Package 'SpectriPy'

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Title Enhancing Cross-Language Mass Spectrometry Data Analysis with R
and Python

Version 1.1.0

Description The SpectriPy package allows integration of Python-based MS
analysis code with the Spectra package. Spectra objects can be converted
into Python MS data structures. In addition, SpectriPy integrates
and wraps the similarity scoring and processing/filtering functions
from the Python matchms package into R.

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  compareSpectriPy   *Spectra similarity calculations using Python's matchms library*

Description

The compareSpectriPy() function allows to calculate spectral similarity scores using the calculate_scores() function of the Python matchms.similarity. module.

Selection and configuration of the algorithm can be performed with one of the *parameter* objects/functions:

- CosineGreedy(): calculate the *cosine similarity score* between spectra. The score is calculated by finding the best possible matches between peaks of two spectra. Two peaks are considered a potential match if their m/z ratios lie within the given tolerance. The underlying peak assignment problem is here solved in a *greedy* way. This can perform notably faster, but does occasionally deviate slightly from a fully correct solution (as with the CosineHungarian algorithm). In practice this will rarely affect similarity scores notably, in particular for smaller tolerances. The algorithm can be configured with parameters tolerance, mz_power and intensity_power (see parameter description for more details). See also matchms CosineGreedy for more information.

- CosineHungarian(): calculate the *cosine similarity score* as with CosineGreedy, but using the Hungarian algorithm to find the best matching peaks between the compared spectra. The algorithm can be configured with parameters tolerance, mz_power and intensity_power (see parameter description for more details). See also [matchms CosingHungarian](#) for more information.

- ModifiedCosine(): The modified cosine score aims at quantifying the similarity between two mass spectra. The score is calculated by finding the best possible matches between peaks of two spectra. Two peaks are considered a potential match if their m/z ratios lie within the given tolerance, or if their m/z ratios lie within the tolerance once a mass shift is applied. The mass shift is simply the difference in precursor-m/z between the two spectra. See also [matchms ModifiedCosine](#) for more information.

- NeutralLossesCosine(): The neutral losses cosine score aims at quantifying the similarity between two mass spectra. The score is calculated by finding the best possible matches between peaks of two spectra. Two peaks are considered a potential match if their m/z ratios lie within the given tolerance once a mass shift is applied. The mass shift is the difference in precursor-m/z between the two spectra. See also [matchms NeutralLossesCosine](#) for more information.

- FingerprintSimilarity(): Calculate similarity between molecules based on their fingerprints. For this similarity measure to work, fingerprints are expected to be derived by running *add_fingerprint()*. See also [matchms FingerprintSimilarity](#) for more information.

Usage

```
CosineGreedy(tolerance = 0.1, mz_power = 0, intensity_power = 1)

CosineHungarian(tolerance = 0.1, mz_power = 0, intensity_power = 1)

ModifiedCosine(tolerance = 0.1, mz_power = 0, intensity_power = 1)

NeutralLossesCosine(
  tolerance = 0.1,
  mz_power = 0,
  intensity_power = 1,
  ignore_peaks_above_precursor = TRUE
)

## S4 method for signature 'Spectra,Spectra,CosineGreedy'
compareSpectriPy(x, y, param, ...)

## S4 method for signature 'Spectra,missing,CosineGreedy'
compareSpectriPy(x, y, param, ...)
```

Arguments

tolerance   numeric(1): tolerated differences in the peaks' m/z. Peaks with m/z differences <= tolerance are considered matching.

mz_power   numeric(1): the power to raise m/z to in the cosine function. The default is 0, in which case the peak intensity products will not depend on the m/z ratios.

intensity_power

> numeric(1): the power to raise intensity to in the cosine function. The default is 1.

ignore_peaks_above_precursor

> For NeutralLossesCosine(): logical(1): if TRUE (the default), peaks with m/z values larger than the precursor m/z are ignored.

x   A Spectra::Spectra() object.

y   A Spectra::Spectra() object to compare against. If missing, spectra similarities are calculated between all spectra in x.

param   One of the parameter classes listed above (such as CosineGreedy) defining the similarity scoring function in Python and its parameters.

...   ignored.

Value

compareSpectriPy() Returns a numeric matrix with the scores, with the number of rows equal to length(x) and the number of columns equal to length(y).

