Testing Plan for baselineARPLss package (DATA501)

Installation

The following steps should work either on your own computer or on a free project / instance in the R Cloud (https://posit.cloud/)

The steps to download the package and install it are the following:

```
install.packages('remotes')
library(remotes)
remotes::install_github("econdatatech/baselineARPLss")
```

Please try these steps and report the result. The expected result is an installation without errors.

Usage

Usage with supplied sample data

Baseline estimation

Try the following instructions on in your R environment and report the result. The execution might take a couple of minutes and should finish without an error.

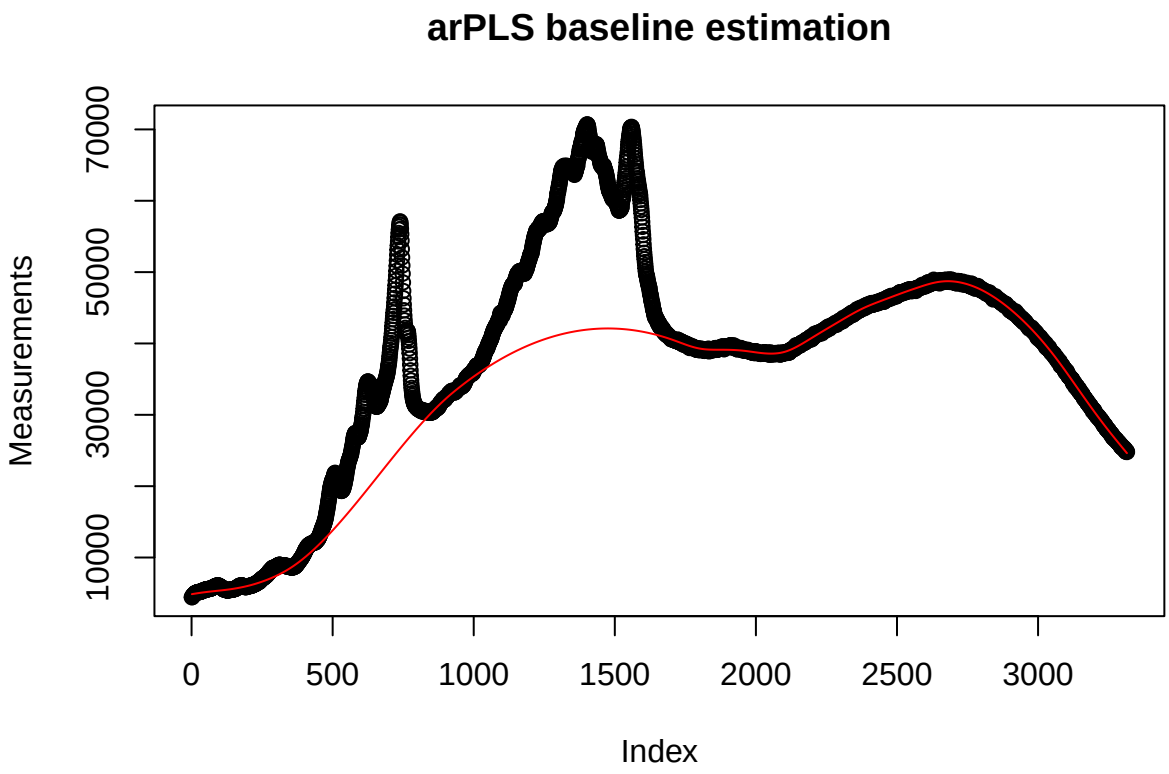
```
library(baselineARPLss)
data("Abelsonite")

res<-baseline_estimation(Abelsonite$measurement)
```

Result plot

Issue the below command and compare the result with the picture below.

```
plot(res)
```



Issue the below command and compare the result with the output below.

```
summary(res)
```

```
## [1] "The lambda parmeter value used was:  1e+06"
## [1] "The ratio parameter value used was:  1e-06"
## [1] "The max_iter parameter value used was:  50"
## [1] "The alogrithm stopped after the following number or iterations:  50"
## [1] "The last weight ratio value was:  0.000153623596796175"
## [1] "It appears that the algorithm stopped because the maximum number of iterations was reached"
```

Try to obtain the help page for the baseline_estimation function.

```
?baseline_estimation
```

```
## starting httpd help server ... done
```

Give your opinion. E.g. is anything unclear or anything missing?

Usage with new data

Select a substance or mineral of your choice from this following URL https://rruff.info/*/display=default/ (The site might take a bit to load) Click on the magnifiying glass on the right hand side of the screen for the substance of your choice. On the next page look for the following section "BROAD SCAN WITH SPECTRAL ARTIFACTS" and download the "Raman Data (RAW)" file. If such a file is not available, choose a different substance in the previous screen and try to obtain a "Raman Data (RAW)" for this substance.

Read the downloaded file into a dataframe (with a command similar to the one below)

```
df<-read.table('C:\\Users\\corvini\\Downloads\\Actinolite__R040063__Broad_Scan__532__0__unoriented__Rama
```

Try to estimate the baseline for the spectrum of this substance with the help of the documentation available (e.g. help files and vignette and manual) Report your findings.

Input validation

The baseline_estimation function has a lot of parameters. Most (apart from the input data in form of the raw spectrum) have default parameters.

```
baseline_estimation <- function(y, lambda = 1e6, ratio = 1e-6, max_iter =50,verbose=FALSE,algo="banded"
```

- y: Numeric vector representing the spectrum.
- lambda: Smoothing parameter. flaoting point number
- ratio: Stopping criterion based on changes in weight vector per iteration. floating point number
- max_iter: Maximum number of iterations. Integer number
- verbose: Boolean to print intermediary outputs
- algo: String to choose solver between Armadillo CPP armaInv ("cpp") and native solver function "native" and limSolve::Solve.banded solver ("banded")

Try different values than the default value for each parameter and report your findings. Furthermore try to feed the parameters with wrong data types and report your findings.

Performance testing

Run the performance test below involving different solver algorithms. Report back the values for nativesolve, cppsolve and bandedsolve. CAVE: This will take quite a long time!

```
start_time <- Sys.time()
rn<-baseline_estimation(Abelsonite$measurement,algo="native")
end_time<- Sys.time()
nativesolve<-(end_time - start_time)
nativesolve
start_time <- Sys.time()
rc<-baseline_estimation(Abelsonite$measurement,algo="cpp")
end_time<- Sys.time()
cppsolve<-(end_time - start_time)
cppsolve
start_time <- Sys.time()
rb<-baseline_estimation(Abelsonite$measurement,algo="banded")
end_time<- Sys.time()
bandedsolve<-(end_time - start_time)
bandedsolve
```