hyperSpec Plotting functions

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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.

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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 ± 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)
```

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

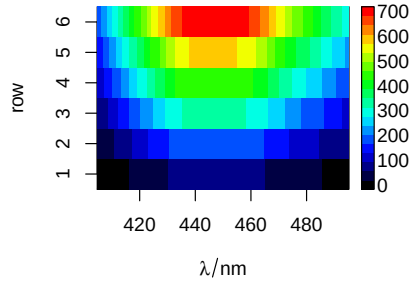
`plotc` calibration plot, time series, depth profile
`plotc` is a *lattice* function

`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?).

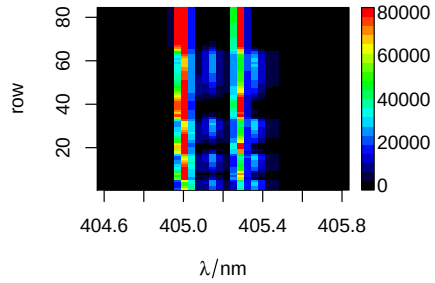
plotspc



plots the spectra, i. e. the intensities `$spc` over the wavelengths `@wavelength`.

```
> plotspc (flu)
```

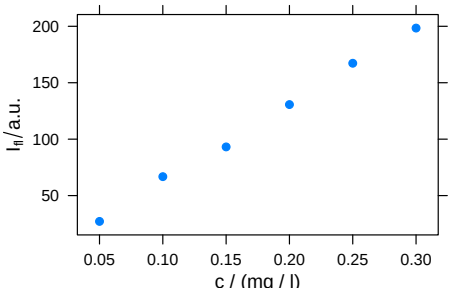
plotmat



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

```
> plotmat (flu)
```

plotc

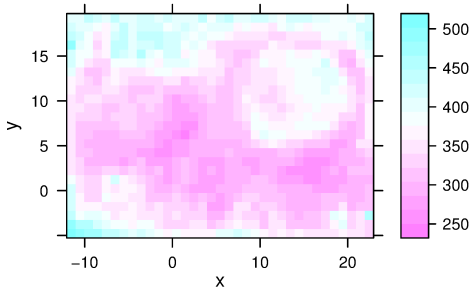


plots an intensity over a single other data column, e. g.

- calibration
- time series
- depth profile

```
> plotc (flu)
```

levelplot

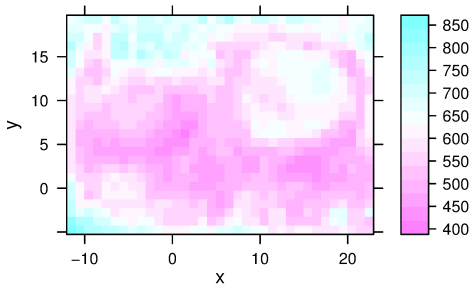


plots a false colour map, defined by a formula.

```
> levelplot (spc ~ x * y, chondro, aspect = "iso")
```

Warning: `Only first wavelength is used for plotting`

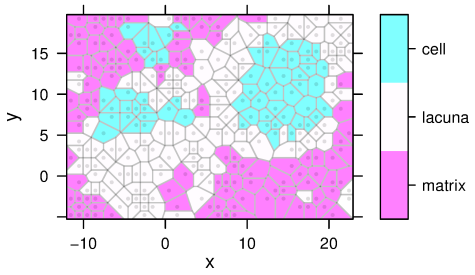
plotmap



plotmap is a specialized version of levelplot. 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)
```

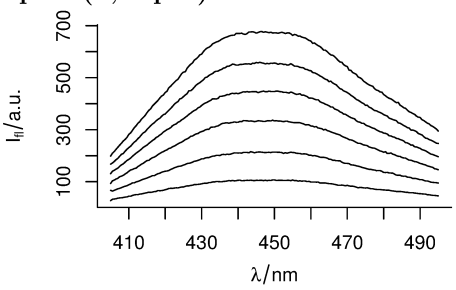
```
PLEASE NOTE:  The components "delsgs" and "summary" of the
object returned by deldir() are now DATA FRAMES rather than
matrices (as they were prior to release 0.0-18).
See help("deldir").

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.

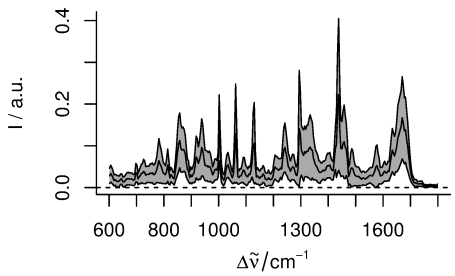
plot (x, "spc")



is equivalent to `plotspc (flu)`

```
> plot (flu, "spc")
```

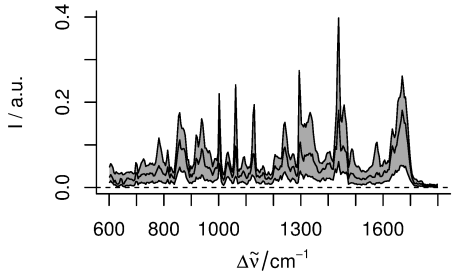
plot (x, "spcmeansd")



plots mean spectrum ± 1 standard deviation