Note

Parameters and algorithms are named as originally defined in the *matchms* library (i.e. all parameters in *snake_case* while *CamelCase* is used for the algorithms.

Author(s)

Carolin Huber, Michael Witting, Johannes Rainer, Helge Hecht, Marilyn De Graeve

See Also

Spectra::compareSpectra() in the *Spectra* package for pure R implementations of spectra similarity calculations.

Examples

```
library(Spectra)
## Create some example Spectra.
DF <- DataFrame(
    msLevel = c(2L, 2L, 2L),
    name = c("Caffeine", "Caffeine", "1-Methylhistidine"),
    precursorMz = c(195.0877, 195.0877, 170.0924)
)
DF$intensity <- list(
    c(340.0, 416, 2580, 412),
    c(388.0, 3270, 85, 54, 10111),
    c(3.407, 47.494, 3.094, 100.0, 13.240)
)
DF$mz <- list(
    c(135.0432, 138.0632, 163.0375, 195.0880),
    c(110.0710, 138.0655, 138.1057, 138.1742, 195.0864),
    c(109.2, 124.2, 124.5, 170.16, 170.52)
```

```
)
sps <- Spectra(DF)

## Calculate pairwise similarity beween all spectra within sps with
## matchms' CosineGreedy algorithm
## Note: the first compareSpectriPy will take longer because the Python
## environment needs to be set up.
res <- compareSpectriPy(sps, param = CosineGreedy())
res

## Next we calculate similarities for all spectra against the first one
res <- compareSpectriPy(sps, sps[1], param = CosineGreedy())

## Calculate pairwise similarity of all spectra in sps with matchms'
## ModifiedCosine algorithm
res <- compareSpectriPy(sps, param = ModifiedCosine())
res

## Note that the ModifiedCosine method requires the precursor m/z to be
## known for all input spectra. Thus, it is advisable to remove spectra
## without precursor m/z before using this algorithm.
sps <- sps[!is.na(precursorMz(sps))]
compareSpectriPy(sps, param = ModifiedCosine())
```

---

conversion *Converting between R and Python MS data structures*

Description

The rspec_to_pyspec() and pyspec_to_rspec() functions allow to convert (translate) MS data structures between R and Python. At present the R Spectra::Spectra() objects can be either translated into a list of matchms Python matchms.Spectrum objects or spectrum_utils Python spectrum_utils.spectrum.MsmsSpectrum objects. For better integration with the *reticulate* R package also a r_to_py.Spectra() method is available.

The mapping of spectra variables (in R) to (Python) spectra metadata can be configured and defined with the setSpectraVariableMapping() and spectraVariableMapping(). These get and set the *global* (system wide) setting and are thus also used by the r_to_py() method.

Properties for translation to the MS data objects of the different Python libraries are:

- *matchms*: the matchms.Spectrum objects support arbitrary metadata, so any spectra variable can be translated and stored in these objects.

- *spectrum_utils*: the spectrum_utils.spectrum.MsmsSpectrum object supports metadata variables *identifier* (character), *precursor_mz* (numeric), *precursor_charge* (integer) and optionally also *retention_time* (numeric).

See the indivudual function's documentation for more details.

Function to convert R Spectra objects into a Python list of matchms Spectrum objects using the reticulate package.

Usage

```
## S4 method for signature 'character'
spectraVariableMapping(object, x = character(), ...)

## S4 method for signature 'missing'
spectraVariableMapping(object, ...)

setSpectraVariableMapping(x)

defaultSpectraVariableMapping()

## S3 method for class 'Spectra'
r_to_py(x, convert = FALSE)

rspec_to_pyspec(
  x,
  mapping = spectraVariableMapping(),
  pythonLibrary = c("matchms", "spectrum_utils")
)

pyspec_to_rspec(
  x,
  mapping = spectraVariableMapping(),
  pythonLibrary = c("matchms", "spectrum_utils")
)
```

Arguments

object	For spectraVariableMapping(): not used.
x	Spectra object.
...	For spectraVariableMapping(): not used.
convert	Boolean; should Python objects be automatically converted to their R equivalent? Defaults to FALSE.
mapping	named character() vector defining which spectra variables/metadata should be translated between R and Python and how they should be renamed. Defaults to spectraVariableMapping().
pythonLibrary	For rspec_to_pyspec() and pyspec_to_rspec(): character(1) defining the Python library to which (or from which) data structures the data should be converted. Possible options are "matchms" or "spectrum_utils" with "matchms" being the default.

