hyperSpec Plotting functions

Claudia Beleites <chemometrie@beleites.de>
CENMAT and DI3, University of Trieste
Spectroscopy · Imaging, IPHT Jena e.V.

June 7, 2013

Vignette under Development

This file is currently undergoing a thorough revision. Changes may happen frequently.

Reproducing the Examples in this Vignette

All spectra used in this manual are installed automatically with *hyperSpec*. Note that some definitions are executed in vignette.defs, and others invisibly at the beginning of the file in order to have the code as similar as possible to interactive sessions.

Contents

1	Predefined functions	2
2	Arguments for plot	4
3	Spectra 3.1 Stacked spectra	7 9
4	Calibration Plots, (Depth) Profiles, and Time Series Plots 4.1 Calibration plots	11 11 13
5	Levelplot	13
6	Spectra Matrix	14
7	False-Colour Maps: plotmap	15
8	3 D (with rgl)	17
9	Using ggplot2 with hyperSpec objects	18
10	Troubleshooting 10.1 No output is produced	19 19

11	Interactive Graphics	1
	11.1 spc.identify: finding out wavelength, intensity and spectrum	2
	11.2 map.identify: finding a spectrum in a map plot	2
	11.3 map.sel.poly: selecting spectra inside a polygon in a map plot	2
	11.4 Related functions provided by base graphics and lattice	2
	11.5 Interactively changing graphics	2

Suggested Packages

latticeExtra: available deldir: available rgl: available ggplot2: available

In addition tripack, playwith, and latticist are mentioned, but not used in this vignette.

Preliminary Calculations

For some plots of the chondro dataset, the pre-processed spectra and their cluster averages \pm one standard deviation are more suitable:

```
> chondro.preproc <- chondro - spc.fit.poly.below (chondro)
Fitting with npts.min = 15
> chondro.preproc <- sweep (chondro.preproc, 1, mean, "/")
> chondro.preproc <- sweep (chondro.preproc, 2, apply (chondro.preproc, 2, quantile, 0.05), "-")
> cluster.cols <- c ("dark blue", "orange", "#C02020")
> cluster.meansd <- aggregate (chondro.preproc, chondro$clusters, mean_pm_sd)
> cluster.means <- aggregate (chondro.preproc, chondro$clusters, mean)</pre>
```

For details about the pre-processing, please refer to the example work flow in vignette ("chondro"), or the help? chondro.

1 Predefined functions

hyperSpec comes with 6 major predefined plotting functions.

plot main switchyard for most plotting tasks
levelplot hyperSpec has a method for lattice[?] function levelplot

plotspc plots spectra

plotmat plots the spectra matrix

plotc calibration plot, time series, depth profile

plotc is a lattice function

plotmap more specialized version of levelplot for map or image plots.

plotmap is a lattice function

plotvoronoi more specialized version of plotmap that produces Voronoi tesselations. plotvoronoi is a *lattice* function

plotmap, plotvoronoi, and levelplot are *lattice* functions. Therefore, in loops, functions, Sweave chunks, etc. the lattice object needs to be printed explicitly by e.g. print (plotmap (object)) (R FAQ: Why do lattice/trellis graphics not work?).



plots the spectra, i.e. the intensities $\protect\operatorname{\mathtt{\$spc}}$ over the wavelengths $\protect\operatorname{\mathtt{\mathtt{@wavelength}}}.$

> plotspc (flu)

$\operatorname{plotmat}$



plots the spectra, i. e. the colour coded intensities \$spc over the wavelengths @wavelength and the row number.

> plotmat (flu)

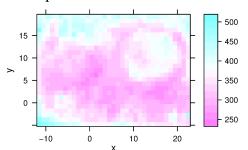


c / (ma / I)

plots an intensity over a single other data column, e.g.

