Enabling analysis of large scale metabolomics/proteomics data: on-the-fly data access in MSnbase

Johannes Rainer

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Introduction

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- Updates to `MSnbase`, `mzR` and `xcms` packages:
  - *on-the-fly* data access.
  - Mass spectrometry (MS) data write support.
  - towards a common MS infrastructure: `xcms` re-uses classes from `MSnbase`.

onDisk *vs* inMem data; why?

- Keeping all data in memory prevents analysis of large experiments.
- Example: load a MS file

```
library(MSnbase)
library(pryr)

## Read a single MS level 1 file
msd <- readMSData("data/150616_POOL_IntraP_S_POS_6.mzML", mode = "onDisk")

## Object size?
object_size(msd)
```

```
602 kB
```

- Memory footprint: 977 MB (inMem) *vs* 600 kB (onDisk).
- Reading data on demand: *relatively* fast for indexed mzML files.

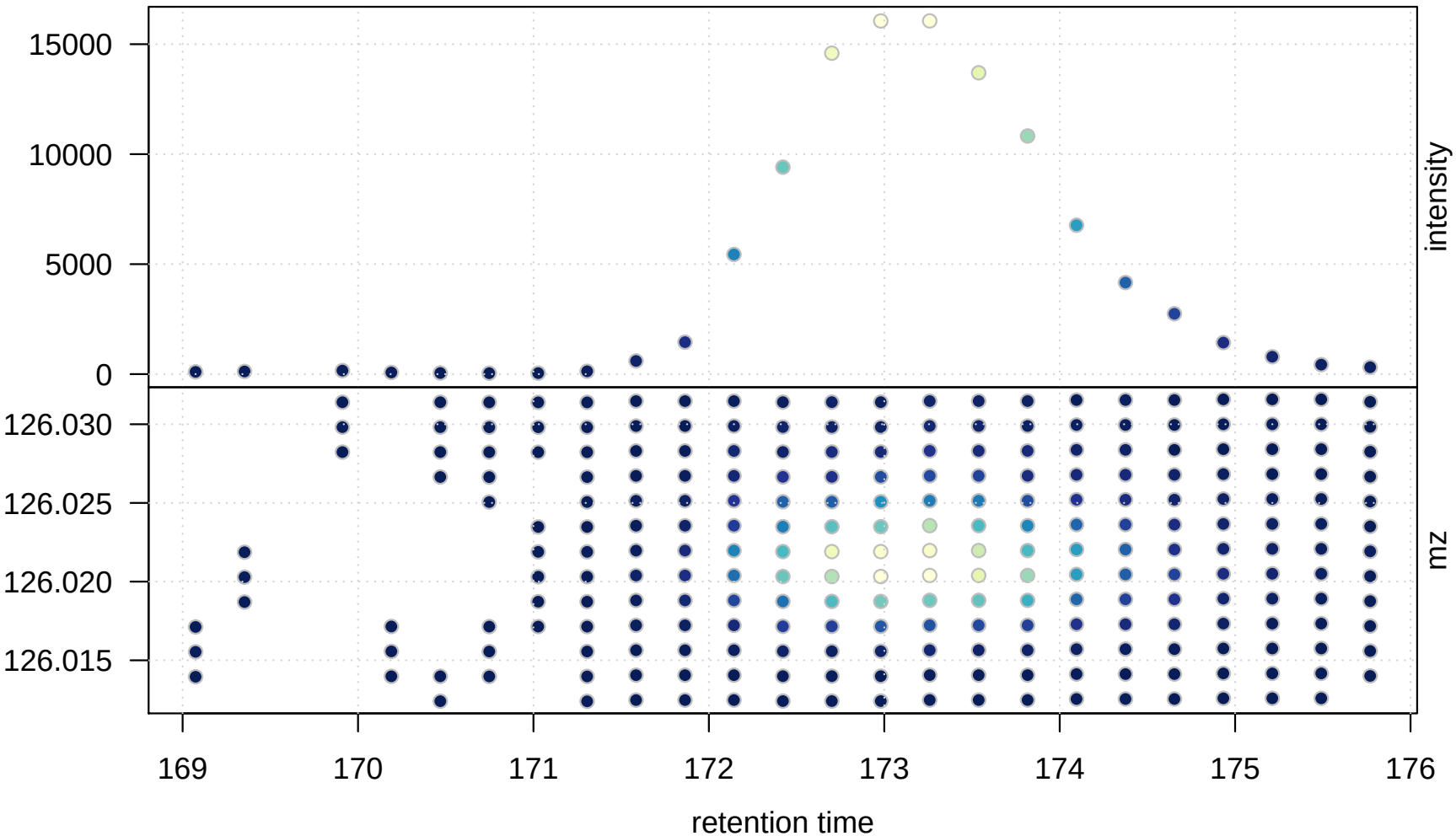
Application example: *centroiding* of *profile* MS data