Value

For r_to_py.Spectra() and rspec_to_pyspec(): Python list of MS data structures, either matchms.Spectrum or spectrum_utils.spectrum.MsmsSpectrum objects. For pyspec_to_rspec(): Spectra::Spectra() with the MS data of all matchms.Spectrum objects in the submitted list.

Translation of MS data objects

MS data structures can be translated between R and Python using the rspec_to_pyspec() and pyspec_to_rspec() functions, or with the r_to_py() method.

- rspec_to_pyspec() translates an R [Spectra::Spectra()](#) object into a list of Python MS data objects, which can be, depending on parameter pythonLibrary, matchms.Spectrum objects (for pythonLibrary = "matchms", the default) or spectrum_utils.spectrum.MsmsSpectrum objects (for pythonLibrary = "spectrum_utils"). Parameter mapping allows to specify which spectra variables from the Spectra object x should be converted in addition to the peaks data (m/z and intensity values). It defaults to mapping = spectraVariableMapping() (See the respective help below for more information on the variable mapping). While being fast, this function first loads all peaks and spectra data into memory before translating to Python data structures. A less memory intense operation could be to call this function in a loop to only load parts of the data at a time into memory.

- pyspec_to_rspec() translates a single, or a list of matchms.Spectrum objects (with parameter pythonLibrary = "matchms", the default) or a list of spectrum_utils.spectrum.MsmsSpectrum objects (with parameter pythonLibrary = "spectrum_utils") to a [Spectra::Spectra()](#) object. Parameter mapping allows to specify the metadata variables that should be translated and mapped in addition to the peaks data. The library used to represent the MS data in Python needs to be specified with parameter pythonLibrary.

- r_to_py.Spectra() is equivalent to rspec_to_pyspec(pythonLibrary = "matchms"). The spectra variables that should be converted can be configures with setSpectraVariableMapping() (see documentation below).

Mapping of spectra variables (metadata)

Metadata for MS spectra are represented and stored as *spectra variables* in the R [Spectra::Spectra()](#) objects. Also Python MS data structures store such metadata along with the mass peak data. While spectra metadata is thus supported by data structures in both programming languages, different names and naming conventions are used. The spectraVariableMapping() and setSpectraVariableMapping() functions allow to define how the names of spectra metadata (spectra variables) should be translated between R and Python. To support also the different naming conventions used by the Python libraries *matchms* and *spectrum_utils*, spectraVariableMapping() defines different mapping schemes for these, using by default the mapping for *matchms*. Note also that *spectrum_utils* supports only few selected metadata/spectra variables, so any additional spectra variables defined by the mapping will be ignored. The r_to_py() and py_to_r() functions will use the selected naming scheme to name the spectra variables accordingly. Also, only spectra metadata/variables in spectraVariableMapping() will be translated. The initial mapping is based on this [definition in matchms](#).

- defaultSpectraVariableMapping(): returns the *default* mapping between spectra variables and Python metadata names for the *matchms* library.

- spectraVariableMapping(): returns the currently defined spectra variable mapping as a named character vector, with names representing the names of the spectra variables in R and elements the respective names of the spectra metadata in Python. Use [Spectra::spectraVariables()](#) on the Spectra object that should be converted with r_to_py() to list all available spectra variables. r_to_py() and py_to_r() for MS data structures will use this default mapping. Calling spectraVariableMapping() defining also the Python library (e.g., spectraVariableMapping("matchms")

or spectraVariableMapping("spectrum_utils")) will return the variable mapping for the specified Python library. Optional parameter x allows to specify a (potentially names) character vector with the names of the spectra variables that should in addition be included in the mapping.

- setSpectraVariableMapping(): sets/replaces the currently defined mapping of spectra variable names to Python metadata names. Setting setSpectraVariableMapping(character()) will only convert the mass peaks data (m/z and intensity values) but no spectra metadata.