```
> plot (chondro.preproc, "spcmeansd")
```

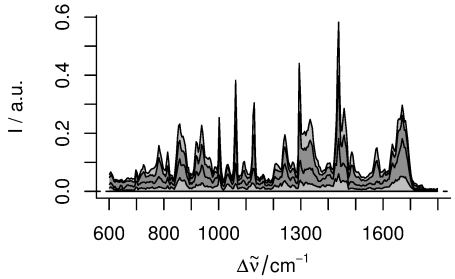
plot (x, "spcprctile")



plots median, 16^{th} and 84^{th} percentile for each wavelength. For Gaussian distributed data, 16^{th}, 50^{th} and 84^{th} percentile are equal to mean ± 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")
```

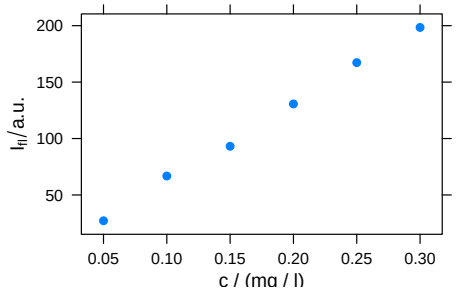
plot (x, "spcprctl5")



like `"spcprctl"` plus 5^{th} and 95^{th}percentile.

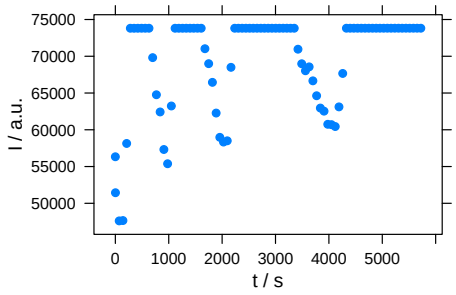
```
> plot (chondro.preproc, "spcprctl5")
```

plot (x, "c")



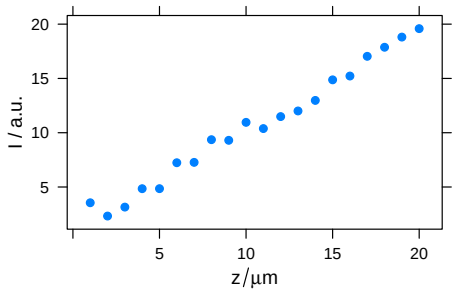

```
> plot (flu, "c")
```
is equivalent to `plotc (flu)`

plot (x, "ts")



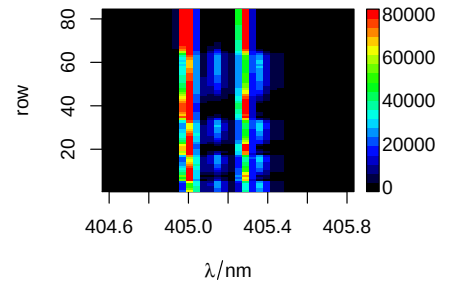
plots a time series plot
```
> plot (laser [,, 405], "ts")
```
equivalent to `plotc (laser, spc ~ t)`

plot (x, "depth")



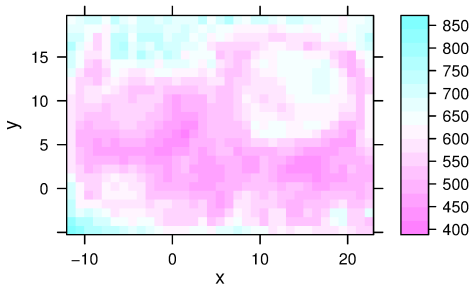
plots a depth profile plot
```
> depth.profile <- new ("hyperSpec",
+     spc = as.matrix (rnorm (20) + 1:20),
+     data = data.frame (z = 1 : 20),
+     labels = list (spc = "I / a.u.",
+        z = expression (`/` (z, mu*m)),
+        .wavelength = expression (lambda)))
> plot (depth.profile, "depth")
```
the same as `plotc (laser, spc ~ z)`

plot (x, "mat")



plots the spectra matrix.
```
> plot (laser, "mat")
```
Equivalent to
```
> plotmat (laser)
```
A lattice alternative is:
```
> levelplot (spc ~ .wavelength * .row, laser)
```

