Unstable Laser Emission
Vignette for the Data Set `laser` of the R package hyperSpec

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Reproducing the Examples in this Vignette

All spectra used in this manual are installed automatically with *hyperSpec*.
The source data files can be found with the command:
```
> Sys.glob (paste (.libPaths (), "hyperSpec/doc/rawdata/laser.txt", sep = "/"))
```

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1 Introduction

This data set consists of a time series of 84 spectra of an unstable laser emission at 405 nm recorded during ca. 1.5 h.

The spectra were recorded during the installation of the 405 nm laser at a Raman spectrometer. There is no Raman scattering involved in this data, but the Raman software recorded the abscissa of the spectra as Raman shift in wavenumbes.

2 Loading the Data and Preprocessing

```
> library (hyperSpec)
> laser <- scan.txt.Renishaw ("rawdata/laser.txt", data = "ts")
> plot (laser, "spcprctl5")
```

As the laser emission was recorded with a Raman spectrometer, the wavelength axis initially is the Raman shift in wavenumbers (cm^{-1}).

As most of the spectra do not show any signal (fig. 1a), so the spectral range can be cut to -75 – 0 cm^{-1}. Note that negative numbers in the spectral range specification with the tilde do not exclude the spectral range but rather mean negative values of the wavelength axis. The results are shown in figure 1b.

```
> laser <- laser [,,-75~0]
> plot (laser, "spcprctl5")
```

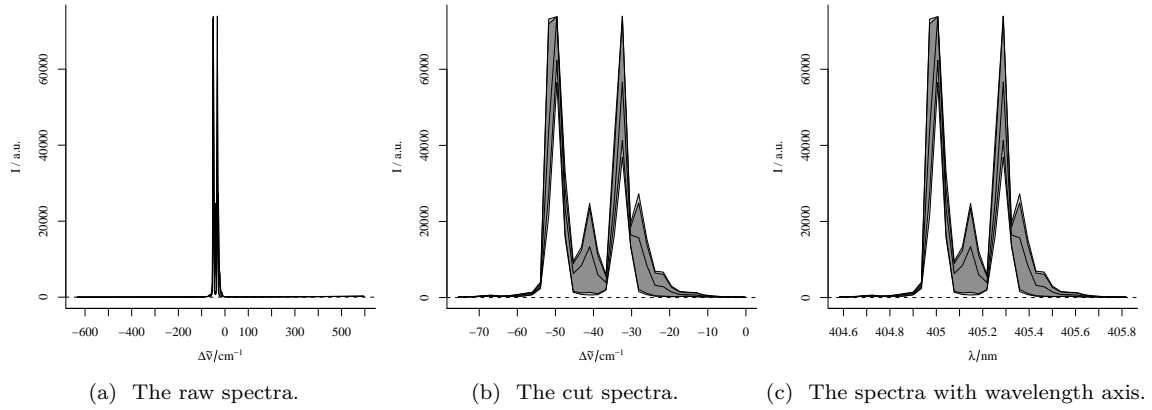| (a) The raw spectra. | (b) The cut spectra. | (c) The spectra with wavelength axis. |

Figure 1: The laser emission spectra.

The wavelength axis was recorded as Raman shift from 405 nm. However, the spectra were taken before calibrating the wavelength axis. The band at -50 cm⁻¹ is known to be at 405 nm.

```
> wl (laser) <- wl (laser) + 50
```

Furthermore, as the spectra are not Raman shift but emission, the wavelength axis should be converted to proper wavelengths in nm.

The Raman shift is calculated from the wavelength as follows:

$$\Delta\tilde{\nu} = \frac{1}{\lambda_0} - \frac{1}{\lambda}$$

with $\Delta\tilde{\nu}$ being the Raman shift, and λ_0 the excitation wavelength for a Raman process, here 405 nm.

