Article

Philipp Baumann | philipp.baumann@usys.ethz.ch

2019-12-01

Intro

Albert Einstein would probably not have felt the necessity for simplerspec, as he would have followed his quote *"Everything should be made as simple as possible, but not simpler"*. In line with this recommendation, I was told that spectral analysis in R is standard practice and straight forward using the famous partial least squares (PLS) regression when I started my MSc back in July 2015. I was given the honour of the exciting task to sample and model both soils and yam plants from 20 fields in 4 landscapes across the West African yam belt (see here for details). Since I was both fascinated by R, statistics, soils, and their interplay with plants, I started my first scientific journey with the premise that I just had to deepen a bit my R knowledge. I thought that the tools out there are simple enough for achieving my neat MSc task.

Being a big fan of R and other open source tools, I was happy to find quite a bit of chemometrics and other modeling toolsets, many of them for example available via CRAN and listed in the CRAN Task View Chemometrics and Computational Physics or Machine Learning & Statistical Learning. I would consider most of them good at solving single tasks, but I somehow missed a clean common interface that interlinked the key steps required for spectral processing and modeling. While doing first analysis steps, my intuition told me that streamlining all analysis steps would aid in more efficiently estimating the composition and properties of natural materials. More importantly, it would allow a sustainable basis for model development and sharing with collaborators.

However, I was far from being there (now still). Soon I realized that while extending explorations of various options along modeling steps, such as pre-processing to achieve robust and accurate models, I ended up writing more and more verbose code for repetitive or only slighly different tasks. I felt I could do better at some point and get rid of the verbose boilerplate coding I was doing. To solve this more elegantly, I started continously building the simplerspec package with the goal of delivering beginner-friendly and standardized functions. In short, to provide a rapid prototyping pipeline for various spectroscopy applications that share common tasks.

Prepare the R environment for spectral analysis

Enough of the personal talking, let's start. To reproduce the entire analysis in this hands-on, I would advise two main procedures:

1. Installing exact package versions and sources using the renv package and the snapshot file `renv.lock`
2. Manual installation of R packages with specific version tags

To restore and reproduce this entire analysis and document, first clone this repository to your local computer. Then install renv and restore R packages based on the `renv.lock` file in an isolated project library in two lines of code.

```r
## Option 1 for installation
install.packages("renv")
renv::restore("renv.lock")
```

Option 1 is probably the easiest as it makes automatically sure that all dependencies are met and the computational environment is the same (apart from operating system and system tools).

To install and attach all required R packages used in this article with more manual care and less guarantees, you can run the following lines:

```r
## Option 2 for installation
pkgs <- c("simplerspec", "here", "tidyverse", "data.table",
  "future", "doFuture", "remotes")
# install.packages(pkgs)
# remotes::install_github("philipp-baumann/simplerspec")}
```

Hands-on

Now we are ready to proceed to the fundamentals of the package. We use the example data set from my MSc thesis. First, let's load required packages. The tidyverse is optional, so if you feel it is not required you won't need to load it.

```r
# Load required packages
# `walk()` is like `lapply()`, but returns invisibly
suppressPackageStartupMessages(
  purrr::walk(pkgs, library, character.only = TRUE, quietly = TRUE)
)
```

A typical simple spectroscopy modeling project has the following components:

1. Soil sampling and sample preparation
2. Spectral measurements
3. Selection of calibration samples
4. Soil analytical reference analyses
5. a. Calibration or Recalibration
   b. Estimation of properties of new soils based on new spectra and established models.