Author(s)

Michael Witting, Johannes Rainer, Wout Bittremieux, Thomas Naake

Examples

```
## Import a MGF file as a `Spectra` object
library(MsBackendMgf)
library(SpectriPy)
s <- Spectra(
    system.file("extdata", "mgf", "spectra2.mgf", package = "SpectriPy"),
    source = MsBackendMgf())
s


###########################
## Conversion R to Python

## A `Spectra` can be translated to a `list` of `matchms.Spectrum` objects
## using either the `r_to_py()` method or the `rspec_to_pyspec()` function:
s_py <- r_to_py(s)
s_py

## The `s_py` can now be used like any other Python variable within the R
## *reticulate* framework. Below we extract the m/z values of the first
## spectrum
s_py[0]$mz

## Extracting that information from the `Spectra` object in R
s[1]$mz

## The `spectraVariableMapping()` defines which spectra variables (metadata)
## should be translated between R and Python:
spectraVariableMapping()

## The names of that character vector represent the names of the spectra
## variables in R, the elements the name of the metadata variable in Python.
## Below we list the available metadata information from the first
## Spectrum in Python
s_py[0]$metadata

## `setSpectraVariableMapping()` allows to replace the default mapping
## of variables. Below we e.g. add a new spectra variable to the `Spectra`
## object.
s$new_col <- 1:4
```

```
## To translate that variable to Python we need to include it to the
## `spectraVariableMapping()`. Below we define to translate only the
## precursor m/z and the new spectra variable to Python. Be aware that
## `setSpectraVariableMapping()` **globally** sets the default for any
## spectra variable mapping between R and Python. Thus, any subsequent
## calls mapping calls will use the same mapping. It is suggested to
## eventually *restore* the default mapping again after the call or
## use the `rspec_to_pyspec()` function instead, that allows to configure
## the mapping using a parameter `mapping`.
setSpectraVariableMapping(
    c(precursorMz = "precursor_mz", new_col = "new_col"))
s_py <- r_to_py(s)

s_py[0]$metadata

## Restoring the global spectra variable mapping configuration to
## the default mapping:
setSpectraVariableMapping(defaultSpectraVariableMapping())

## As an alternative to the `r_to_py()` we can use the `rspec_to_pyspec()`
## function and provide a custom mapping using the `mapping` parameter:
s_py <- rspec_to_pyspec(
    s, mapping = c(precursorMz = "precursor_mz", new_col = "new_col"))

## Convert to MS data objects from the spectrum_utils Python library
s_py2 <- rspec_to_pyspec(
    s, mapping = spectraVariableMapping("spectrum_utils"),
    pythonLibrary = "spectrum_utils")

## Convert the data back to R
pyspec_to_rspec(s_py2, pythonLibrary = "spectrum_utils")


#########################
## Conversion Python to R

## A `list` of `matchms.Spectrum` objects in Python can be translated into
## the corresponding MS data structure in R (i.e. a `Spectra`) object using
## the `pyspec_to_rspec()` function:
res <- pyspec_to_rspec(s_py)
res

## All spectra from Python are thus converted into a single `Spectra` object.

## Or providing a custom variable mapping:
res <- pyspec_to_rspec(
    s_py, mapping = c(precursorMz = "precursor_mz", new_col = "new_col"))
res$new_col
```

---

filterSpectriPy   *Filter Spectra using Python's matchms library*

Description

The `filterSpectriPy()` function allows to filter/process a `Spectra` object using the `select_by_intensity()`, `select_by_mz()`, `remove_peaks_around_precursor_mz()`, and `normalize_intensities()` functions of the Python matchms.filtering module.

Selection and configuration of the algorithm can be performed with one of the parameter objects (equivalent to *matchms*' function names):

- `select_by_intensity()`: Keeps only the peaks within defined intensity range (keep if `intensity_from` >= intensity >= intensity_to). See also the respective documentation in *matchms*.

- `select_by_mz()`: Keeps only the peaks between `mz_from` and `mz_to` (keep if `mz_from` >= m/z >= `mz_to`). See also the respective documentation in *matchms*.

- `remove_peaks_around_precursor_mz()`: Removes the peaks that are within `mz_tolerance` (in Da) of the precursor mz, excluding the precursor peak.

- `normalize_intensities()`: Normalizes the intensities of peaks (and losses) to unit height.