The wavelengths corresponding to the wavenumbers are thus:

$$\lambda = \frac{1}{\frac{1}{\lambda_0} - \Delta\tilde{\nu}}$$

Taking into account that $1 \text{ cm} = 10^7$ nm, we arrive at the new wavelength axis:

```
> wl (laser) <- list (
+    wl = 1e7 / (1/405e-7 - wl (laser)),
+    label = expression (lambda / nm)
+    )
```

```
> plot (laser, "spcprctl5")
```

Note that the new wavelength axis label is immediately assigned as well.

Now, save laser as the laser data set shipped with *hyperSpec*.

```
> save (laser, file = "laser.rda")
> laser
```

2

```
hyperSpec object
   84 spectra
   2 data columns
   36 data points / spectrum
wavelength: lambda/nm [numeric 36]  404.6 404.6 ... 405.8
data:  (84 rows x 2 columns)
   (1) t: t / s [numeric 84] range 0 2 ... 5722
   (2) spc: I / a.u. [AsIs matrix 84 x 36] range 98.04 98.06 ... 73934
```

3 Inspecting the time dependency of the laser emission

The maxima of the different emission lines encountered during this measurement are data points 13, 17, 21, and 23 (fig. 2a):

```
> wl2i (laser, locator()$x)
```

```
> plot (laser, "spcmeansd")
> abline (v = wl (laser)[c (13, 17, 21, 23)], col = c("black", "blue", "red", "darkgreen") )
```

plotc can also be used to plot time-series. In that case, the abscissa needs to be specified in parameter use.c. The collection time is stored in column $t in seconds from start of the measurement, and can be handed over as the column name. The resulting time series are shown in figure 2b variable,

```
> plotc (laser[,,13, wl.index = TRUE], use.c = "t",
+      plot.args = list (type = "b", col = "black", ylim = range (laser), pch = 20))
> plotc (laser[,,17, wl.index = TRUE], use.c = "t", add = TRUE,
+      plot.args = list (type = "b", col = "blue", ylim = range (laser), pch = 20))
> plotc (laser[,,21, wl.index = TRUE], use.c = "t", add = TRUE,
+          plot.args = list (type = "b", col = "red", ylim = range (laser), pch = 20))
> plotc (laser[,,23, wl.index = TRUE], use.c = "t", add = TRUE,
+          plot.args = list (type = "b", col = "darkgreen", ylim = range (laser), pch = 20))
```


(a)   (b)
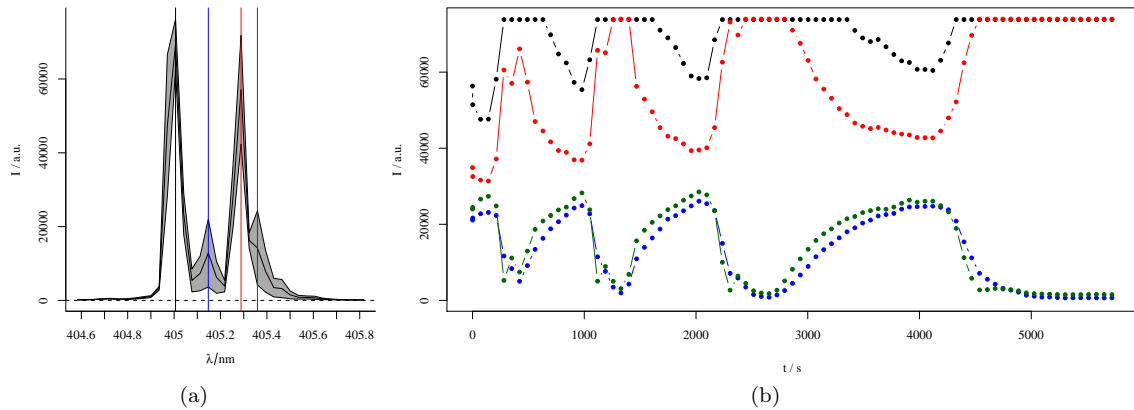
Figure 2: The laser emission time series. 2a shows the spectral position of the bands. The time series are plotted in corresponding colors in 2b.