conversion
src	source unit
dst	destination unit
laser	laser wavelength (required for work with Raman shift)
x	wavelength points for conversion
...	ignored

Functions

- nm2raman: conversion **nanometers -> Raman shift (relative wavenumber)**
- nm2invcm: conversion **nanometers -> inverse cm (absolute wavenumber)**
- nm2ev: conversion **nanometers -> electronvolt**

- nm2freq: conversion **nm -> frequency in THz**
- invcm2raman: conversion **inverse cm (absolute wavenumber) -> Raman shift (relative wavenumber)**
- invcm2nm: conversion **inverse cm (absolute wavenumber) -> nanometers**
- invcm2ev: conversion **inverse cm (absolute wavenumber) -> electronvolt**
- invcm2freq: conversion **inverse cm (absolute wavenumber) -> frequency in THz**
- raman2invcm: conversion **Raman shift (relative wavenumber) -> inverse cm (absolute wavenumber)**
- raman2nm: conversion **Raman shift (relative wavenumber) -> nanometers**
- raman2ev: conversion **Raman shift (relative wavenumber) -> electronvolt**
- raman2freq: conversion **Raman shift (relative wavenumber) -> frequency in THz**
- ev2raman: conversion **electronvolt -> Raman shift (relative wavenumber)**
- ev2invcm: conversion **electronvolt -> inverse cm (absolute wavenumber)**
- ev2nm: conversion **electronvolt -> nanometers**
- ev2freq: conversion **electronvolt -> frequency in THz**
- freq2nm: conversion **frequency in THz -> nanometers**
- freq2invcm: conversion **frequency in THz -> inverse cm (absolute wavenumber)**
- freq2ev: conversion **frequency in THz -> electronvolt**
- freq2raman: conversion **frequency in THz -> Raman shift (relative wavenumber)**

Author(s)

R. Kiselev

Examples

```
wlconv (3200, "Raman shift", "nm", laser = 785.04)
wlconv( 785, "nm", "invcm")
```

[,hyperSpec-method *Extract and Replace parts of hyperSpec objects*

Description

These Methods allow to extract and replace parts of the hyperSpec object.

Usage

```
## S4 method for signature 'hyperSpec'
x[i, j, l, ..., wl.index = FALSE, drop = FALSE]

## S4 method for signature 'hyperSpec'
x[[i, j, l, ..., wl.index = FALSE, drop = FALSE]]

## S4 method for signature 'hyperSpec'
x$name

## S4 replacement method for signature 'hyperSpec'
x[i, j, ...] <- value

## S4 replacement method for signature 'hyperSpec'
x[[i, j, l, wl.index = FALSE, ...]] <- value

## S4 replacement method for signature 'hyperSpec'
x$name <- value
```

Arguments

x	a hyperSpec Object
i	row index: selects spectra [[and code[[<- accept indexing with logical matrix or a n by 2 integer index matrix. In this case the indexing is done inside the spectra matrix. See the examples below.
j	selecting columns of x@data
l	selecting columns of the spectra matrix. If l is numeric, the default behaviour is treating l as wavelengths, *not* as indices.
...	ignored
wl.index	If TRUE (default), the value(s) in l are treated as column indices for the spectral matrix. Otherwise, the numbers in l are treated as wavelengths and the corresponding column indices are looked up first via wl2i.
drop	For [[: drop unnecessary dimensions, see drop and Extract. Ignored for [, as otherwise invalid hyperSpec objects might result.
name	name of the data column to extract. $spc yields the spectra matrix.
value	the replacement value

Details

They work with respect to the spectra (rows of x), the columns of the data matrix, and the wavelengths (columns of the spectra matrix).

Thus, they can be used for selecting/deleting spectra, cutting the spectral range, and extracting or setting the data belonging to the spectra.

Convenient shortcuts for access of the spectra matrix and the data.frame in slot data are provided.

Extracting: `[`, `[[`, *and* `$`.

The version with single square brackets (`[`) returns the resulting `hyperSpec` object.

`[[` yields `data.frame` of slot `@data` of that corresponding `hyperSpec` object returned with the same arguments by `[` if columns were selected (i.e. `j` is given), otherwise the spectra `matrix` `x@data$spc`.

`$` returns the selected column of the `data.frame` in slot `@data`.

Shortcuts. Three shortcuts to conveniently extract much needed parts of the object are defined:

`x[[]]` returns the spectra matrix.