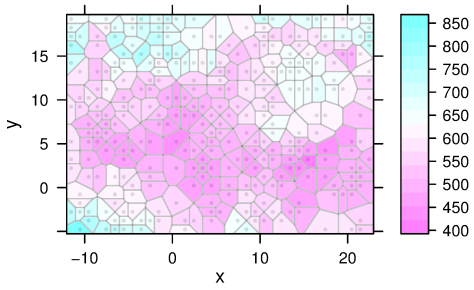
plot (x, "map")



is equivalent to `plotmap (chondro)`

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

plot (x, "voronoi")




```
> plot (sample (chondro, 300), "voronoi")
```

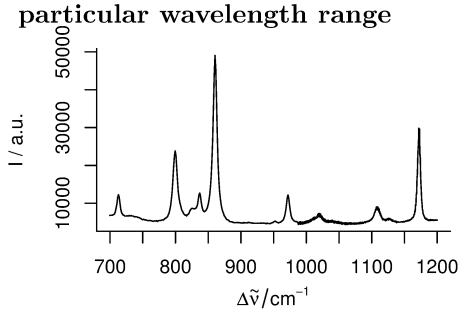
See `plotvoronoi`

3 Spectra

`plotspc`

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

particular wavelength range

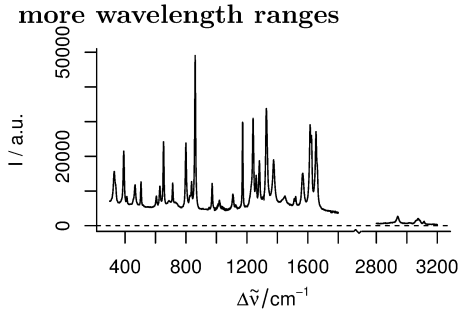


if only one wavelength range is needed, the extract command (see `vignette ("introduction")`) is handiest:

```
> plotspc (paracetamol [,, 700 ~ 1200])
```

wavelengths. If `wl.range` already contains indices use `wl.index = TRUE`.

more wavelength ranges

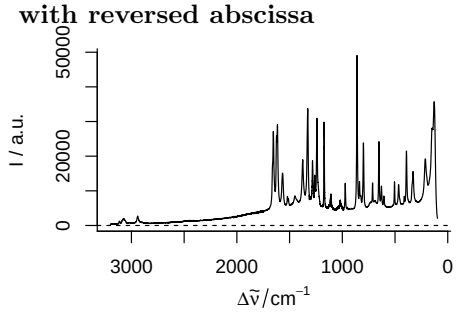


use `wl.range = list (600 ~ 1800, 2800 ~ 3100)`. Cut the wavelength axis appropriately with `xoffset = 750`

```
> plotspc (paracetamol,
+          wl.range = c (300 ~ 1800, 2800 ~ max),
+          xoffset = 750)
```

If available, the package *plotrix*[1] is used to produce the cut mark.

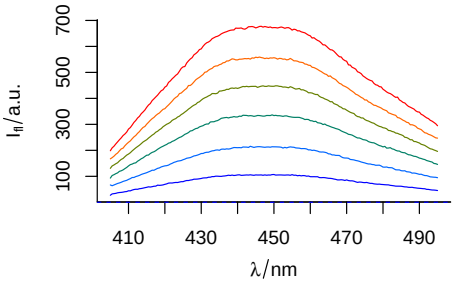
with reversed abscissa



use `wl.reverse = TRUE`

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

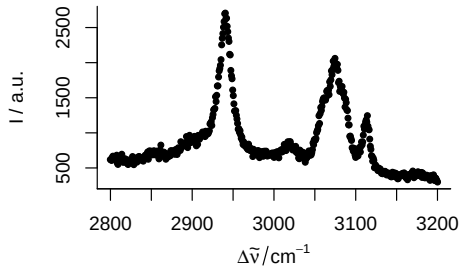
in different colours



use `col = vector.of.colours`

```
> plotspc (flu, col = matlab.dark.palette (6))
```