Usage

```
select_by_intensity(intensity_from = 10, intensity_to = 200)

select_by_mz(mz_from = 0, mz_to = 1000)

remove_peaks_around_precursor_mz(mz_tolerance = 17)

normalize_intensities()

## S4 method for signature 'Spectra,filter_param'
filterSpectriPy(object, param, mapping = spectraVariableMapping(), ...)
```

Arguments

intensity_from	numeric(1): Set lower threshold for peak intensity. Default is 10.
intensity_to	numeric(1): Set upper threshold for peak intensity. Default is 200.
mz_from	numeric(1): Set lower threshold for m/z peak positions. Default is 0.
mz_to	numeric(1): Set upper threshold for m/z peak positions. Default is 1000.
mz_tolerance	numeric(1): Tolerance of m/z values that are not allowed to lie within the precursor mz. Default is 17 Da.
object	A `Spectra::Spectra()` object.
param	one of parameter classes listed above (such as select_by_intensity()) defining the filter/processing function in Python and its parameters.
mapping	named `character()` defining which spectra variables/metadata should be converted between R and Python and how they should be renamed. Defaults to spectraVariableMapping(). See `setSpectraVariableMapping()` for more information.
...	ignored.

Value

filterSpectriPy() returns a Spectra object on which the filtering/processing function has been applied

Note

The first call to the filterSpectriPy() function can take longer because the Python environment needs to be first set up.

filterSpectriPy() first translates the Spectra to Python, applies the filter functions from the *matchms* Python libraries and then translates the filtered data back to a Spectra object. Thus, any spectra variables other than those that are translated between R and Python will be lost during the processing. Use setSpectraVariableMapping() to define which spectra variables should be transferred/converted between R and Python. See also examples below for more information.

The Spectra::Spectra() object returned by filterSpectriPy() will **always** use an in-memory backend (i.e. the Spectra::MsBackendMemory()), independently of the backend used by the backend used by the input Spectra.

Author(s)

Thomas Naake

See Also

- Spectra::filterIntensity(), Spectra::filterMzRange(), Spectra::scalePeaks() in the Spectra package for pure R implementations of filtering/processing calculations.

- rspec_to_pyspec() or pyspec_to_rspec() for the functions used to translated the MS data between R and Python.

Examples

```
library(Spectra)

## create some example Spectra
DF <- DataFrame(
    msLevel = c(2L, 2L, 2L),
    name = c("Caffeine", "Caffeine", "1-Methylhistidine"),
    precursorMz = c(195.0877, 195.0877, 170.0924)
)
DF$intensity <- list(
    c(340.0, 416, 2580, 412),
    c(388.0, 3270, 85, 54, 10111),
    c(3.407, 47.494, 3.094, 100.0, 13.240))
DF$mz <- list(
    c(135.0432, 138.0632, 163.0375, 195.0880),
    c(110.0710, 138.0655, 138.1057, 138.1742, 195.0864),
    c(109.2, 124.2, 124.5, 170.16, 170.52))
sps <- Spectra(DF)

## Filter: select_by_intensity
```

```
res <- filterSpectriPy(
    sps, select_by_intensity(intensity_from = 15, intensity_to = 300))
## Only mass peaks with intensities between the specified limits are
## retained
intensity(res)
## Compared to the original intensities
intensity(sps)

## Note that the spectra variable `"name"` was lost during conversion of
## the MS data between R and Python:
sps$name
any(spectraVariables(res) == "name")

## Only spectra variables defined by `spectraVariableMapping()` are
## converted and thus retained:
spectraVariableMapping()

## We can also pass a custom *spectra variable mapping* with the `mapping`
## parameter to the `filterSpectriPy()` function. Below we create such
## a mapping by adding the translation of a spectra variable `"name"` to
## a metadata name `"compound_name"` to the default spectra variable
## mapping `defaultSpectraVariableMapping()`.
map <- c(defaultSpectraVariableMapping(), name = "compound_name")
map

## Repeat the filtering operation passing this mapping information:
res <- filterSpectriPy(
    sps, select_by_intensity(intensity_from = 15, intensity_to = 300),
    mapping = map)
res$name
```

MsBackendPy   *A MS data backend for MS data stored in Python*

Description

The MsBackendPy allows to access MS data stored as matchms.Spectrum or spectrum_utils.spectrum.MsmsSpectrum objects from the *matchms* respectively *spectrum_utils* Python library directly from R. The MS data (peaks data or spectra variables) are translated on-the-fly when accessed. Thus, the MsBackendPy allows a seamless integration of Python MS data structures into Spectra::Spectra() based analysis workflows.

The MsBackendPy object supports replacing values for peaks variables (*m/z* and intensity) and adding/replacing or removing spectra variables. The changes are immediately translated and written back to the Python variable.