Simplerspec focuses on the key tasks and provides user-friendly modules in the form of a standardized function pipeline. This pipeline builds upon common design principles of spectral R objects which are shared between function inputs and outputs.

```r
# Read final reference analysis data
# see data/reference-data/metadata_soilchem_yamsys.txt for further details
reference_data <- fread(
  file = here("data", "reference-data", "soilchem_yamsys.csv")) %>%
  as_tibble()
# number of rows and columns
dim(reference_data)
```

```
## [1] 94 36
```

```
reference_data[1:5, ]
```

```
## # A tibble: 5 x 36
##   sample_ID country site  material     S     C     N ex_Ca ex_Mg  ex_K
##   <chr>     <chr>   <chr> <chr>    <dbl> <dbl> <dbl> <dbl> <dbl> <dbl>
## 1 BF_lo_01~ BF      lo    soil      71.3  6.92 0.438  488   62.5 113
## 2 BF_lo_02~ BF      lo    soil      87    5.73 0.447  656   47.5 140
## 3 BF_lo_03~ BF      lo    soil      72.   3.41 0.233  270   21.9  61.6
## 4 BF_lo_04~ BF      lo    soil      73    5.37 0.423  532.  49.5 110.
## 5 BF_lo_05~ BF      lo    soil      70    9.03 0.624  604   92.6 115
## # ... with 26 more variables: ex_Al <dbl>, ex_Na <dbl>, ex_Fe <dbl>,
## #   ex_Mn <dbl>, pH_BaCl2 <dbl>, CEC_eff <dbl>, BS_eff <dbl>, pH <dbl>,
## #   P_resin <dbl>, Fe_tot <dbl>, Si_tot <dbl>, Al_tot <dbl>, P_tot <dbl>,
## #   K_tot <dbl>, Ca_tot <dbl>, Mn_tot <dbl>, Zn_tot <dbl>, Cu_tot <dbl>,
## #   Zn_DTPA <dbl>, Cu_DTPA <dbl>, Fe_DTPA <dbl>, Mn_DTPA <dbl>,
## #   sand <dbl>, clay <dbl>, silt <dbl>, site_comb <chr>
```

First, you may want to read files from spectra that you measured on your spectrometer. Spectral inputting is the first step done when doing spectral analysis prior to the standard chemical analysis. This is useful when you have a lot of samples and you want to save some time and money to to do reference analysis, and then predict the remaining samples only with infrared spectroscopy.

Here we read from a Bruker Alpha mid-Infrared spectrometer. Currently, the package is limited to Bruker and ASD devices, however support for reading files from other devices and formats is planned within the package simplerspec.io.

```
# multicore would work on UNIX/Darwin, however not supported for RStudio
# and the future package due to stability reasons
plan(multisession)
registerDoFuture()
# availableCores()

# files to read
files_spc <- list.files(
  here("data", "spectra", "example-yamsys"), full.names = TRUE)
# path to one example file
# files_spc[[1]]
# read the files
suppressMessages(
  spc_list <- read_opus_univ(fnames = files_spc, extract = c("spc"),
    parallel = TRUE)
)
length(spc_list)
```

```
## [1] 284
```

```
names(spc_list[[1]])
```

```
##  [1] "metadata"          "spc"               "spc_nocomp"
##  [4] "sc_sm"             "sc_rf"             "ig_sm"
##  [7] "ig_rf"             "wavenumbers"       "wavenumbers_sc_sm"
## [10] "wavenumbers_sc_rf"
```