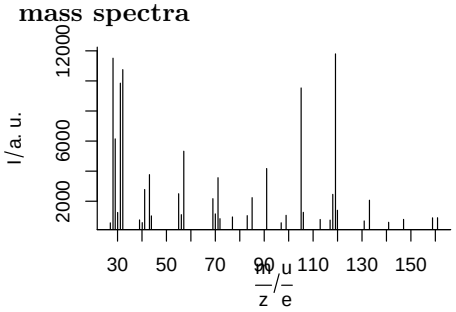
dots instead of lines



use `lines.args = list (pch = 20, type = "p")`

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

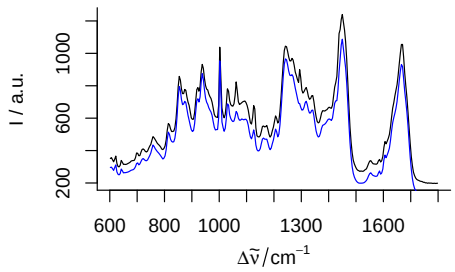
mass spectra



use `lines.args = list (type = "h")`

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

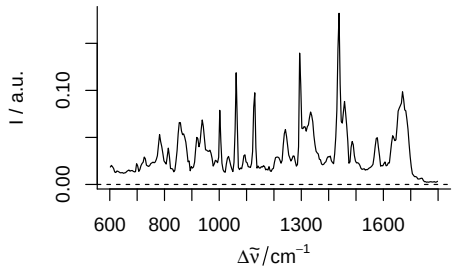
more spectra into an existing plot



use `add = TRUE`

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

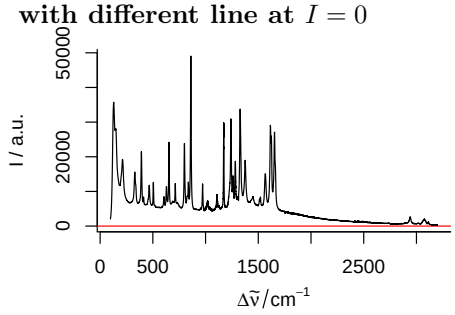
Summary characteristics



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)
```

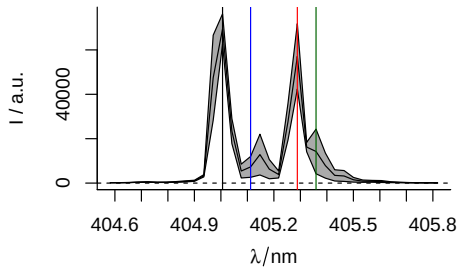
with different line at $I = 0$



zeroline takes a list with parameters to `abline`, `NA` suppresses the line.

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

adding to a spectra plot

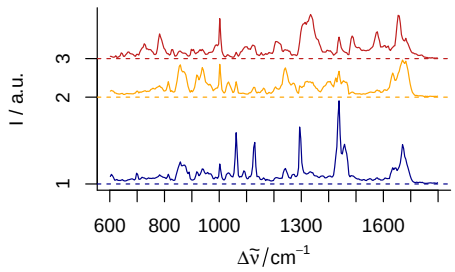


`plotspc` uses base graphics. After plotting the spectra, more content may be added to the graphic by `abline`, `lines`, `points`, etc.

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

3.1 Stacked spectra

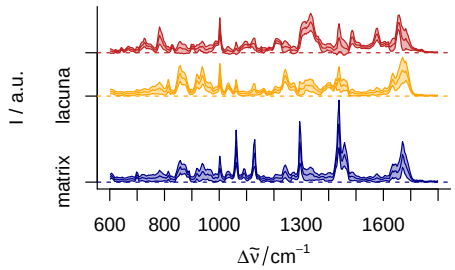
stacked



use `stacked = TRUE`

```
> plotspc (cluster.means,
+          col = cluster.cols,
+          stacked = TRUE)
```

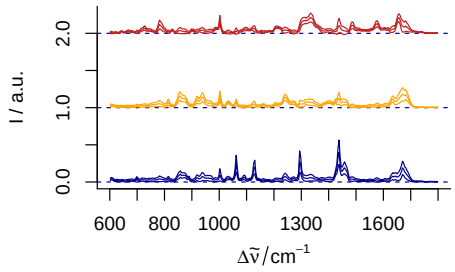
Stacking groups of spectra



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)
```

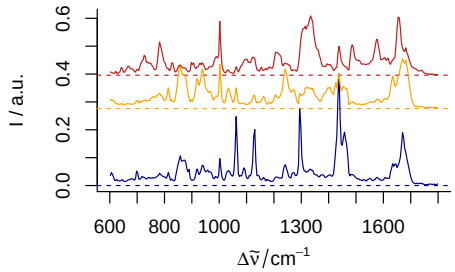
Manually giving yoffset



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))
```

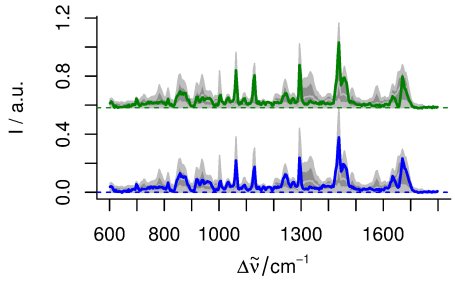
Dense stacking



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