- Profile MS data?
- Example: plot MS data for a metabolite:

```
library(xcms)
library(magrittr)

## m/z for Taurine [M+H]+
taur_mz <- 126.02194
taur_rt <- c(169, 176)

## Extract the MS data for this ion
taur_msd <- msd %>%
    filterRt(rt = taur_rt) %>%
    filterMz(mz = c(taur_mz - 0.01, taur_mz + 0.01)) %>%
    extractMsData

plotMsData(taur_msd[[1]])
```

Application example: *centroiding* of *profile* MS data

- Profile-mode MS data for Taurine [M+H]+ ion.



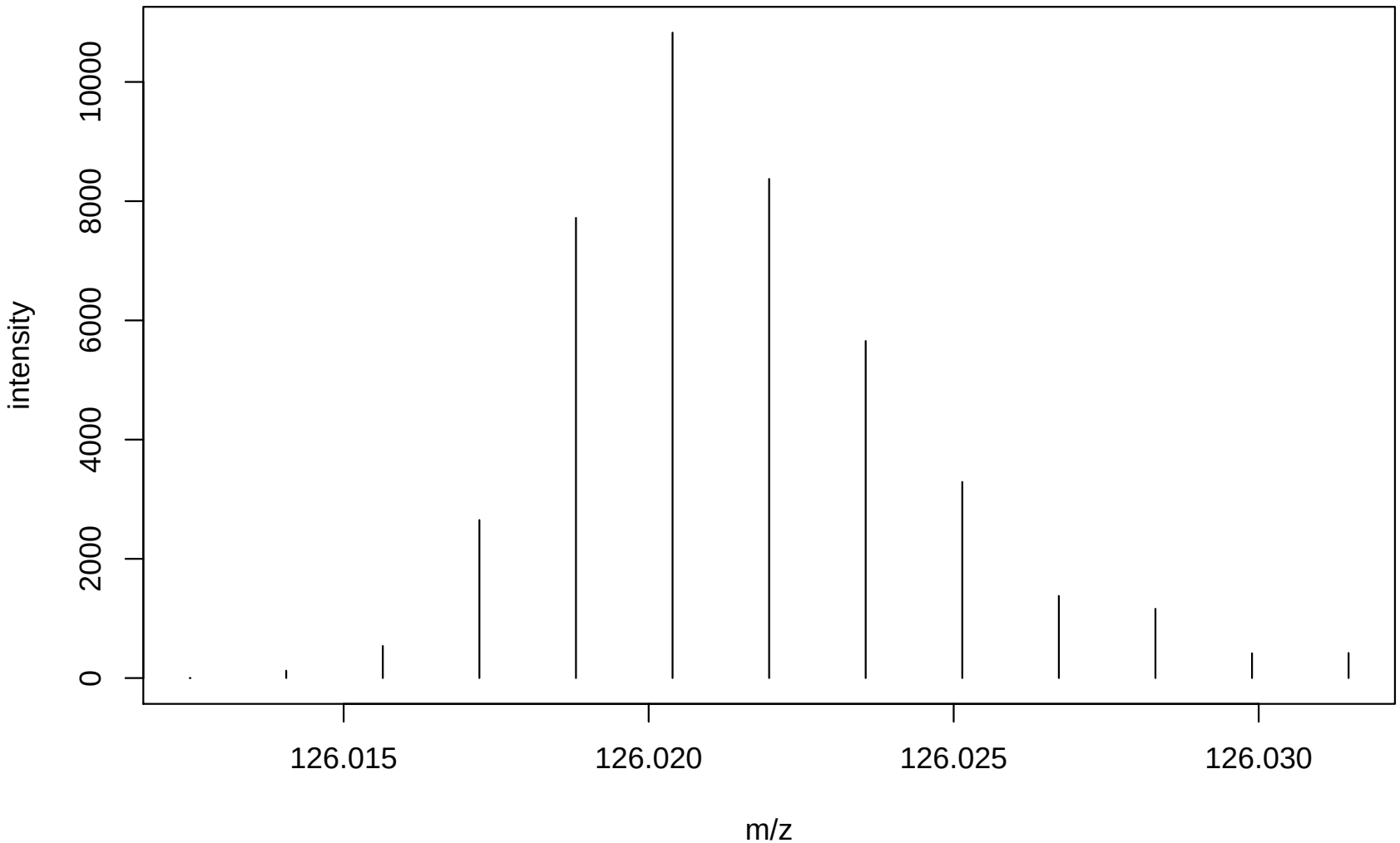
Application example: *centroiding* of *profile* MS data