Typically, list information is nicely ordered, however printing is really verbose. Therefore, we can gather the list into a so-called spectral tibble (`spc_tbl`).

```
# Gather from list into tibble data.frame
(spc_tbl <-
  spc_list %>%
  gather_spc())
```

```
## # A tibble: 284 x 6
##    unique_id        file_id    sample_id   metadata   spc       wavenumbers
##    <chr>            <chr>      <chr>       <named li> <named l> <named lis>
##  1 BF_lo_01_soil_c~ BF_lo_01_~ BF_lo_01_s~ <tibble [~ <df[,171~ <dbl [1,71~
##  2 BF_lo_01_soil_c~ BF_lo_01_~ BF_lo_01_s~ <tibble [~ <df[,171~ <dbl [1,71~
##  3 BF_lo_01_soil_c~ BF_lo_01_~ BF_lo_01_s~ <tibble [~ <df[,171~ <dbl [1,71~
##  4 BF_lo_02_soil_c~ BF_lo_02_~ BF_lo_02_s~ <tibble [~ <df[,171~ <dbl [1,71~
##  5 BF_lo_02_soil_c~ BF_lo_02_~ BF_lo_02_s~ <tibble [~ <df[,171~ <dbl [1,71~
##  6 BF_lo_02_soil_c~ BF_lo_02_~ BF_lo_02_s~ <tibble [~ <df[,171~ <dbl [1,71~
##  7 BF_lo_03_soil_c~ BF_lo_03_~ BF_lo_03_s~ <tibble [~ <df[,171~ <dbl [1,71~
##  8 BF_lo_03_soil_c~ BF_lo_03_~ BF_lo_03_s~ <tibble [~ <df[,171~ <dbl [1,71~
##  9 BF_lo_03_soil_c~ BF_lo_03_~ BF_lo_03_s~ <tibble [~ <df[,171~ <dbl [1,71~
## 10 BF_lo_04_soil_c~ BF_lo_04_~ BF_lo_04_s~ <tibble [~ <df[,171~ <dbl [1,71~
## # ... with 274 more rows
```

Instead of appending a matrix of spectra as a single column in a data.frame, spectra in a spectral tibble form a list-column. A list-column is basically a column consisting of a list instead of an atomic vector. With this we can extract this list column of spectra.

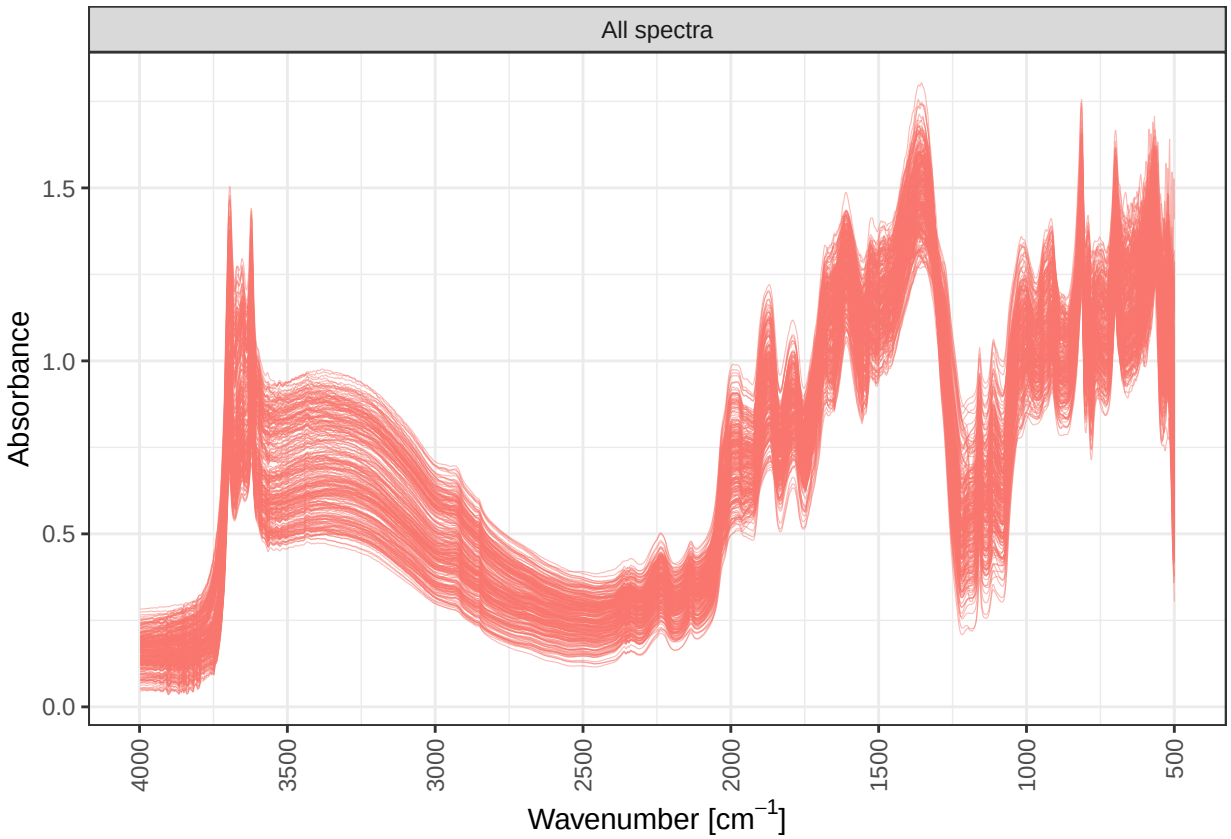
```
spc_dt <- data.table::rbindlist(spc_tbl$spc)
dim(spc_dt); class(spc_dt)
```

```
## [1]  284 1716
```