```
> yoffset <- apply (chondro.preproc, 2, quantile, c(0.05, 0.95))
> yoffset <- range (yoffset)
> plot(chondro.preproc[1],
+      plot.args = list (ylim = c (0, 2) * yoffset),
+      lines.args = list( type = "n"))
> yoffset <- (0:1) * diff (yoffset)
> for (i in 1 : 3){
+   plot(chondro.preproc, "spcprctl5", yoffset = yoffset [i],
+        col = "gray", add = TRUE)
+   plot (chondro.preproc [i], yoffset = yoffset [i],
+         col = matlab.dark.palette (3) [i], add = TRUE,
+         lines.args = list (lwd = 2))
+ }
```

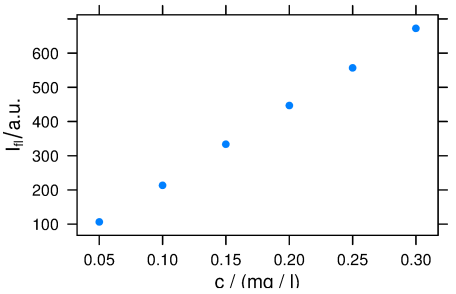
`plotspc` allows fine grained customization of almost all aspects of the plot. This is possible by giving arguments to the functions that actually perform the plotting `plot` for setting up the plot area, `lines` for the plotting of the lines, `axis` for the axes, etc. The arguments for these functions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

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

`plotc`

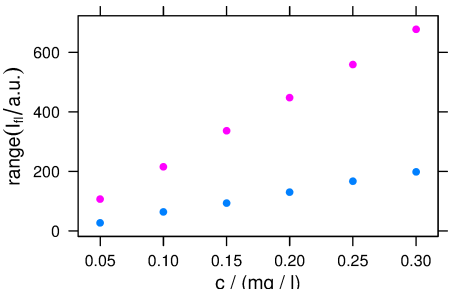
4.1 Calibration plots

Intensities over concentration



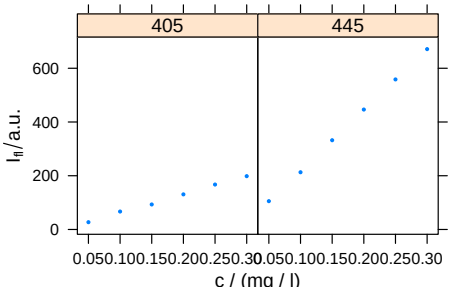
Plotting the Intensities of one wavelength over the concentration for univariate calibration:
`> plotc (flu [,, 450])`
The default is to use the first intensity only.

Summary Intensities over concentration



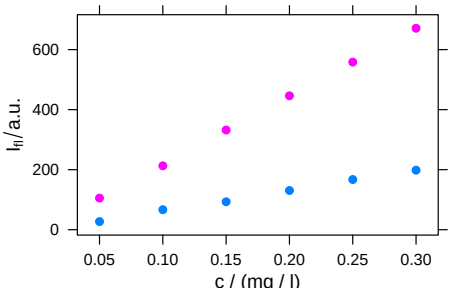
A function to compute a summary of the intensities before drawing can be used:
`> plotc (flu, func = range, groups = .wavelength)`
If `func` returns more than one value, the different results are accessible by `.wavelength`.

Conditioning: plotting more traces separately



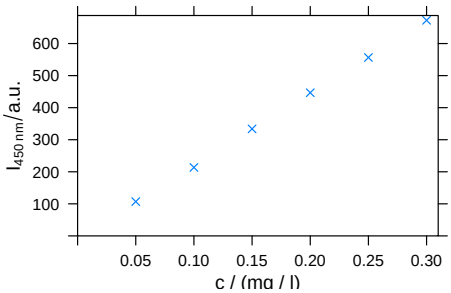

```
> plotc (flu [,, c (405, 445)], spc ~ c | .wavelength,
+        cex = .3, scales = list (alternating = c(1, 1)))
```

Grouping: plot more traces in one panel




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

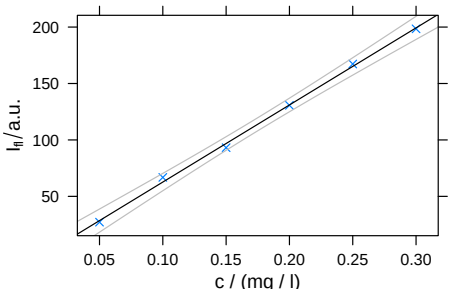
Changing Axis Labels (and other parameters)



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

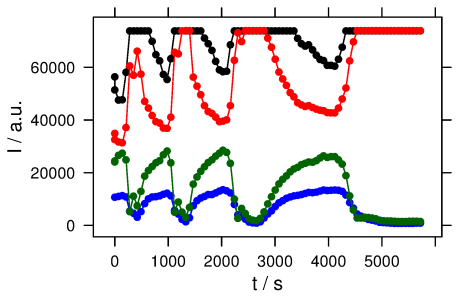


As `plotc` uses the *lattice* function `xyplot`, additions to the plot must be made via the panel function:

```
> 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:

```
>  plotc (laser [,, c(405.0063, 405.1121, 405.2885, 405.3591)],
+         spc ~ t,
+         groups = .wavelength,
+         type = "b",
+         col = c ("black", "blue", "red", "darkgreen"))
```

5 Levelplot

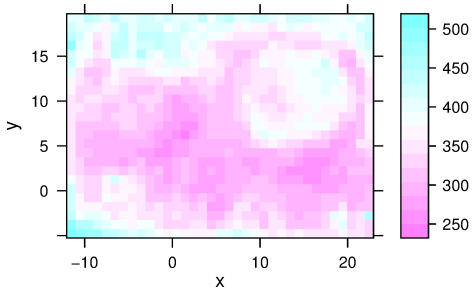
hyperSpec's *levelplot* can use two special column names:

.wavelength for the wavelengths

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

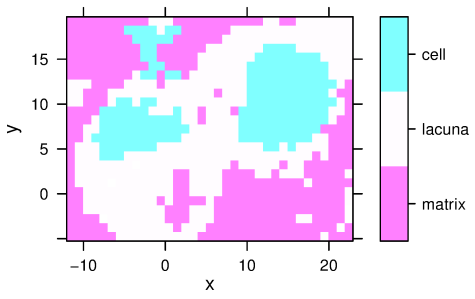
Besides that, it behaves exactly like *levelplot*. Particularly, the data is given as the *second* argument:

levelplot




```
>  levelplot (spc ~ x * y, chondro)
```

factors as z



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

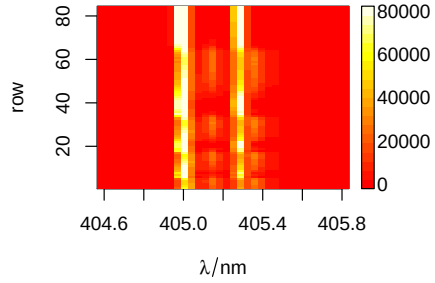
```
>  levelplot (clusters ~ x * y, chondro)
```

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.

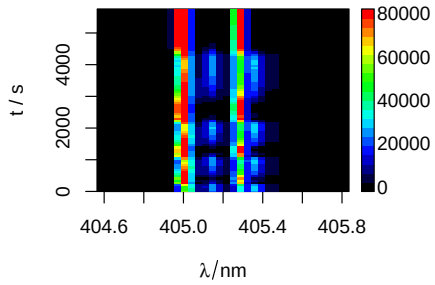
This can be done by `plot (object, "mat")`. The actual plotting is done by `image`, but `levelplot` can produce spectra matrix plots as well and these plots can be grouped or conditioned.

different palette




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

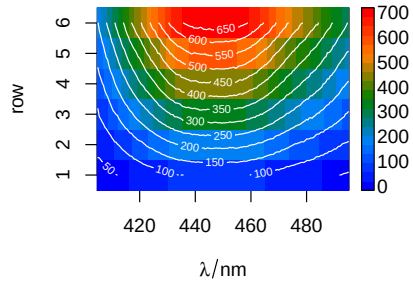
different y axis



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

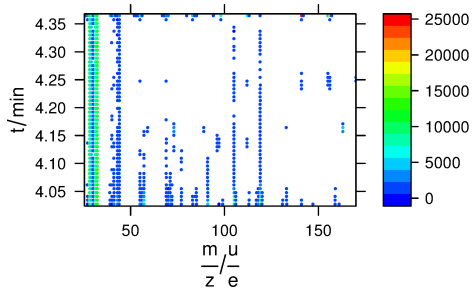
```
> plotmat (laser, y = laser$t, ylab = labels (laser, "t"))
```

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**

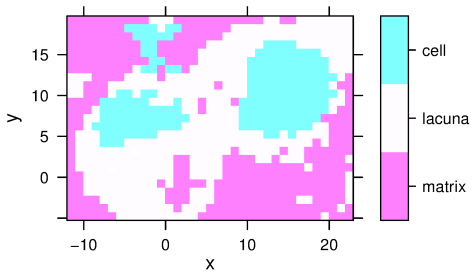



```
> require ("latticeExtra")
> barb <- do.call (collapse, barbiturates[1:50])
> barb <- orderwl (barb)
> levelplot (spc ~ .wavelength * z, barb,
+            panel = panel.levelplot.points,
+            cex = .33, col.symbol = NA,
+            col.regions = matlab.palette)
```

7 False-Colour Maps: `plotmap`

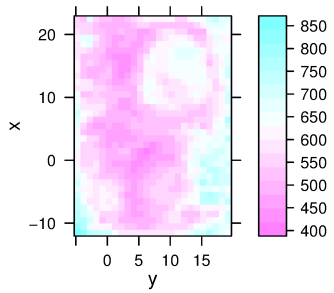
`plotmap` is a specialized version of `levelplot`. The spectral intensities may be summarized by a function before plotting (default: `mean`). The same scale is used for x and y axes (*aspect = "iso"*).

plotting map




```
> plotmap (chondro)
```

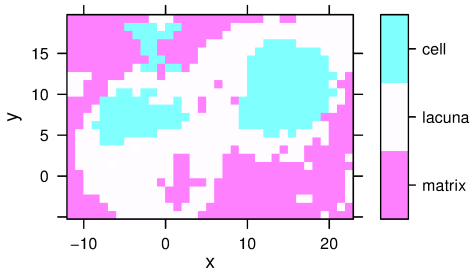
plotting maps with other than x and y



specify the colour-coded variable, abscissa and ordinate as formula: `colour.coded ~ abscissa * ordinate`

```
> plotmap (chondro, spc ~ y * x)
```