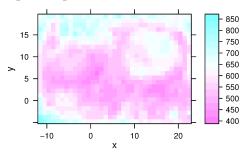
- calibration
- time series
- depth profile
- > plotc (flu)

levelplot



plots a false colour map, defined by a formula.
> levelplot (spc ~ x * y, chondro, aspect = "iso")
Warning: Only first wavelength is used for plotting

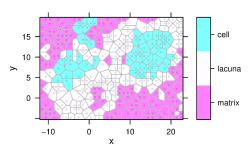
plotmap



plotmap is a specialized version of level plot. It uses a single value (e.g. average intensity or cluster membership) over two data columns (default x and y

> plotmap (chondro)

plotvoronoi



plotmap is a specialized version of levelplot. It uses a single value (e.g. average intensity or cluster membership) over two data columns (default \$x\$ and \$y)

> plotvoronoi (sample (chondro, 300), clusters ~ x * y)
 PLEASE NOTE: The components "delsgs" and "summary" of the
 object returned by deldir() are now DATA FRAMES rather than
 matrices (as they were prior to release 0.0-18).
 See help("deldir").

PLEASE NOTE: The process that deldir() uses for determining duplicated points has changed from that used in version 0.0-9 of this package (and previously). See help("deldir").

2 Arguments for plot

hyperSpec's plot method uses its second argument to determine which of the specialized plots to produce. This allows some handy abbreviations. All further arguments are handed over to the function actually producing the plot.



is equivalent to plotspc (flu)
> plot (flu, "spc")



plots mean spectrum \pm 1 standard deviation > plot (chondro.preproc, "spcmeansd")



plots median, $16^{\rm th}$ and $84^{\rm th}$ percentile for each wavelength. For Gaussian distributed data, $16^{\rm th}$, $50^{\rm th}$ and $84^{\rm th}$ percentile are equal to mean \pm standard deviation. Spectroscopic data frequently are not Gaussian distributed. The percentiles give a better idea of the true distribution. They are also less sensitive to outliers.

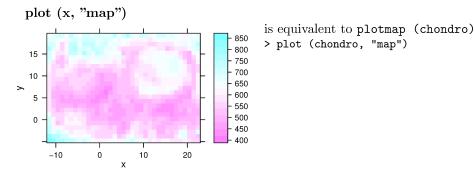
> plot (chondro.preproc, "spcprctile")

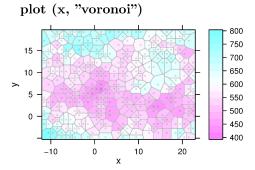


like "spcprctl" plus $5^{\rm th}$ and $95^{\rm th}$ percentile. > plot (chondro.preproc, "spcprctl5")

```
plot (x, "c")
  200
                                             > plot (flu, "c")
                                             is equivalent to plotc (flu)
  150
l<sub>ff</sub>/a.u.
   50
       0.05
             0.10
                   0.15
                        0.20
                              0.25
                                    0.30
                   c / (ma / I)
 plot (x, "ts")
                                             plots a time series plot
  75000
                                             > plot (laser [,, 405], "ts")
  70000
                                             equivalent to plotc (laser, spc ~ t)
  65000
  60000
  55000
  50000
             1000 2000 3000 4000 5000
 plot (x, "depth")
                                             plots a depth profile plot
                                               depth.profile <- new ("hyperSpec",</pre>
                                                    spc = as.matrix (rnorm (20) + 1:20),
  15
                                                    data = data.frame (z = 1 : 20),
1/a.u.
                                                    labels = list (spc = "I / a.u.",
                                                       z = expression ('/' (z, mu*m)),
                                                       .wavelength = expression (lambda)))
                                             > plot (depth.profile, "depth")
                                             the same as plotc (laser, spc \tilde{z})
                     10
                             15
                                     20
                    z/\mu m\,
 plot (x, "mat")
                                             plots the spectra matrix.
                                  80000
    80
                                             > plot (laser, "mat")
                                  60000
    9
                                             Equivalent to
ΓŌW
                                             > plotmat (laser)
                                  40000
    40
                                             A lattice alternative is:
    20
                                  20000
                                             > levelplot (spc ~ .wavelength * .row, laser)
       404.6
              405.0
                     405.4
                            405.8
```

 λ/nm

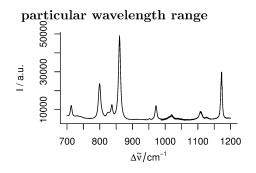




> plot (sample (chondro, 300), "voronoi") See plotvoronoi

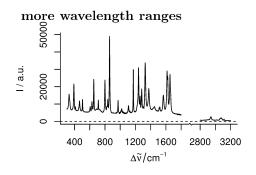
3 Spectra

plotspc offers a variety of parameters for customized plots. To plot ...



