Package 'LCF'

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Title Linear Combination Fitting

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Author Florian Werner [aut, cre]

Maintainer Florian Werner <florian.werner@wzw.tum.de>

Description Baseline correction, normalization and linear combination fitting (LCF) of X-ray absorption near edge structure (XANES) spectra. The package includes data loading of .xmu files exported from 'ATHENA' (Ravel and Newville, 2005) <doi:10.1107/S0909049505012719>. Loaded spectra can be background corrected and all standards can be fitted at once. Two linear combination fitting functions can be used: (1) fit_athena(): Simply fitting combinations of standards as in ATHENA, (2) fit_float(): Fitting all standards with changing baseline correction and edge-step normalization parameters.

Depends R (>= 3.2.1)

License GPL-3

Imports quadprog

Repository CRAN

LazyData true

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R topics documented:

`bkg_corr` *Background correction function*

Description

This function allows you to base-line correct and edge-step normalize XANES spectra (background correction). Raw spectra are loaded, then base-line corrected and edge-step normalized. The spectrum is flattened after E0. The function returns the corrected, normalized and flattened spectrum

Usage

```
bkg_corr(raw.spec, corr.norm)
```

Arguments

`raw.spec`	Raw spectrum
`corr.norm`	Vector of the base-line correction and edge-step normalization values (vector of length 4)

Examples

```
data(stdmix)
corr.spec.samples <- initial_load(specdat[5:8],
  corr.norm = c(-36, -15, 37, 58))
corr.spec <- bkg_corr(raw.spec = corr.spec.samples[[1]],
  corr.norm = c(-36, -15, 37, 58))
print(corr.spec)
```

`fit_athena` *Porting of 'ATHENA' linear combination fitting*

Description

The function can be used to check which combinations of standards produce a good fit and if output from 'ATHENA' is similar.

Usage

```
fit_athena(all.samples, all.standards, LC.vals, amoSTD, ex.smaller = NULL,
  file.output = NULL, best.fits = NULL)
```

Arguments

all.samples	List of all samples
all.standards	List of all standards
LC.vals	The fitting range values for the linear combination fitting
amoSTD	Use at most X standards
ex.smaller	Exclude portions smaller than a given value (decimal form), default to NULL
file.output	Possibility to have a file output, default to NULL
best.fits	Possibility to output more than the best fit (e.g. the first 10 best fits), default to 1

Examples

```
data(stdmix)
corr.spec.standards  <- initial_load(specdat[1:4],
  corr.norm = c(-36, -15, 37, 58))
corr.spec.samples    <- initial_load(specdat[5:8],
  corr.norm = c(-36, -15, 37, 58))
athena.fit <- fit_athena(all.samples = corr.spec.samples,
  all.standards = corr.spec.standards, LC.vals = c(-14, 46), amoSTD = 4)
## exclude portions smaller 5% = 0.05
athena.fit.exlcude <- fit_athena(all.samples = corr.spec.samples,
  all.standards = corr.spec.standards,
  LC.vals = c(-14, 46), amoSTD = 4, ex.smaller = 0.05)
```

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fit_float *Central fitting function with float environment*

Description

This function allows to process all samples, especially written for the float environment.

Usage

```
fit_float(all.samples, all.standards, LC.vals, float, ex.smaller = NULL,
  file.output = NULL, best.fits = NULL)
```

Arguments

all.samples	List of all samples
all.standards	List of all standards
LC.vals	The fitting range values for the linear combination fitting
float	Let vary the energy range paramerters
ex.smaller	Exclude portions smaller than a given value (decimal form), default to NULL
file.output	Possibility to have a file output, default to NULL
best.fits	Possibility to output more than the best fit (e.g. the first 10 best fits), default to 1

