



# hyperSpec: working with spectroscopic data

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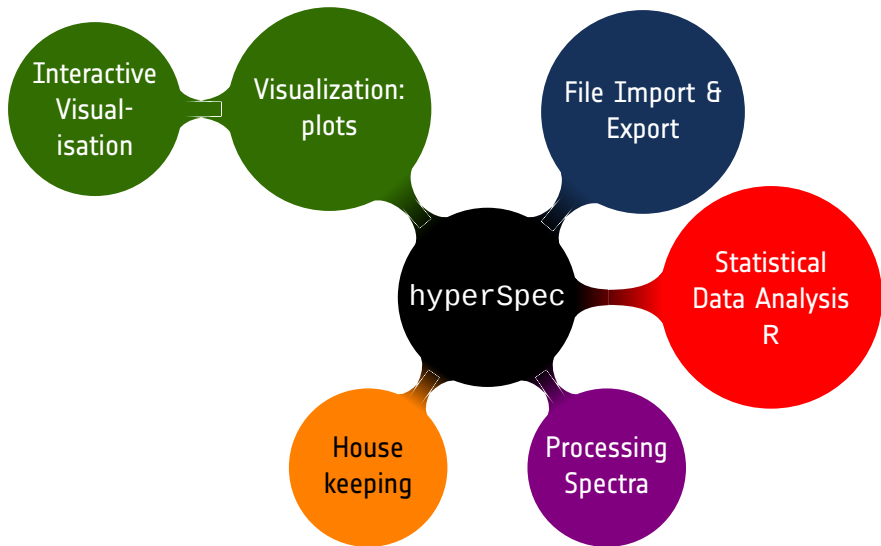
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<sup>2</sup>Institute of Photonic Technology, Jena/Germany

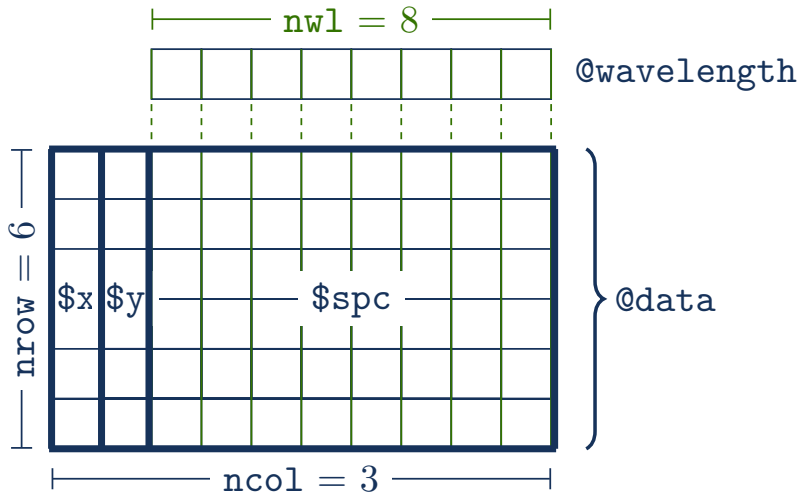
<sup>3</sup>Abbe Center of Photonics, University Jena/Germany

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# hyperSpec's Data Structure



# hyperSpec's Data Structure

```
> chondro
```

```
hyperSpec object
```

```
  875 spectra
```

```
  4 data columns
```

```
  300 data points / spectrum
```

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

```
data: (875 rows x 4 columns)
```

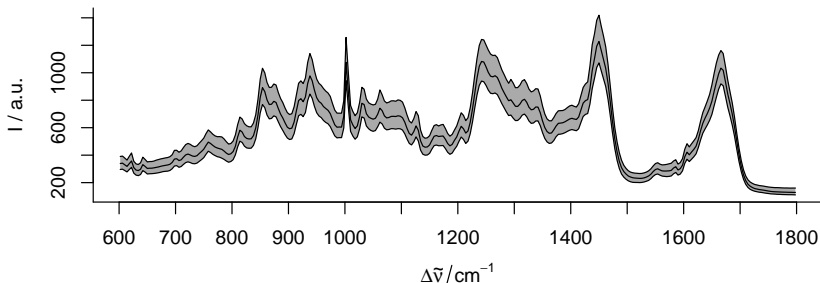
```
  1. y: y/(mu * m) [numeric] -4.77 -4.77 ... 19.23
```

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

```
  3. clusters: clusters [factor] matrix matrix ... lacuna + NA
```

```
  4. spc: I / a.u. [matrix300] 501.8194 500.4552 ... 169.2942
```

# Pre-Processing



```
> baselines <- spc.fit.poly.below (chondro)
```

```
Fitting with npts.min = 15
```

```
> chondro <- chondro - baselines
```