if only one wavelength range is needed, the extract command
 (see vignette ("introduction")) is handiest:
> plotspc (paracetamol [,, 700 ~ 1200])
 wavelengths. If wl.range already contains indices use
wl.index = TRUE.

plotspc



use wl.reverse = TRUE
> plotspc (paracetamol, wl.reverse = TRUE)

in different colours



use col = vector.of.colours
> plotspc (flu, col = matlab.dark.palette (6))

dots instead of lines



use lines.args = list (pch = 20, type = "p")
> plotspc (paracetamol [,, 2800 ~ 3200],
+ lines.args = list (pch = 20, type = "p"))



use lines.args = list (type = "h")
> plot (barbiturates [[1]], lines.args = list (type = "h"))

more spectra into an existing plot

```
Δῦ/cm<sup>-1</sup>
```

```
use add = TRUE
> plotspc (chondro [ 30,,])
> plotspc (chondro [300,,], add = TRUE, col = "blue")
```

Summary characteristics



func may be used to calculate summary characteristics prior to plotting. To plot e.g. the standard deviation of the spectra, use:

> plotspc (chondro.preproc, func = sd)



zero line takes a list with parameters to ${\tt abline}, \, {\tt NA} \, \, {\tt suppresses}$ the line.

> plotspc (paracetamol,
+ zeroline = list (col = "red"))

adding to a spectra plot



plotspc uses base graphics. After plotting the spectra, more content may be added to the graphic by abline, lines, points, etc.

> plot (laser, "spcmeansd")
> abline (v = c(405.0063, 405.1121, 405.2885, 405.3591),
+ col = c("black", "blue", "red", "darkgreen"))

3.1 Stacked spectra

stacked



Stacking groups of spectra



The spectra to be stacked can be grouped: stacked = factor. Alternatively, the name of the grouping extra data column can be used:

```
> plot (cluster.meansd,
+ stacked = ".aggregate",
+ fill = ".aggregate",
+ col = cluster.cols)
```

Manually giving yoffset



Stacking values can also be given manually as numeric values in yoffset:

```
> plotspc (cluster.meansd,
+ yoffset = rep (0:2, each = 3),
+ col = rep (cluster.cols, each = 3))
```

Dense stacking



```
To obtain a denser stacking:
> yoffsets <- apply (cluster.means [[]], 2, diff)
> yoffsets <- - apply (yoffsets, 1, min)
> plot (cluster.means, yoffset = c (0, cumsum (yoffsets)),
+ col = cluster.cols)
```

Elaborate example

plotspc allows fine grained customization of almost all aspects of the plot. This is possible by giving arguments to the functions that actually perform the plotting plot for setting up the plot area, lines for the plotting of the lines, axis for the axes, etc. The arguments for these functions should be given in lists as plot.args, lines.args, axis.args, etc.

4 Calibration Plots, (Depth) Profiles, and Time Series Plots

plotc

4.1 Calibration plots

Intensities over concentration



Plotting the Intensities of one wavelength over the concentration for univariate calibration:

> plotc (flu [,, 450])

The default is to use the first intensity only.

Summary Intensities over concentration



A function to compute a summary of the intensities before drawing can be used:

> plotc (flu, func = range, groups = .wavelength)
If func returns more than one value, the different results are accessible by .wavelength.

Conditioning: plotting more traces separately



```
> plotc (flu [,, c (405, 445)], spc ~ c | .wavelength,
+ cex = .3, scales = list (alternating = c(1, 1)))
```

Grouping: plot more traces in one panel



> plotc (flu [,, c (405, 445)], groups = .wavelength)

Changing Axis Labels (and other parameters)



```
Arguments for xyplot can be given to plotc:

> plotc (flu [,, 450],

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

+ xlim = range (0, flu$c + .01),

+ ylim = range (0, flu$spc + 10),

+ pch = 4)
```