- *centroiding*: represent mass peaks by their *centroid* (largest signal for each mass peak).
- Example: plot mass peak for taurin from one spectrum.

```
## Identify values corresponding to one spectrum
idx <- grep("F1.S0623", rownames(taur_msd[[1]]))

## Plot the m/z and intensity
par(mfrow = c(1, 1), mar = c(4.5, 4, 1, 1))
plot(taur_msd[[1]]$mz[idx], taur_msd[[1]]$i[idx],
     type = "h", xlab = "m/z", ylab = "intensity")
```

Application example: *centroiding* of *profile* MS data

- Taurin ion mass peak in one spectrum.



Application example: *centroiding* of *profile* MS data

- onDisk data: lazy execution of data manipulations. Example: Data smoothing (smooth) and centroiding (pickPeaks).

```
## 1) smooth the spectrum data
## 2) perform centroiding
cntr <- msd %>% smooth(method = "MovingAverage", halfWindowSize = 2L) %>%
    pickPeaks()

## ... not executed yet ...
cntr@spectraProcessingQueue
```

```
[[1]]
Object of class "ProcessingStep"
 Function: smooth
 Arguments:
  o method = MovingAverage
  o halfWindowSize = 2

[[2]]
Object of class "ProcessingStep"
 Function: pickPeaks
 Arguments:
  o method = MAD
  o halfWindowSize = 3
  o SNR = 0
  o ignoreCentroided = TRUE
  o refineMz = none
```

