

# (Interactive) Spike Correction of Raman Spectra

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## 1 Introduction

Raman spectra are often affected by cosmic rays hitting the CCD camera. These and similar sharp high intensity artifacts are called *spikes*.

- Spikes are often assumed to affect only one pixel
- this is not always the case: the camera at Uni. Trieste frequently produces wider spikes. (Possibly due to orientation in space?)

```
> library (hyperSpec)
> load ("cartilage-raw.RData")
```

## 2 Typical strategy for semi-automatic spike correction

spikefilter.R defines a semi-automatic spike finder:

```
> source ("spikefilter.R")
```

Function spikefilter filters each spectrum with  $c(-1, 2, -1)$ , spikefilter2d applies the same filter also among spectra. This is useful if the spectra are rather similar: in that case, sharp bands are better distinguished from spikes that occur only in one spectrum.

A pre-processing that removes typical spectroscopic information may help. Particularly spikefilter2d benefits from making the spectra as similar as possible.

So I normalize the spectra to their median and then subtract the median spectrum:

```
> tmp <- sweep (cartilage, 1, median, `/\`) # special abbreviation for hyperSpec's sweep:
>                                           # instead of a vector, we can give a function
> tmp <- sweep (tmp, 2, median , `-\`)
```

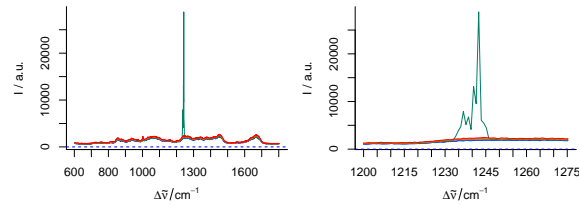


Figure 1: Spike in Raman spectrum: the green spectrum is affected by a spike. right: detail

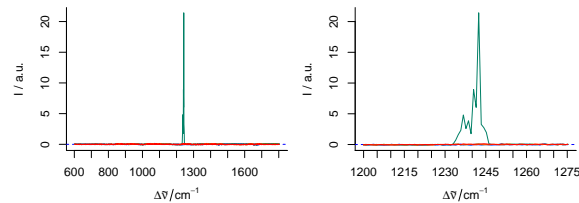


Figure 2: Pre-processing to enhance the spikes

Now the SNR with respect to the spikes is already greatly enhanced ( 2).

now generate spikiness scores:

```
> system.time (
+       scores <- spikefilter2d (spcmatrix= tmp [[]])
+ )
```

User	System	verstrichen
9.990	1.160	18.139

now the interactive filtering, I take just the 1st 100 spectra to see the principle:

```
> spikes <- spikes.interactive (cartilage [1:100], scores [1:100, ])
```

Note that suspicion no. 17 (spectrum 1) is a real sharp signal of an inorganic salt (carbonate), no spike.

After about 25 suspicions, the procedure can be ended: no more spikes but only real signals are found.