See the descripion of the backendInitialize() method below for creation and initialization of objects from this class. Also, the setBackend() method for Spectra::Spectra() objects internally uses backendInitialize(), thus the same parameters can (and have) to be passed if the backend of a Spectra object is changed to MsBackendPy using the setBackend() method. Special care

should also be given to parameter spectraVariableMapping, that defines which spectra variables should be considered/translated and how their names should or have to be converted between R and Python. See the description for backendInitialize() and the package vignette for details and examples.

Usage

```
## S4 method for signature 'MsBackendPy'
backendInitialize(
  object,
  pythonVariableName = character(),
  spectraVariableMapping = defaultSpectraVariableMapping(),
  pythonLibrary = c("matchms", "spectrum_utils"),
  ...,
  data
)

## S4 method for signature 'MsBackendPy'
length(x)

## S4 method for signature 'MsBackendPy'
spectraVariables(object)

## S4 method for signature 'MsBackendPy'
spectraData(object, columns = spectraVariables(object), drop = FALSE)

## S4 replacement method for signature 'MsBackendPy'
spectraData(object) <- value

## S4 method for signature 'MsBackendPy'
peaksData(object, columns = c("mz", "intensity"), drop = FALSE)

## S4 replacement method for signature 'MsBackendPy'
peaksData(object) <- value

## S4 method for signature 'MsBackendPy'
x$name

## S4 replacement method for signature 'MsBackendPy'
x$name <- value

## S4 replacement method for signature 'MsBackendPy'
intensity(object) <- value

## S4 replacement method for signature 'MsBackendPy'
mz(object) <- value

## S4 replacement method for signature 'MsBackendPy'
spectraVariableMapping(object) <- value
```

```
## S4 method for signature 'MsBackendPy'
spectraVariableMapping(object, value)

reindex(object)
```

Arguments

object	A MsBackendPy object.
pythonVariableName	
	For backendInitialize(): character(1) with the name of the variable/Python attribute that contains the list of matchms.Spectrum objects with the MS data.
spectraVariableMapping	
	For backendInitialize(): named character with the mapping between spectra variable names and (matchms.Spectrum) metadata names. See [defaultSpectraVariableMapping()](#) and the description of the backendInitialize() function for MsBackendPy for more information and details.
pythonLibrary	For backendInitialize(): character(1) specifying the Python library used to represent the MS data in Python. Can be either pythonLibrary = "matchms" (the default) or pythonLibrary = "spectrum_utils".
...	Additional parameters.
data	For backendInitialize(): DataFrame with the full MS data (peaks data and spectra data) such as extracted with the [Spectra::spectraData()](#) method on another MsBackend instance. Importantly, the DataFrame must have columns "mz" and "intensity" with the full MS data.
x	A MsBackendPy object
columns	For spectraData(): character with the names of columns (spectra variables) to retrieve. Defaults to spectraVariables(object). For peaksData(): character with the names of the peaks variables to retrieve.
drop	For spectraData() and peaksData(): logical(1) whether, when a single column is requested, the data should be returned as a vector instead of a data.frame or matrix.
value	Replacement value(s).
name	For $: character(1) with the name of the variable to retrieve.

Details

The MsBackendPy keeps only a reference to the MS data in Python (i.e. the name of the variable in Python) as well as an index pointing to the individual spectra in Python but no other data. Any data requested from the MsBackendPy is accessed and translated on-the-fly from the Python variable. The MsBackendPy is thus an interface to the MS data, but not a data container. All changes to the MS data in the Python variable (performed e.g. in Python) immediately affect any MsBackendPy instances pointing to this variable.

Special care must be taken if the MS data structure in Python is subset or its order is changed (e.g. by another process). In that case it might be needed to re-index the backend using the reindex() function: object <- reindex(object). This will update (replace) the index to the individual spectra in Python which is stored within the backend.

Value

See description of individual functions for their return values.

MsBackendPy **methods**

The MsBackendPy supports all methods defined by the [Spectra::MsBackend()](#) interface for access to MS data. Details on the invidual functions can also be found in the main documentation in the *Spectra* package (i.e. for [Spectra::MsBackend()](#)). Here we provide information for functions with specific properties of the backend.