Examples

```
data(stdmix)
corr.spec.standards  <- initial_load(specdat[1:4],
  corr.norm = c(-36, -15, 37, 58))
corr.spec.samples    <- initial_load(specdat[5:8],
  corr.norm = c(-36, -15, 37, 58))
## Select parameters for baseline correction and edge-step normalization
param.float <- expand.grid(pre.adj.1 = seq(-42,-30,6),
  pre.adj.2 = seq(-19,-9,5), post.adj.1 = seq(35,40,5),
  post.adj.2 = seq(50,65,5))
length(param.float[,1])
float.fit <- fit_float(all.samples = corr.spec.samples,
  all.standards = corr.spec.standards,
  LC.vals = c(-14, 46), float = param.float, best.fits = 20)
print(float.fit)

###### Using next configuration can be very time consuming

param.float.2 <- expand.grid(pre.adj.1 = seq(-43,-30,1),
  pre.adj.2 = seq(-19,-9,.5), post.adj.1 = seq(34,40,.5),
  post.adj.2 = seq(50,65,1))
```

---

initial_load *Initial loading of spectra*

Description

This function loads and initially normalizes the raw spectra. Output is a list with the raw and initially corrected spectra.

Usage

```
initial_load(raw.spec = NULL, file = NULL, corr.norm, use.eshift = NULL)
```

Arguments

raw.spec	List of files already loaded with read_raw_spec()
file	Vector with file names
corr.norm	Initial correction and normalization parameters
use.eshift	Set TRUE, if using energy shift value, defaults to NULL

Examples

```
data(stdmix)
corr.spec.standards  <- initial_load(specdat[1:4],
  corr.norm = c(-36, -15, 37, 58))
corr.spec.samples    <- initial_load(specdat[5:8],
  corr.norm = c(-36, -15, 37, 58))
```

LCF_solve_QP *Linear combination fitting solve function*

Description

Quadratic programming solution function for linear combination fitting (LCF)

Usage

```
LCF_solve_QP(LCF.stds, LCF.samp)
```

Arguments

LCF.stds	Standards for LCF
LCF.samp	Sample for LCF

Examples

```
data(stdmix)
corr.spec.standards  <- initial_load(specdat[1:4],
  corr.norm = c(-36, -15, 37, 58))
corr.spec.samples    <- initial_load(specdat[5:8],
  corr.norm = c(-36, -15, 37, 58))
fit.standards <- std_df(sample = corr.spec.samples[[1]],
  all.standards = corr.spec.standards)
corr.spec <- bkg_corr(raw.spec = corr.spec.samples[[1]],
  corr.norm = c(-36, -15, 37, 58))
## set fitting range parameters relative to E zero
E.zero <- corr.spec.samples[[1]]$data$E0
LC.pre <- -14
LC.post <- 46
## find ranges that have to be fitted
abs.pre <- abs(corr.spec[["energy"]]-(E.zero+LC.pre))
abs.post <- abs(corr.spec[["energy"]]-(E.zero+LC.post))
range.pre <- which(abs.pre == min(abs.pre))
range.post <- which(abs.post == min(abs.post))
## extract standards and sample in given range
LC.sample <- corr.spec["cor.absorption"][range.pre:range.post,]
LC.standards <- fit.standards[range.pre:range.post,]
## actual fitting
fit.result <- LCF_solve_QP(LCF.stds = LC.standards, LCF.samp = LC.sample)
print(fit.result)
```

LC_fit *Linear combination fitting function*

Description

This function performs the LC fitting of the input sample/samples. It outputs the fitting results with the R-Factors as fitting statistics.