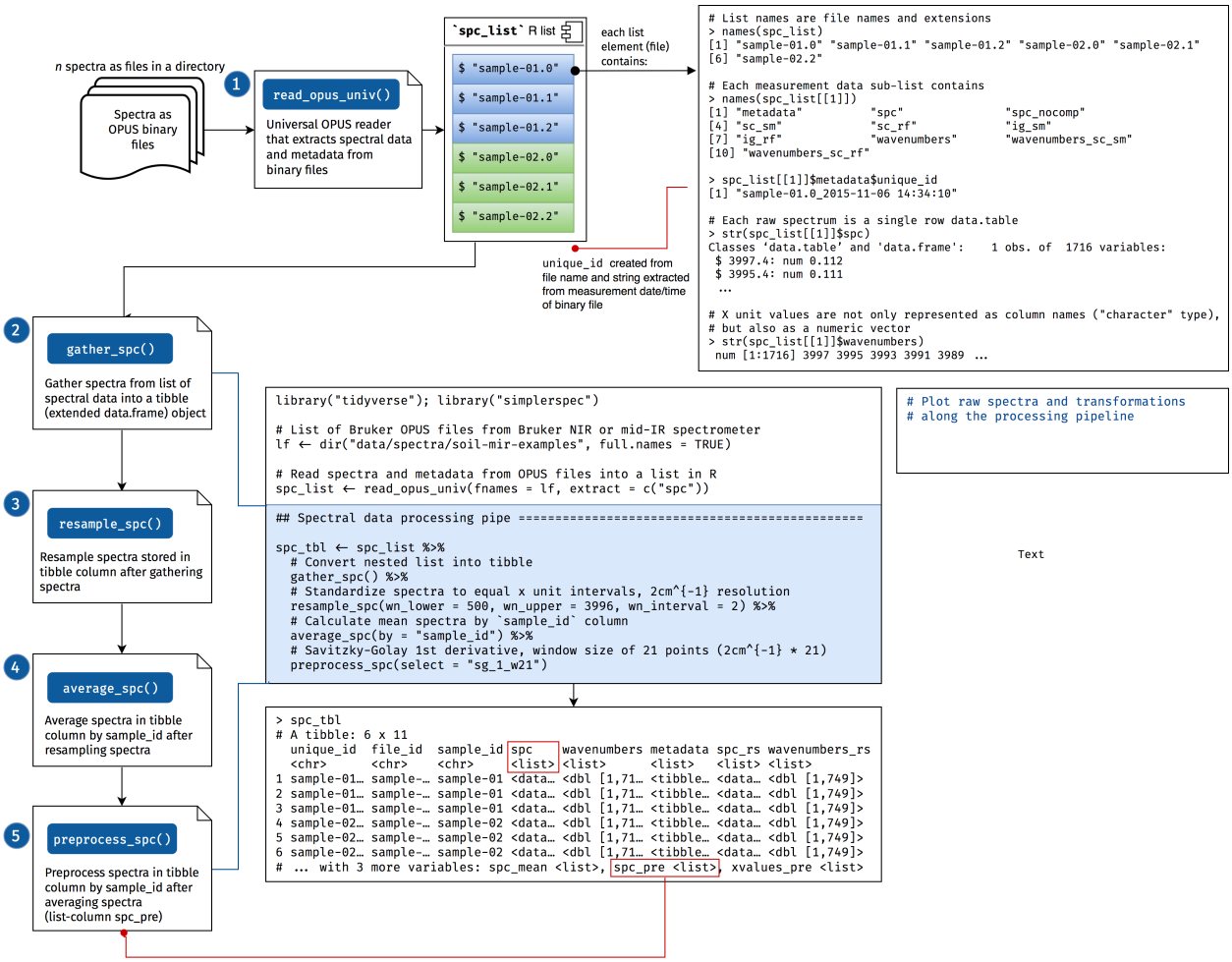
```
## [1] "data.table" "data.frame"
```

