An R workflow for lipidomics data

Lisa Schneider

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Data creation

Samples

- Grass fed cattle
- Stall fed cattle
- Deer
- Roe deer
- Salmon (farmed)

Standards

- Equi Lipido SplashMix
  - deuterium labelled standards with lipid ratios similar to human plasma

LC-MS/MS

- positive ionization mode

Feature selection and lipid identification

Using Thermo Scientific TraceFinder * identification via exact mass * positive mode

What the data looked like

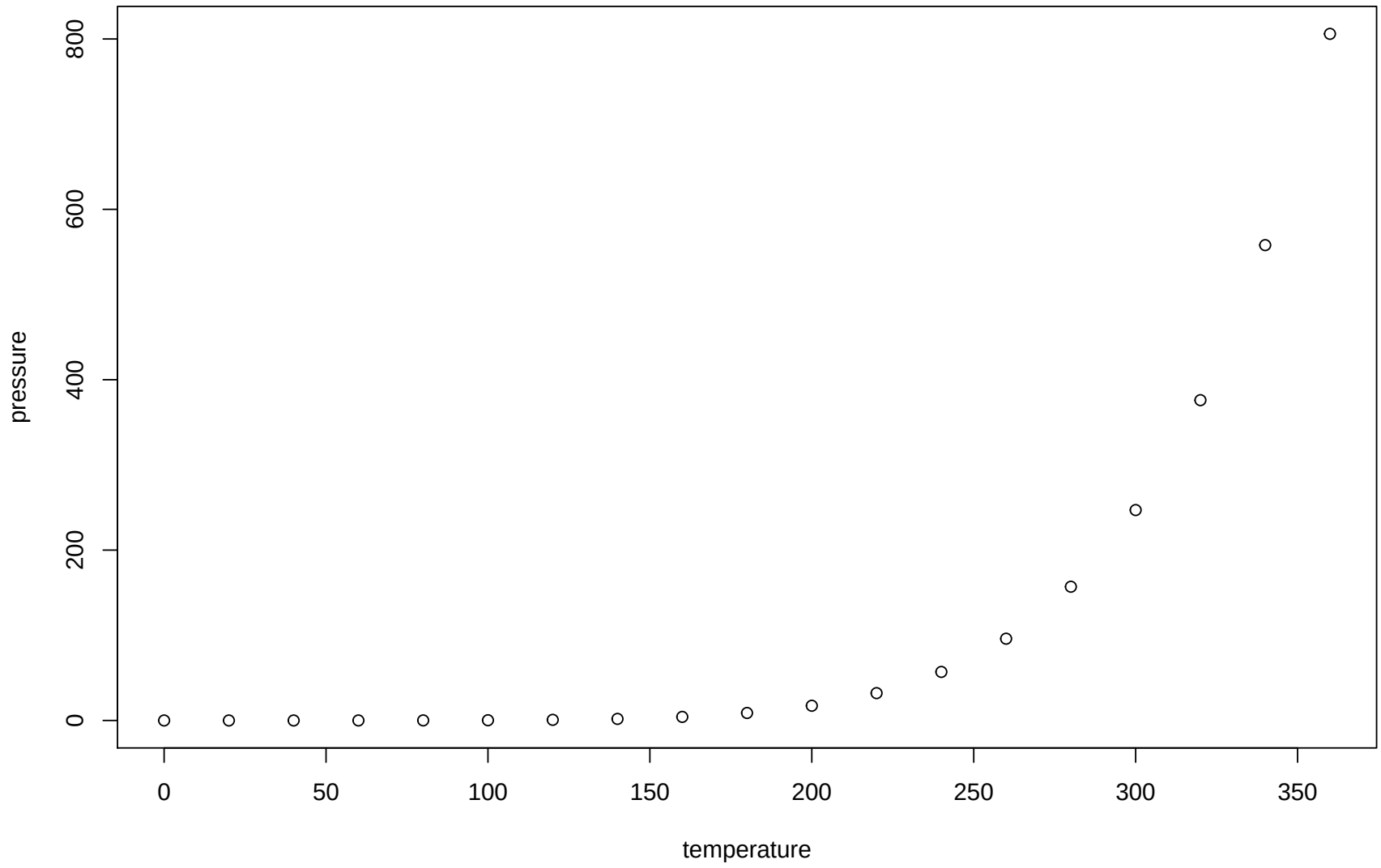
```
## meat data
### data processing

meat_data <- read.csv(meat_data_path, sep = ",", dec = "."
head(meat_data)
```

```
##                      Compound                    RT
## 1                  dCer (15:0)                 12.98 Internal S
## 2   dCholEster (33:1)_19.11 19.11,19.11,19.11 Internal S
## 3 dCholesterol (33:1)_11.21 11.21,11.21,11.21 Internal S
## 4                 dDG (33:1)       15.58,15.58 Internal S
## 5              dLPC (18:1)_1    4.28,4.28,4.28 Internal S
## 6              dLPC (18:1)_2    4.55,4.55,4.55 Internal S
##                                Filename    Status Group   Ar
```

Slide with R Output

```
## set variables
working_directory <- "/home/lisa/FH/Masterarbeit/LipidomeCo
setwd(working_directory)

test_path <- "/home/lisa/FH/Masterarbeit/LipidomeComparison
meat_data_path <- "/home/lisa/FH/Masterarbeit/LipidomeCompa

plot_path <- paste(working_directory, "/plots", sep = "")
plot_name <- paste(plot_path, "/meat_data", sep = "")

## meat data
### data processing

meat_data <- read.csv(meat_data_path, sep = ",", dec = "."
# meat_data
meat_data <- subset(meat_data, select = c(Compound, Type, I
meat_data <- subset(meat_data, Status == "Processed")
# meat_data[meat_data==''] <- NA
```

Slide with Plot



Next Slide

- Theory
- My Workflow
  - Create data matrix
  - Log-Transformation
  - Normalization
  - Imputation
  - Exploratory data analysis
  - Univariate analysis
  - PCA
  - Hierarchical clustering
- What next?
  - Supervised learning
  - Lipid set enrichment analysis