`x$.` returns the complete slot `@data`, including the spectra matrix in column `$spc`, as a `data.frame`.

`x$..` returns a `data.frame` like `x$.` but without the spectra matrix.

Replacing: `[<-`, `[[<-`, *and* `$<-`.

```
## S4 method for signature 'hyperSpec':
x [i, j, l, \dots] <- value

## S4 method for signature 'hyperSpec':
x [[i, j, l, wl.index = FALSE, \dots]] <- value

## S4 method for signature 'hyperSpec':
x$name <- value
```

`value` gives the values to be assigned.

For `$`, this can also be a list of the form `list(value = value, label = label)`, with `label` containing the label for data column `name`.

`[[<-` replaces parts of the spectra matrix.

`[<-` replaces parts of the `data.frame` in slot `x@data`.

`$<-` replaces a column of the `data.frame` in slot `x@data`. The `value` may be a list with two elements, `value` and `label`. In this case the label of the data column is changed accordingly.

`$..<-` is again an abbreviation for the data.frame without the spectra matrix.

Value

For `[`, `[<-`, `[[<-`, and `$<-` a `hyperSpec` object,

for `[[` a matrix or `data.frame`, and

for `$` the column of the `data.frame` `@data`.

`x[[]]` returns the complete spectra matrix.

`x$.` returns the complete slot `@data`,

`x$..` returns the `data.frame` in `@data` but without the column `@data$spc` containing the spectra matrix.

See Also

`wl2i` on conversion of wavelength ranges to indices.

`drop` and `Extract` on `drop`.

Examples

```
## index into the rows (spectra) -------------------------------------
## make some "spectra"

## numeric index
plot (flu, "spc", lines.args = list (lty = 2))
plot (flu[1:3], "spc", add = TRUE, col = "red")     # select spectra
plot (flu[-(1:3)], "spc", add = TRUE, col = "blue") # delete spectra

## logic index
plot (flu, "spc", lines.args = list (lty = 2))
index <- rnorm (6) > 0
index
plot (flu[index], "spc", add = TRUE, col = "red")   # select spectra
plot (flu[!index], "spc", add = TRUE, col = "blue") # select spectra

## index into the data columns ---------------------------------------
range (chondro[[,"x"]])
colnames (chondro[[,1]])
dim (chondro[[,c(TRUE, FALSE, FALSE)]])
chondro$x


## the shortcut functions --------------------------------------------

## extract the spectra matrix
flu[[]]

## indexing via logical matrix
summary (flu [[flu < 125]])

## indexing the spectra matrix with index matrix n by 2
ind <- matrix (c (1, 2, 4, 406, 405.5, 409), ncol = 2)
ind
flu [[ind]]

ind <- matrix (c (1, 2, 4, 4:6), ncol = 2)
ind
flu [[ind, wl.index = TRUE]]

pca <- prcomp (flu[[]])

## result is data.frame, if j is given:
result <- flu [[, 1:2, 405 ~ 410]]
result
class (result)
colnames (result)

## extract the data.frame including the spectra matrix
flu$.
dim(flu$.)
```

```
colnames (flu$.)
flu$.$spc

calibration <- lm (spc ~ c, data = flu[,,450]$.)
calibration

flu$..
colnames (flu$..)

## replacement functions
spc <- flu
spc$.
spc[, "c"] <- 16 : 11
## be careful:
plot (spc)
spc [] <- 6 : 1
spc$..
plot (spc)

spc <- flu [,, 405 ~ 410]
spc [[]]
spc [[3]] <- -spc[[3]]
spc [[]]
spc [[,,405 : 410]] <- -spc[[,,405 : 410]]
spc [[]]
spc [[,,405 ~ 410]] <- -spc[[,,405 ~ 410]]

## indexing with logical matrix
spc <- flu [,, min ~ 410]
spc < 125
spc [[spc < 125]] <- NA
spc [[]]

## indexing with n by 2 matrix
ind <- matrix (c (1, 2, 4, 406, 405.5, 409), ncol = 2)
ind
spc [[ind]] <- 3
spc [[]]

ind <- matrix (c (1, 2, 4, 4:6), ncol = 2)
ind
spc [[ind, wl.index = TRUE]] <- 9999
spc [[]]

spc$.
spc$z <- 1 : 6
spc
spc$z <- list (1 : 6, "z / a.u.")
```

Index