Let's plot what we have first:

```
spc_tbl %>%
  mutate(
    label_all = "All spectra"
  ) %>%
  plot_spc_ext(
    spc_tbl = .,
    group_id = "label_all",
    ylab = "Absorbance"
  )
```



The spectral pre-processing pipeline of simplerspec comprises basic steps that are often performed for spectral modeling and estimation. Simplerspec uses prospectr for key steps and data.table for simple operations. The following scheme summarizes the steps.



In a nutshell, spectral data processing can be done in one pipeline. Resampling in this context refers to to creating a new a axis interval in spectra. Spectra are averaged because there are 3 replicate measurements for each soil sample. Preprocessing is done to reduce scattering and noise in spectra.

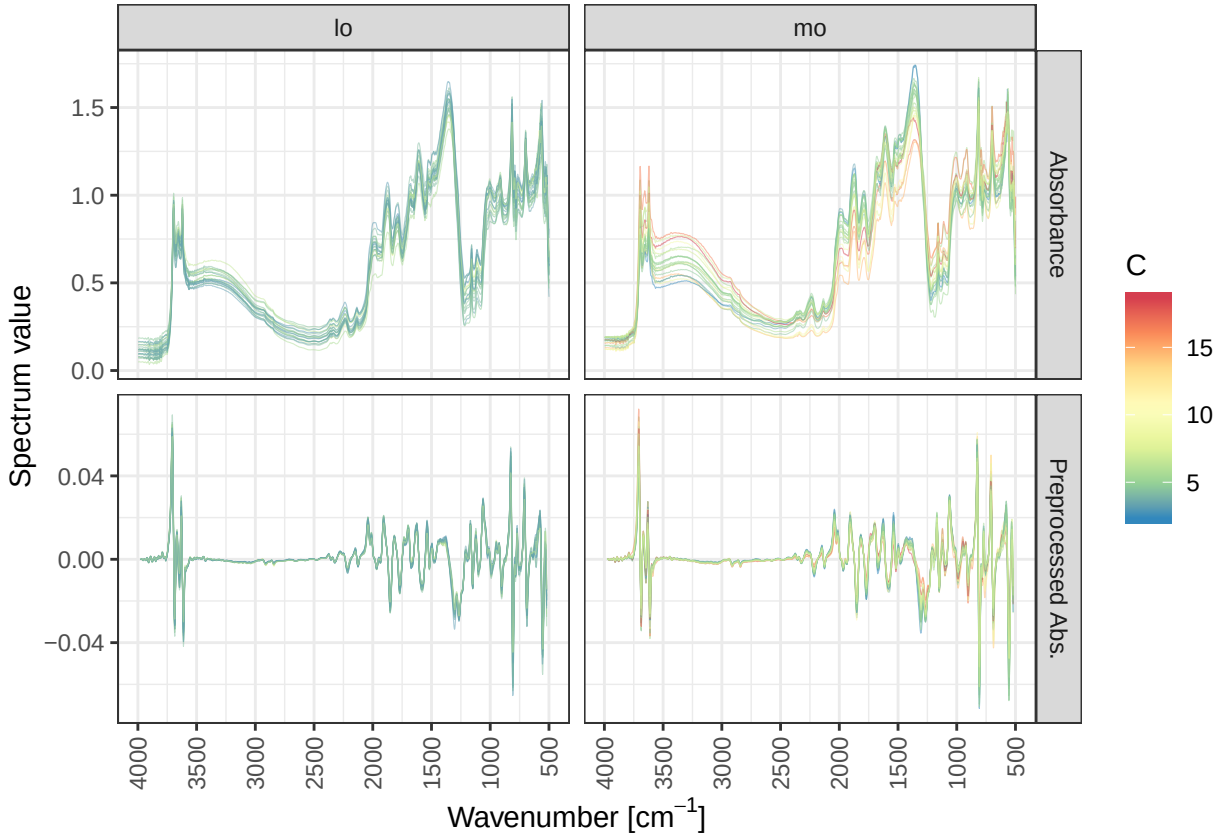
```
spc_proc <-
  spc_tbl %>%
  resample_spc(wn_lower = 500, wn_upper = 3996, wn_interval = 2) %>%
  average_spc(by = "sample_id") %>%
  preprocess_spc(select = "sg_1_w21") %>%
  group_by(sample_id) %>%
  slice(1L)

colnames(spc_proc)
```

```
##  [1] "unique_id"      "file_id"        "sample_id"      "metadata"
##  [5] "spc"            "wavenumbers"    "spc_rs"         "wavenumbers_rs"
##  [9] "spc_mean"       "spc_pre"        "xvalues_pre"
```