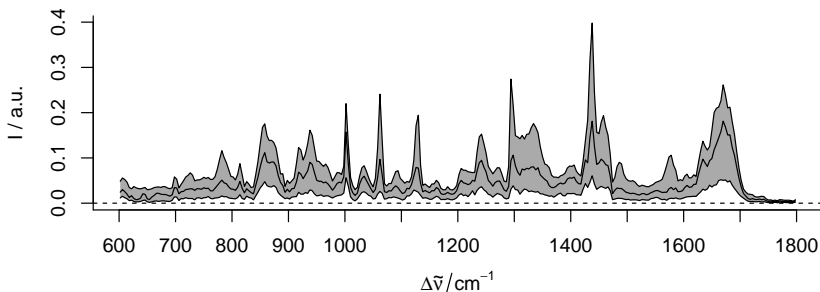
```
> chondro <- sweep (chondro, 1, mean, '/')
```

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

```
> chondro <- sweep (chondro, 2, minspc, '-')
```

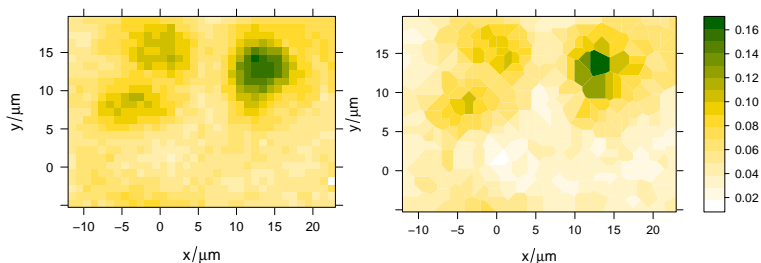
```
> plot (chondro, "spcprctile")
```

# Pre-Processing



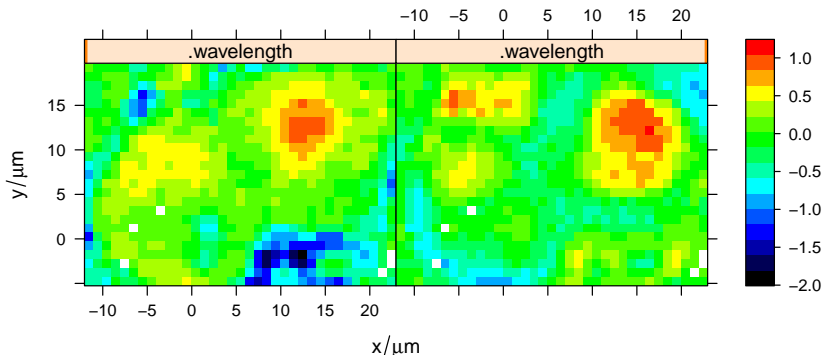
```
> baselines <- spc.fit.poly.below (chondro)
Fitting with npts.min = 15
> chondro <- chondro - baselines
> chondro <- sweep (chondro, 1, mean, '/')
> minspc <- apply (chondro, 2, quantile, 0.05)
> chondro <- sweep (chondro, 2, minspc, '-')
> plot (chondro, "spcprctile")
```

# Plotting Spectral Maps



```
> cols <- colorRampPalette(c("white", "gold", "dark green"), sp  
> DNA <- c(728, 782, 1098, 1240, 1482, 1577)  
> plotmap(chondro[, , DNA], col.regions = cols)  
> spc <- sample(chondro, 300)  
> plotvoronoi(spc[, , DNA], col.regions = cols,  
+             border = NA, points = FALSE)
```

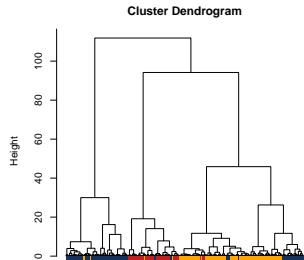
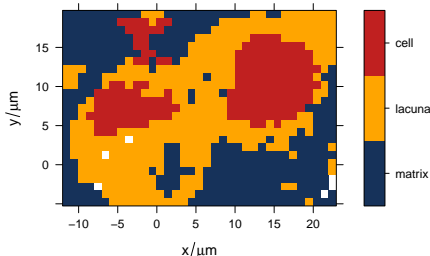
# Modeling with data.frame: PCA



```
> pca <- prcomp (~ spc, chondro$.)
> scores <- decomposition (chondro, pca$x)
> plotmap (scores [, , 1 : 2],
+         spc ~ x * y | .wavelength,
+         func = NULL, col.regions = alois.palette)
```