Adding things to the plot: customized panel function



```
As plotc uses the lattice function xyplot, additions to the plot must be made via the panel function:

> panelcalibration <- function (x, y, ..., clim = range (x), level = .

+ panel.xyplot (x, y, ...)

+ lm <- lm (y ~ x)

+ panel.abline (coef (lm), ...)

+ cx <- seq (clim [1], clim [2], length.out = 50)

+ cy <- predict (lm, data.frame (x = cx),

+ interval = "confidence",

+ level = level)

+ panel.lines (cx, cy [,2], col = "gray")

+ panel.lines (cx, cy [,3], col = "gray")

+ }

> plotc (flu [,,405], panel = panelcalibration,

+ pch = 4, clim = c (0, 0.35), level = .99)
```

4.2 Time series and other Plots of the Type Intensity-over-Something

Abscissae other than c



Other abscissae may be specified by explicitly giving the model formula:

5 Levelplot

hyperSpec's levelplot can use two special column names:

.wavelength for the wavelengths

.row for the row index (i. e. spectrum number) in the data

Besides that, it behaves exactly like *levelplot*. Particularly, the data is given as the *second* argument:

levelplot



> levelplot (spc ~ x * y, chondro)

factors as z



If the colour-coded value is a factor, the display is adjusted to this fact:

> levelplot (clusters ~ x * y, chondro)

6 Spectra Matrix

It is often useful to plot the spectra against an additional coordinate, e.g. the time for time series, the depth for depth profiles, etc.

This can be done by plot (object, "mat"). The actual plotting is done by image, but levelplot can produce spectra matrix plots as well and these plots can be grouped or conditioned.

different palette



```
> plot (laser, "mat", col = heat.colors (20))
is the same as
> plotmat (laser, col = heat.colors (20))
```

different y axis



Using a different extra data column for the y axis: > plotmat (laser, y = "t") alternatively, y values and axis label can be given separately.

> plotmat (laser, y = laser\$t, ylab = labels (laser, "t"))

contour lines



Contour lines may be added:

- > plotmat (flu, col = matlab.dark.palette (20))
- > plotmat (flu, col = "white",
- + contour = TRUE, add = TRUE)

colour-coded points: levelplot with special panel function



7 False-Colour Maps: plotmap

plotmap is a specialized version of levelplot. The spectral intensities may be summarized by a function before plotting (default: mean). The same scale is used for x and y axes (aspect = "iso").

plotting map



plotting maps with other than x and y



specify the colour-coded variable, abscissa and ordinate as
formula: colour.coded ~ abscissa * ordinate
> plotmap (chondro, spc ~ y * x)

colour-coded factors



> plotmap (chondro, clusters ~ x * y) If the colour-coded variable is a factor, each level gets its own colour, and the legend is labeled accordingly.

different palette



To plot with a different palette, use trellis.args = list (col.regions = palette).

```
> print (plotmap (chondro, clusters ~ x * y,
+ col.regions = cluster.cols))
```

defined wavelengths



To plot a map of the average intensity at particular wavelengths use extraction:

Conditioning



```
> plotmap (chondro,
+          spc ~ y * x | x > 5,
+          col.regions = matlab.palette(20))
```

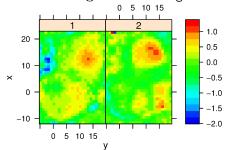
Conditioning on .wavelength



plotmap automatically applies the function in *func* before plotting. This defaults to the mean. In order to suppress this, use func = NULL. This allows conditioning on the wavelengths.

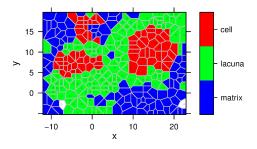
To plot e.g. the first two score maps of a principal component analysis:

Conditioning on .wavelength ${\bf II}$



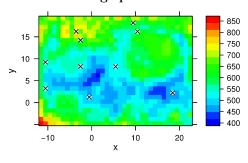
```
Alternatively, use levelplot directly:
> levelplot (spc ~ y * x | as.factor(.wavelength),
+ scores [,,1:2],
+ aspect = "iso",
+ col.regions = matlab.palette(20))
```

Voronoi plot



> plotvoronoi (sample (chondro, 300), clusters ~ x * y, + col.regions = matlab.palette(20)) Voronoi uses panel.voronoi from latticeExtra[2]. The tesselation is calculated by default using deldir[3], but tripack[4] can also be used. tripack seems to faster in general, but may "hang" with certain data sets (particularly regular grids with missing spectra as in this example). Furthermore, it is not FOSS (free and open source software).