We can explore the final processed spectra.

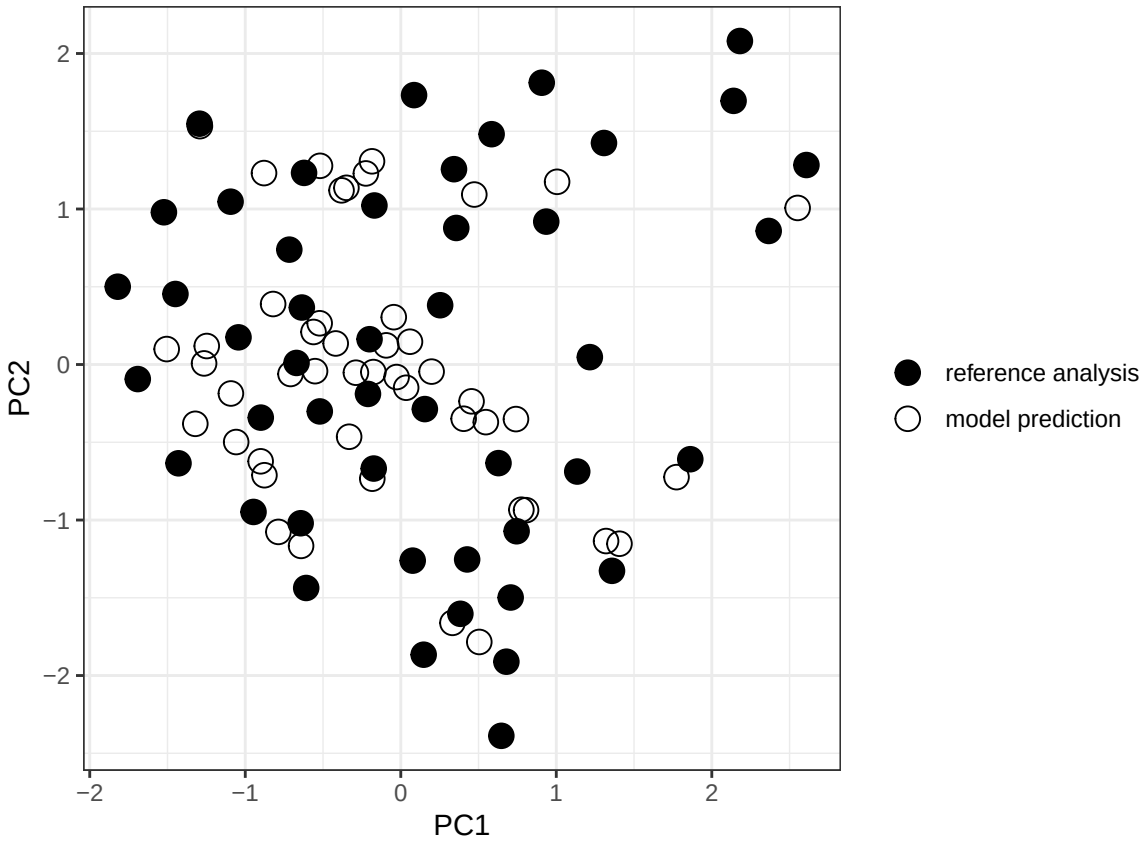
```
spc_proc %>%
  inner_join(
    x = .,
    y = reference_data %>% rename(sample_id = sample_ID)
  ) %>%
  filter(site %in% c("lo", "mo")) %>%
  plot_spc_ext(
    spc_tbl = .,
    lcols_spc = c("spc", "spc_pre"),
    lcol_measure = "C",
    group_id = "site")
```

```
## Joining, by = "sample_id"
```