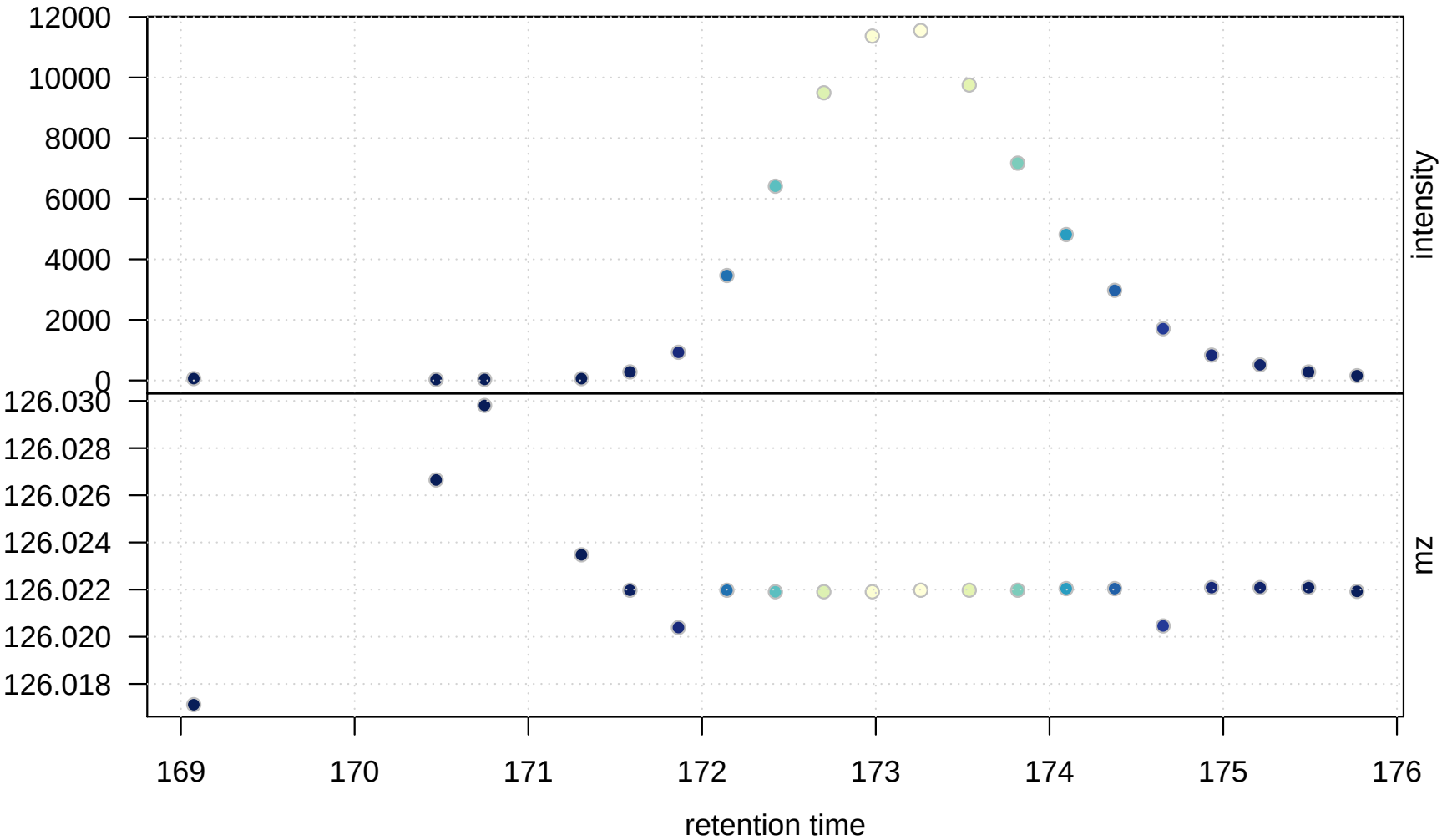
Application example: *centroiding* of *profile* MS data

- Data manipulations are applied *on-the-fly*.

```
## Extract the MS data for our example ion;
## smoothing and centroiding performed on-the-fly
taur_cntr <- extractMsData(cntr, mz = c(taur_mz - 0.01, taur_mz + 0.01),
                           rt = taur_rt)
plotMsData(taur_cntr[[1]])
```

Application example: *centroiding* of *profile* MS data

- Centroided MS data for taurin.



Application example: *centroiding* of *profile* MS data

- *Make persistent*: write to MS data file. Example: write the centroided data to disk.

```
writeMSData(cntr, file = "centroided.mzML", copy = TRUE)

## 1) All processings (smoothing and peak picking) are applied
## 2) Data is exported as mzML
```

Finally

Thank you for your attention!

Collaborative work:

- Johannes Rainer (Eurac Research, Italy); github/twitter: jotsetung
- Laurent Gatto (CPU Cambridge, UK)
- Sebastian Gibb (University Medicine Greifswald, Germany)
- Steffen Neumann (IPB Halle, Germany)

clone me!
`https://github.com/jotsetung/EuroBioc2017-MSnbase.git`