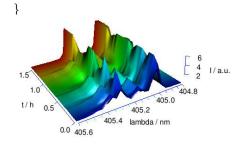
Mark missing spectra



If the spectra come from a rectangular grid, missing positions can be marked with this panel function:

8 3 D (with rgl)

3D plots with rgl

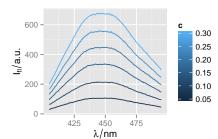


9 Using ggplot2 with hyperSpec objects

hyperSpec objects do not yet directly support plotting with ggplot2 [6]. Nevertheless, ggplot2 graphics can easily be obtained.

In general, as.long.df transforms a *hyperSpec* object into a long-form *data.frame* that is suitable for qplot, ggplot, etc:

plot spectra with as.long.df



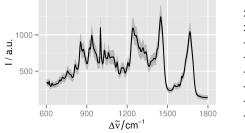
The two special columns .wavelength and .rownames contain the wavelength axis and allow to distinguish the spectra.

Note however, that long data.frames can be very memory consuming as they are of size $nrow \cdot nwl \times (ncol + 2)$ with respect to the dimensions of the hyperSpec object. Thus, e.g. the chondro data set $(2\,\mathrm{MB})$ as hyperSpec object) needs 24 MB as long-format data.frame. It is therefore highly recommended to calculate the particular data to be plotted beforehand. Moreover, depending on the particular plot as.data.frame or as.t.df may be more suitable than as.long.df:

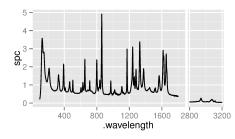
Map with ggplot2

```
> df <- as.long.df (apply (chondro, 1, mean))
> ggplot (df,aes (x = x, y = y, fill = spc)) +
+ geom_tile() +
+ scale_fill_gradientn ("spc", colours = matlab.palette ()) +
+ scale_y_continuous (expand = c (0, 0)) +
+ coord_equal ()
```

Mean \pm standard deviation with ggplot2



Cut spectra with ggplot2



```
Cut axes can be simulated by faceting. A factor is needed that indicates the respective ranges:

> df <- paracetamol [,, c( min ~ 1800, 2800 ~ max)] / 1e4

> df <- as.long.df (df)

> df$range <- factor (df$.wavelength > 2000)

> ggplot (df, aes (x = .wavelength, y = spc)) +

+ geom_line () +

+ facet_grid (. ~ range, labeller = function (...) "",

+ scales = "free", space = "free") +

+ scale_x_continuous (breaks = seq (0, 3200, 400)) +

+ opts (strip.background = theme_blank ())
```

10 Troubleshooting

10.1 No output is produced

plotmap, plotvoronoi, levelplot, and plotc use *lattice* functions. Therefore, in loops, functions, Sweave chunks, etc. the lattice object needs to be printed explicitly by print (plotmap (object)) (R FAQ: Why do lattice/trellis graphics not work?). The same holds for *ggplot2* graphics.

For suggestions how the lattice functions can be redefined so that the result is printed without external print command, see the file vignettes.defs.

11 Interactive Graphics

hyperSpec offers basic interaction, spc.identify for spectra plots, and map.identify and map.sel.poly

for maps. The first two identify points in spectra plots and map plots, respectively. map.sel.poly selects the part of a *hyperSpec* object that lies inside the user defined polygon.

11.1 spc.identify: finding out wavelength, intensity and spectrum

spc.identify allows to measure points in graphics produced by plotspc. It works correctly with reversed and cut wavelength axes.

```
> spc.identify (plotspc (paracetamol, wl.range = c (600 ~ 1800, 2800 ~ 3200), xoffset = 800))
```

The result is a data.frame with the indices of the spectra, the wavelength, and its intensity.

11.2 map.identify: finding a spectrum in a map plot

```
{\tt map.identify} returns the spectra indices of the clicked points.
```

```
> map.identify (chondro)
```

11.3 map.sel.poly: selecting spectra inside a polygon in a map plot

map.sel.poly returns a logical indicating which spectra are inside the polygon drawn by the user:
> map.sel.poly (chondro)

11.4 Related functions provided by base graphics and lattice

For base graphics (as produced by plotspc), locator may be useful as well. It returns the clicked coordinates. Note that these are *not* transformed according to xoffset & Co.