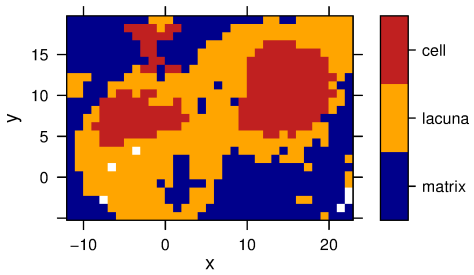
colour-coded factors




```
> 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.

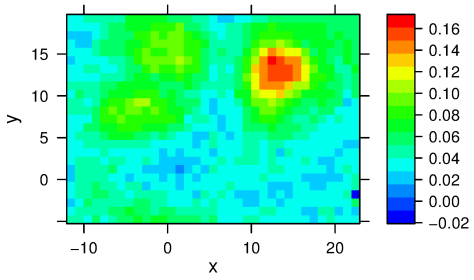
different palette



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

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

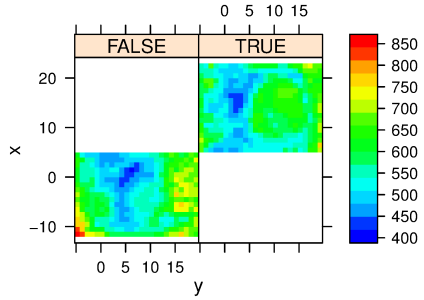
defined wavelengths



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

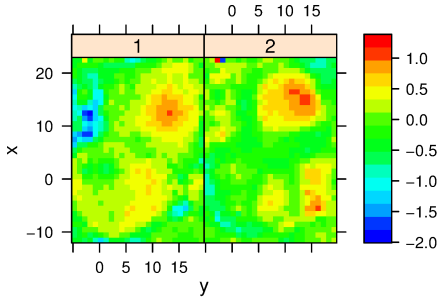
```
> plotmap (chondro.preproc [, , c(728, 782, 1098,
+                                 1240, 1482, 1577)],
+          col.regions = matlab.palette)
```

Conditioning




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

Conditioning on `.wavelength`

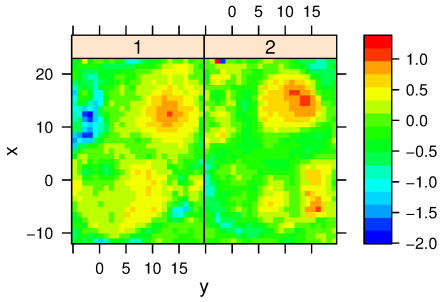


`plotmap` automatically applies the function in *func* before plotting. This defaults to the `mean`. In order to suppress this, use `func = NULL`. This allows conditioning on the wavelengths.

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

```
> pca <- prcomp (~ spc, data = chondro.preproc$.)
> scores <- decomposition (chondro, pca$x,
+                          label.wavelength = "PC",
+                          label.spc = "score /  a.u.")
> plotmap (scores [,,1:2],
+          spc ~ y * x | as.factor(.wavelength),
+          func = NULL,
+          col.regions = matlab.palette(20))
```

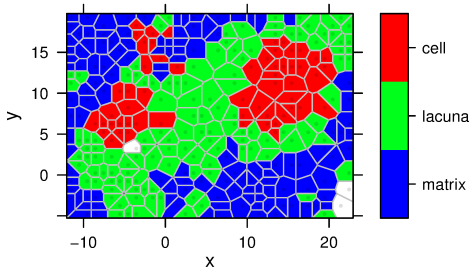
Conditioning on `.wavelength` II



Alternatively, use `levelplot` directly:

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

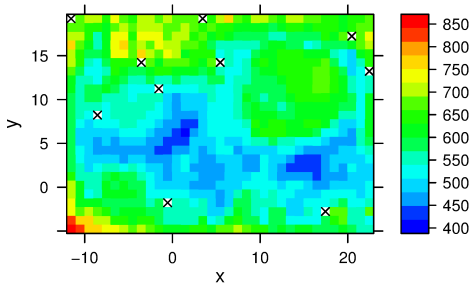
Voronoi plot




```
> 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



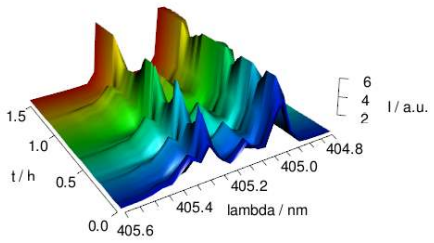
If the spectra come from a rectangular grid, missing positions can be marked with this panel function:

```
> mark.missing <- function (x, y, z, ...){
+   panel.levelplot (x, y, z, ...)
+
+   miss <- expand.grid (x = unique (x), y = unique (y))
+   miss <- merge (miss, data.frame (x, y, TRUE),
+                  all.x = TRUE)
+   miss <- miss [is.na (miss[, 3]),]
+   panel.xyplot (miss [, 1], miss [, 2], pch = 4, ...)
+ }
> plotmap (sample (chondro, 865),
+          col.regions = matlab.palette(20),
+          col = "black",
+          panel = mark.missing)
```

8 3 D (with rgl)

3D plots with *rgl*

}



rgl[5] offers fast 3d plotting in R. As *rgl*'s axis annotations are sometimes awkward, they may better be set manually:

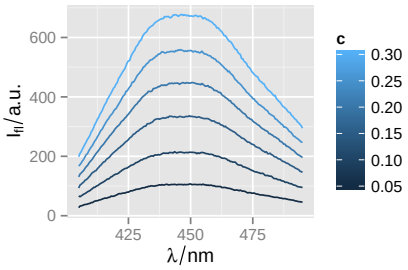
```
> laser <- laser [,,404.8 ~ 405.6] / 10000
> laser$t <- laser$t / 3600
> cols <- rep (matlab.palette (nrow (laser)), nwl (laser))
> surface3d (y = wl (laser), x = laser$t,
+            z = laser$spc, col =  cols)
> aspect3d (c (1, 1, 0.25))
> axes3d (c ('x+-', 'y--', 'z--'))
> axes3d ('y--', nticks = 25, labels= FALSE)
> mtext3d ("t / h", 'x+-', line = 2.5)
> mtext3d ("lambda / nm", 'y--', line = 2.5)
> mtext3d ("I / a.u.", edge = 'z--', line = 2.5)
```

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`

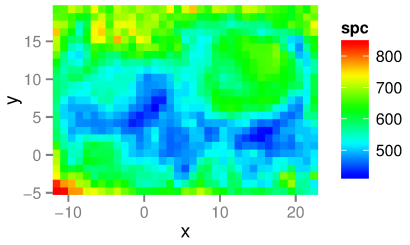



```
> df <- as.long.df (flu, rownames = TRUE)
> ggplot (df, aes (x = .wavelength, y = spc,
+                  colour = c, group = .rownames)) +
+   geom_line () +
+   xlab (labels (flu)$.wavelength) +
+   ylab (labels (flu)$spc)
```

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

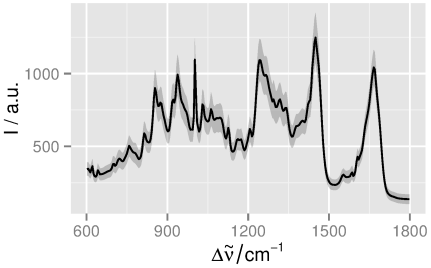
Note however, that long *data.frames* can be *very* memory consuming as they are of size $nrow \cdot nwl \times (ncol + 2)$ with respect to the dimensions of the *hyperSpec* object. Thus, e. g. the `chondro` data set (2 MB) as *hyperSpec* object) needs 24 MB as long-format *data.frame*. It is therefore 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*



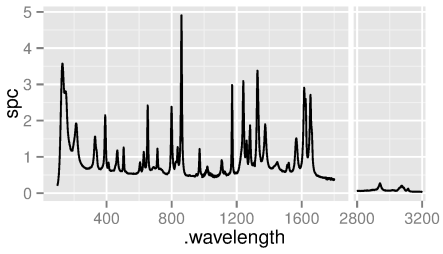

```
> df <- as.long.df (apply (chondro, 1, mean))
> ggplot (df,aes (x = x, y = y, fill = spc)) +
+   geom_tile() +
+   scale_fill_gradientn ("spc", colours = matlab.palette ()) +
+   scale_x_continuous (expand = c (0, 0)) +
+   scale_y_continuous (expand = c (0, 0)) +
+   coord_equal ()
```

Mean ± standard deviation with *ggplot2*




```
> df <- as.t.df (apply (chondro, 2, mean_pm_sd))
> ggplot (df, aes (x = .wavelength)) +
+   geom_ribbon (aes (ymin = mean.minus.sd,
+                     ymax = mean.plus.sd),
+                alpha = 0.25) +
+   geom_line (aes (y = mean)) +
+   xlab (labels (chondro)$.wavelength) +
+   ylab (labels (chondro)$spc)
```

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

`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.*, 2012. URL http://CRAN.R-project.org/package=deldir. R package version 0.0-21.

[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)*, 2012. URL http://CRAN.R-project.org/package=rgl. R package version 0.92.894.

[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]
sysname        "Linux"
release        "3.2.0-38-generic"
version        "#59-Ubuntu SMP Tue Feb 5 17:53:03 UTC 2013"
nodename       "cb-t61p"
machine        "x86_64"
login          "unknown"
user           "cb"
effective_user "cb"

R version 2.15.2 (2012-10-26)
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   base

other attached packages:
[1] ggplot2_0.9.3           deldir_0.0-21           latticeExtra_0.6-24     RColorBrewer_1.0-5
[5] plotrix_3.4-5           hyperSpec_0.98-20130209 mvtnorm_0.9-9994        lattice_0.20-13

loaded via a namespace (and not attached):
 [1] colorspace_1.2-0 dichromat_1.2-4  digest_0.6.1     gtable_0.1.2     labeling_0.1
 [6] MASS_7.3-23      munsell_0.4      plyr_1.8         proto_0.3-10     reshape2_1.2.2
[11] scales_0.2.3     stringr_0.6.2    tools_2.15.2
```