Package 'baselineARPLss'

October 21, 2024

Type Package

Title Baseline correction with arPLS smoothing (Baek 2015)

Version 0.1.0

Description Implements the algorithm for smoothing of spectra from: Sung-June Baek, Aaron Park, Young-Jin Ahna and Jaebum Choo: ``Baseline correction using asymmetrically reweighted penalized least squares smoothing", Analyst, 2015,140, 250-257 <https://pubs.rsc.org/en/content/articlelanding/2015/an/c4an01061b>.

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Encoding UTF-8

LazyData true

Imports Rcpp (>= 1.0.13), limSolve

LinkingTo Rcpp, RcppArmadillo

RoxygenNote 7.3.2

Depends R (>= 2.10)

Suggests knitr, rmarkdown

VignetteBuilder knitr

R topics documented:

`Abelsonite` *Raw Raman spectrum for Abelsonite*

Description

A data frame containing 3315 rows and 2 variables (wavenumber and measurement)

Usage

```
Abelsonite
```

Format

An object of class `data.frame` with 3315 rows and 2 columns.

Author(s)

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Source

https://rruff.info/repository/sample_child_record_raman_full/by_minerals/Abelsonite__R070007__Broad_Scan__532__0__unoriented__Raman_Data_RAW__13756.txt

References

Lafuente B, Downs R T, Yang H, Stone N (2015) The power of databases: the RRUFF project. In: Highlights in Mineralogical Crystallography, T Armbruster and R M Danisi, eds. Berlin, Germany, W. De Gruyter, pp 1-30

Examples

```
data("Abelsonite")
```

---

baseline_estimation *asymmetrically reweighted penalized least squares*

Description

Baseline estimation using asymmetrically reweighted penalized least squares smoothing (Baek et al. 2015).

Usage

```
baseline_estimation(
  y,
  lambda = 1e+06,
  ratio = 1e-06,
  max_iter = 50,
  verbose = FALSE,
  algo = "banded"
)
```

Arguments

y	Numeric vector representing the spectrum.
lambda	Smoothing parameter. The smaller the more curvature (wiggliness). (default: 1e6).
ratio	Stopping criterion based on changes in weight vector per iteration (default: 1e-6).
max_iter	Maximum number of iterations as fall back criterion if no conversion happens (default: 50).
verbose	Boolean to print intermediary outputs (default: FALSE).
algo	String to choose solver between Armadillo CPP armaInv ("cpp") and native solver function "native" and limSolve::Solve.banded solver ("banded") (default: "banded").

Details

The algorithm iteratively estimates a spectral baseline curve by updating a weight vector by means of a generalized logistic function that focuses the estimation efforts on regions where the baseline and the signal are close to each other

Value

object of class arPLSresult:

- rawinput: The original spectrum fed into the algorithm.
- lambda: The lambda parameter fed into the algorithm.
- ratio: The ratio stopping parameter fed into the algorithm.
- max_iter: The maximum iteration stopping parameter fed into the algorithm.
- baseline: The fitted spectral baseline.
- last_iter: The number of iterations the algorithm did before stopping.
- last_ratio: The last value of the ratio stopping criterium before stopping.

Author(s)

Corvin Idler

References

Baek, S.-J., Park, A., Ahn, Y.-J., and Choo, J. (2015). Baseline correction using asymmetrically reweighted penalized least squares smoothing. Analyst, 140:250–257.

Examples

```
{
data("Abelsonite")
baseline <- baseline_estimation(Abelsonite$measurement, max_iter=10, verbose=T)
}
```

plot.arPLSresult — *Take an object of class arPLSresult and plot some results*

Description

This is an S3 generic. To plot an input spectrum and an estimated baseline spectrum.

Usage

```
## S3 method for class 'arPLSresult'
plot(x, ...)
```

Arguments

x	A result object of class arPLSresult (mainly a list).
...	placeholder for arbitrary additional parameters (to stay in line with other generic plot functions)

Examples

```
{
data("Abelsonite")
baseline <- baseline_estimation(Abelsonite$measurement, max_iter=10, verbose=T)
plot(baseline)
}
```

summary.arPLSresult — *Take an object of class arPLSresult and summarize (print) some facts about it*

Description

This is an S3 generic. To summarize (print) some facts about the arPLS baseline estimation that led to it.

Usage

```
## S3 method for class 'arPLSresult'
summary(object, ...)
```

Arguments

object	A result object of class arPLSresult (mainly a list).
...	placeholder for arbitrary additional parameters (to stay in line with other generic summary functions)

Examples

```
{
data("Abelsonite")
baseline <- baseline_estimation(Abelsonite$measurement, max_iter=10, verbose=T)
summary(baseline)
}
```

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