After preprocessing, we can proceed with selecting reference analytical samples based on Kennard-Stone.

```
spc_tbl_selection <- select_ref_spc(spc_tbl = spc_proc, ratio_ref = 0.5)
# PCA biplot
spc_tbl_selection$p_pca
```



Lastly, we develop a partial least squares (PLS) calibration model.

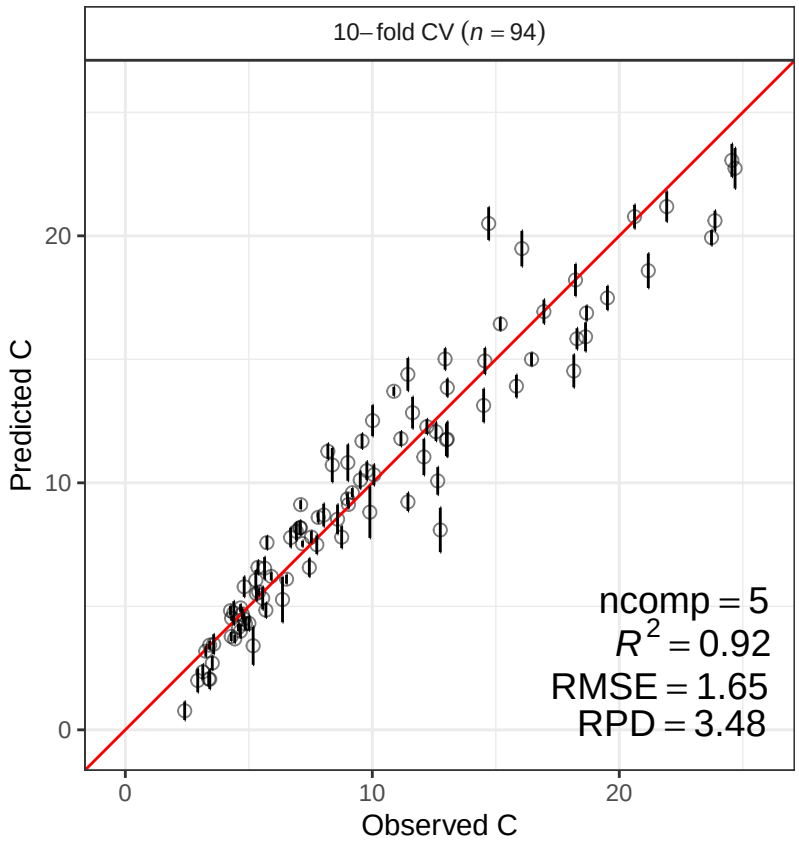
```
# Fuse spectra and reference data
spc_refdata <-
  dplyr::inner_join(
    x = spc_proc,
    y = reference_data %>% rename(sample_id = sample_ID)
  )
```

```
## Joining, by = "sample_id"
```