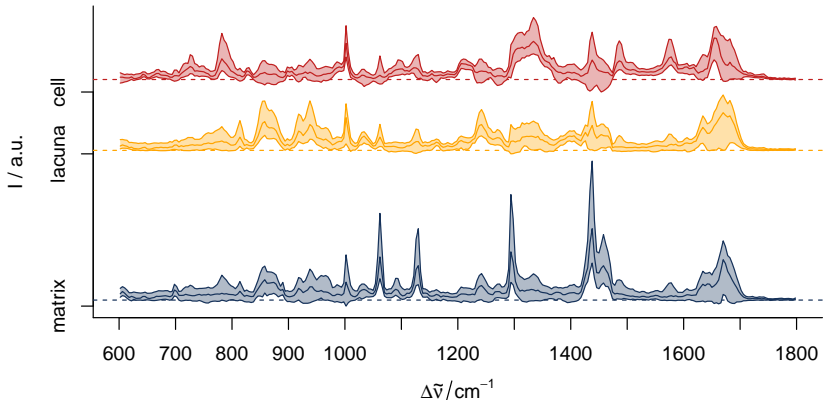


# Modeling with Matrix: HCA



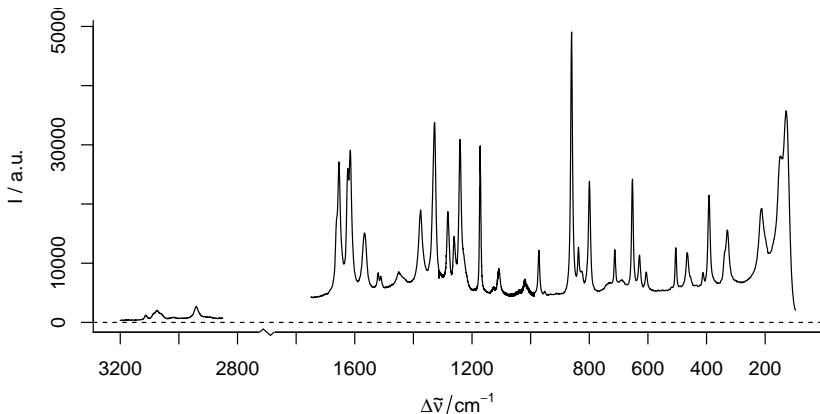
```
> dist <- dist (chondro [,,,])
> dendrogram <- hclust (dist, method = "ward")
> plot (dendrogram, hang = -1, labels = FALSE)
> mark.dendrogram (dendrogram, chondro$clusters,
+                  col = cols, pos.text=NA)
> chondro$cluster <- as.factor (cutree (dendrogram, k = 3))
```

# Plotting Spectra Groupwise



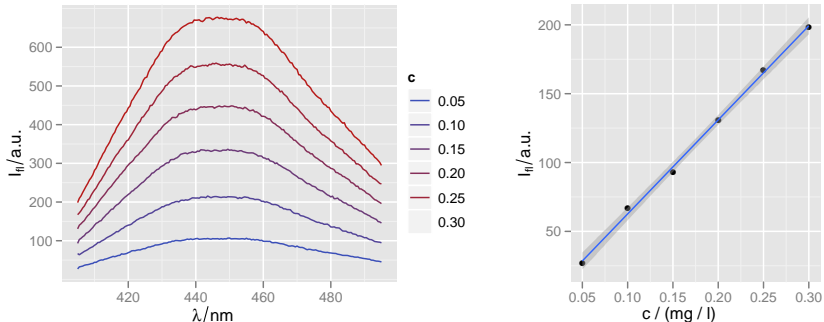
```
> spc <- aggregate (chondro, chondro$clusters,  
+                   quantile, probs = c (.05, .5, .95))  
> plot (spc, col = cols,  
+       stacked = ".aggregate", fill = ".aggregate")
```

# Plotting The Other Way Round



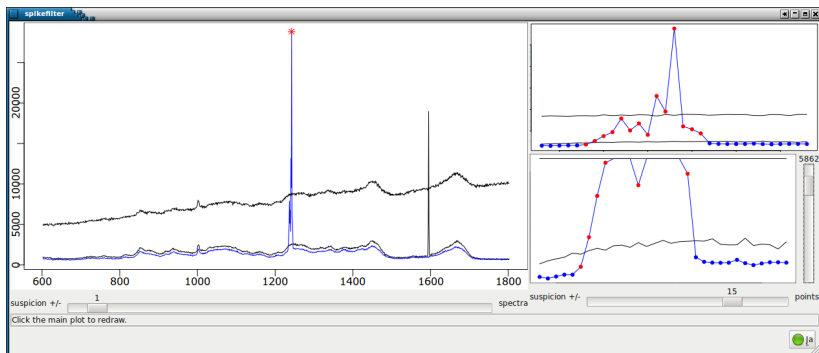
```
> plot (paracetamol, wl.reverse = TRUE,  
+       wl.range = c (min ~ 1750, 2850 ~ 3300), xoffset = 800)
```

## ggplot2



```
> qplotspc (flu) + aes (colour = c)  
> qplotc (flu) + stat_smooth (method = "lm")
```

# Interactive Functions: spike filtering



```

> library ("hyperSpecGUI")
> tmp <- sweep (cartilage, 1, median, '/')
> tmp <- sweep (tmp, 2, median, '-')
> spikiness <- spikefilter2d (spcmatrix = tmp [ [] ])
> suspicions <- make.suspicions (spikiness)
> spikes <- spikes.interactive.cb (cartilage, suspicions)

```

# Acknowledgements



- Homepage:  
`hyperSpec.r-forge.r-project.org`
- Contact:  
`Claudia.Beleites@ipht-jena.de`
- Installation:  
`install.packages ("hyperSpec",  
repos = "http://r-forge.r-project.org")`
- Documentation:  
check out the vignettes

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