For lattice graphics, grid.locator may be used instead. If it is not called in the panel function, a preceding call to trellis.focus is needed:

```
> plot (laser, "mat")
> trellis.focus ()
> grid.locator ()
```

identify (or panel.identify for lattice graphics) allows to identify points of the plot directly. Note that the returned indices correspond to the plotted object.

11.5 Interactively changing graphics

hyperSpec's lattice functions work with playwith[7] and latticist [8]. These packages allow easy customization of the plots and also identification of points.

References

- [1] Lemon J. Plotrix: a package in the red light district of r. R-News, 6(4):8–12, 2006.
- [2] Deepayan Sarkar and Felix Andrews. latticeExtra: Extra Graphical Utilities Based on Lattice, 2012. URL http://CRAN.R-project.org/package=latticeExtra. R package version 0.6-24.
- [3] Rolf Turner. deldir: Delaunay Triangulation and Dirichlet (Voronoi) Tessellation., 2013. URL http://CRAN.R-project.org/package=deldir. R package version 0.0-22.

- [4] Fortran code by R. J. Renka. R functions by Albrecht Gebhardt. With contributions from Stephen Eglen <stephen@anc.ed.ac.uk>, Sergei Zuyev, and Denis White. tripack: Triangulation of irregularly spaced data, 2012. URL http://CRAN.R-project.org/package=tripack. R package version 1.3-5.
- [5] Daniel Adler and Duncan Murdoch. rgl: 3D visualization device system (OpenGL), 2013. URL http://CRAN.R-project.org/package=rgl. R package version 0.93.935.
- [6] Hadley Wickham. ggplot2: elegant graphics for data analysis. Springer New York, 2009. ISBN 978-0-387-98140-6. URL http://had.co.nz/ggplot2/book.
- [7] Felix Andrews. playwith: A GUI for interactive plots using GTK+, 2012. URL http://CRAN.R-project.org/package=playwith. R package version 0.9-54.
- [8] Felix Andrews. latticist: A Graphical User Interface for Exploratory Visualisation, 2012. URL http://latticist.googlecode.com/. R package version 0.9-44.

Session Info

```
[,1]
               "Linux"
sysname
               "3.2.0-45-generic"
release
               "#70-Ubuntu SMP Wed May 29 20:12:06 UTC 2013"
version
               "cbdesktop"
nodename
               "x86_64"
machine
              "unknown"
login
               "cb"
user
effective_user "cb"
R version 3.0.1 (2013-05-16)
Platform: x86_64-pc-linux-gnu (64-bit)
locale:
 [1] LC_CTYPE=de_DE.UTF-8
                               LC NUMERIC=C
                                                           LC_TIME=de_DE.UTF-8
 [4] LC_COLLATE=de_DE.UTF-8
                               LC_MONETARY=de_DE.UTF-8
                                                           LC_MESSAGES=de_DE.UTF-8
 [7] LC_PAPER=C
                               LC_NAME=C
                                                           LC_ADDRESS=C
[10] LC_TELEPHONE=C
                               LC_MEASUREMENT=de_DE.UTF-8 LC_IDENTIFICATION=C
attached base packages:
[1] grid
              stats
                      graphics grDevices utils
                                                     datasets methods
other attached packages:
[1] ggplot2_0.9.3.1
                            deldir_0.0-22
                                                   latticeExtra_0.6-24
                                                                            RColorBrewer_1.0-5
                            hyperSpec_0.98-20130607 mvtnorm_0.9-9995
[5] plotrix_3.4-7
                                                                           lattice_0.20-15
loaded via a namespace (and not attached):
 [1] colorspace_1.2-2 dichromat_2.0-0 digest_0.6.3
                                                        gtable_0.1.2
                                                                        labeling_0.1
 [6] MASS_7.3-26
                     munsell_0.4
                                      plyr_1.8
                                                       proto_0.3-10
                                                                        reshape2_1.2.2
[11] scales_0.2.3
                     stringr_0.6.2
                                      tools_3.0.1
```