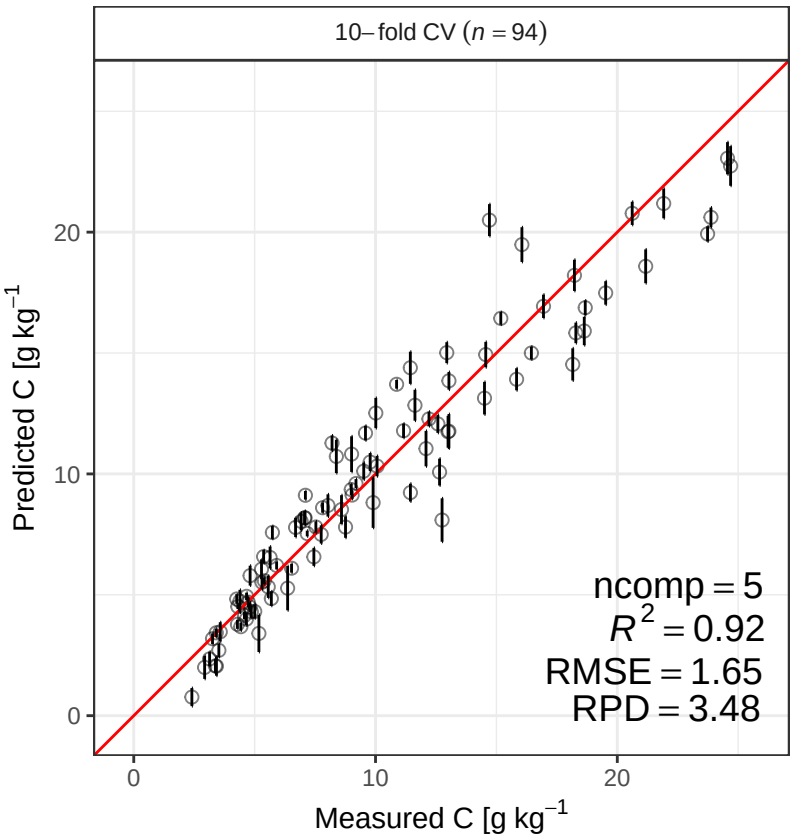
```
# spc_refdata %>%
#   skimr::skim(starts_with("spc"))
```

```
pls_carbon <- fit_pls(spec_chem = spc_refdata, response = C,
  evaluation_method = "resampling", print = FALSE)
```

```
## Adding missing grouping variables: `sample_id`
```




```
pls_carbon$p_model +
  xlab(expression(paste("Measured C [g", ~kg^-1))) +
  ylab(expression(paste("Predicted C [g", ~kg^-1)))
```



Outro

Simplerspec are some first baby steps in spectral adventures. The package deals with simplifying standard tasks and now has mainly exploration and teaching purposes. As an example, the Congo spectral platform uses some of its functionality. It would be great to further develop streamlining packages which are good at doing single things. It would also be fantastic to co-develop a new set of programs that automatically tune spectral machine learning pipelines. Complex problems require targeted learning. For example, one could create a custom graph learner using mlr3 and a preprocessing wrapper targeted to spectral analysis, in connection with a proper database system. If you have ideas, just send me an email or interact via github. Last but not least, I would like to give a big thanks to my generous supervisor for providing me infinite freedom in my science bubble. A big thank goes also to my main advisor and many more part and full-time advisors in my PhD committee. Working without constraints and waking up every day with thinking "alright — what am I going to do today?" feels amazing.