Usage

```
LC_fit(sample, standards, LC.vals, float = NULL, E.zero = NULL,
  ex.smaller = NULL)
```

Arguments

sample	The sample spectrum
standards	The standards spectra
LC.vals	Values for ranges of linear combination fitting, with respect to the edge-step
float	Set float parameters, defaults to NULL
E.zero	Set E0, defaults to NULL
ex.smaller	Set value to exclude small portions (as portion of 1), defaults to NULL

Examples

```
data(stdmix)
corr.spec.standards  <- initial_load(specdat[1:4],
  corr.norm = c(-36, -15, 37, 58))
corr.spec.samples    <- initial_load(specdat[5:8],
  corr.norm = c(-36, -15, 37, 58))
fit.standards <- std_df(sample = corr.spec.samples[[1]],
  all.standards = corr.spec.standards)
fit.result <- LC_fit(sample = corr.spec.samples[[1]],
  standards = fit.standards, LC.vals = c(-14, 46))
print(fit.result)
```

plot_LCF *Plot sample data, linear combination fit and residual spectrum*

Description

This function allows plotting (png or tiff image files) of the corrected sample spectrum, the linear combination fit and the residual.

Usage

```
plot_LCF(all.samples, all.standards, LCF.res, LC.vals, corr.norm,
  float = NULL, exclude = NULL, use.tiff = NULL, E.zero = NULL,
  set.plot.ymax = NULL, file.output = NULL)
```

Arguments

all.samples	List of all samples
all.standards	List of all standards
LCF.res	Results from function fit_float()
LC.vals	The fitting range values for the linear combination fitting
corr.norm	Vector of the base-line correction and edge-step normalization values (vector of length 4)
float	Logical, default to FALSE
exclude	Logical, default to FALSE
use.tiff	Logical, default to FALSE
E.zero	Set E0, defaults to NULL
set.plot.ymax	Set maximum of plot y axis, defaults to NULL
file.output	Logical, default to FALSE

Examples

```
data(stdmix)
corr.spec.standards  <- initial_load(specdat[1:4],
  corr.norm = c(-36, -15, 37, 58))
corr.spec.samples    <- initial_load(specdat[5:8],
  corr.norm = c(-36, -15, 37, 58))
param.float <- expand.grid(pre.adj.1 = seq(-45,-30,5),
  pre.adj.2 = seq(-19,-9,5), post.adj.1 = seq(34,40,2),
  post.adj.2 = seq(50,65,5))
float.fit <- fit_float(all.samples = corr.spec.samples[1],
  all.standards = corr.spec.standards, LC.vals = c(-14, 46),
  float = param.float, ex.smaller = 0.05)
par(pty="s")
plot_LCF(all.samples = corr.spec.samples[1],
  all.standards = corr.spec.standards,
  LCF.res = float.fit[1,], LC.vals = c(-14,46),
  corr.norm = c(-36, -15, 37, 58))
```

read_raw_spec *Read raw spectra*

Description

This function reads the raw .xmu file, extracts E0 and energy shift and returns a list with name, E0, energy shift, and the raw spectrum

Usage

```
read_raw_spec(file, use.eshift = NULL)
```

Arguments

file	The raw .xmu file
use.eshift	Set TRUE, if using energy shift value, defaults to NULL

Examples

```
## any .xmu file as output from ATHENA (>=0.9.25)
```

specdat *Phosphorus K-edge XANES spectral data for LCF*

Description

Data from an experiment on the quality of XANES spectrscopy for phosphorus speciation

Usage

```
data(stdmix)
```

Format

List of four standard spectra comounds and four spectra of mixtures of these standard compounds, output objects of function read_raw_spec().

References

Werner & Prietzel 2015, Environ. Sci. Technol. (49), 10521-10528 (DOI)

Examples

```
data(stdmix)
specdat[[1]]
specdat[[5]]
```

std_df *Create a data frame of all standards*

Description

The function creates a data frame with all standards in one data frame. The data frame has the same energy values as the sample that is loaded.

Usage

```
std_df(sample, all.standards)
```

Arguments

sample	A raw sample
all.standards	List of all standards

Examples

```
data(stdmix)
corr.spec.standards  <- initial_load(specdat[1:4],
  corr.norm = c(-36, -15, 37, 58))
corr.spec.samples    <- initial_load(specdat[5:8],
  corr.norm = c(-36, -15, 37, 58))
fit.standards <- std_df(sample = corr.spec.samples[[1]],
  all.standards = corr.spec.standards)
print(fit.standards)
```

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