- backendInitialize(): this method can be used to either initialize the backend with data from a referenced and **existing ** MS data structure in Python, or, through parameter data, first convert and store the provided data to a Python MS data structure and then initialize the backend pointing to this referenced variable (Python attribute). In both cases, the name of the Python attribute needs to be provided with the parameter pythonVariableName. The mapping between the spectra variable names in R and the related Python metadata variables can be specified with the spectraVariableMapping parameter. It has to be a named character with names being the spectra variables and the values the respective name for the metadata in the Python MS data structure. It defaults to [defaultSpectraVariableMapping()](#) which returns the mapping of some core spectra variables for the *matchms* Python library. Be aware that only those spectra variables specified with this parameter are mapped and translated between R and Python. For backendInitialize() with parameter data provided, only the variables defined by spectraVariableMapping, and available in data, are converted and stored in Python. Also note that, for efficiency reasons, core spectra variables (those listed by [Spectra::coreSpectraVariables()](#)) defined with spectraVariableMapping but that have only missing values, are ignored. Parameter pythonLibrary must be used to specify the Python library representing the MS data in Python. It can be either pythonLibrary = "matchms" (the default) or pythonLibrary = "spectrum_utils". The function returns an initialized instance of MsBackendPy. See examples below for different settings and conversion of spectra variables.

- intensity(), intensity()<-: get or replace the intensity values. intensity() returns a NumericList of length equal to the number of spectra with each element being the intensity values of the individual mass peaks per spectrum. intensity()<- takes the same list-like structure as input parameter. Both the number of spectra and the number of peaks must match the length of the spectra and the number of existing mass peaks. To change the number of peaks use the peaksData()<- method instead that replaces the *m/z* and intensity values at the same time. Calling intensity()<- will replace the full MS data (spectra variables as well as peaks variables) of the associated Python variable.

- mz(), mz()<-: get or replace the *m/z* values. mz() returns a NumericList of length equal to the number of spectra with each element being the *m/z* values of the individual mass peaks per spectrum. mz()<- takes the same list-like structure as input parameter. Both the number of spectra and the number of peaks must match the length of the spectra and the number of existing mass peaks. To change the number of peaks use the peaksData()<- method instead that replaces the *m/z* and intensity values at the same time. Calling mz()<- will replace the full MS data (spectra variables as well as peaks variables) of the associated Python variable.

- peaksData(): extracts the peaks data matrices from the backend. Python code is applied to the data structure in Python to extract the *m/z* and intensity values as a list of (numpy) arrays. These are then translated into an R list of two-column numeric matrices. Because Python

does not allow to name columns of an array, an additional loop in R is required to set the column names to ″mz″ and ″intensity″.

- peaksData()<-: replaces the full peaks data (i.e., *m/z* and intensity values) for all spectra. Parameter value has to be a list-like structure with each element being a numeric matrix with one column (named ″mz″) containing the spectrum's *m/z* and one column (named ″intensity″) with the intensity values. This method will replace the full data of the associated Python variable (i.e., both the spectra as well as the peaks data).

- spectraData(): extracts the spectra data from the backend. Which spectra variables are translated and retrieved from the Python objects depends on the backend's spectraVariableMapping(). All metadata names defined are retrieved and added to the returned DataFrame (with eventually missing *core* spectra variables filled with NA).

- spectraData()<-: replaces the full spectra (+ peaks) data of the backend with the values provided with the submitted DataFrame. The number of rows of this DataFrame has to match the number of spectra of object (i.e., being equal to length(object)) and the DataFrame must also contain the spectras' *m/z* and intensity values.

- spectraVariables(): retrieves available spectra variables, which include the names of all metadata attributes in the matchms.Spectrum objects and the *core* spectra variables Spectra::coreSpectraVariables

- spectraVariableMapping(): get the currently defined mapping for spectraVariables() of the backend.

- spectraVariableMapping<-: replaces the spectraVariableMapping of the backend (see setSpectraVariableMapping() for details and description of the expected format).

- $, $<-: extract or add/replace values for a spectra variable from/in the backend. Replacing or adding values for a spectra variable cause the full data to be replaced. In detail, first the full data is retrieved from Python, then the values are added/replaced and then the data is again transferred to Python.

Additional helper and utility functions

- reindex(): update the internal *index* to match 1:length(object). This function is useful if the original data referenced by the backend was subset or re-ordered by a different process (or a function in Python).

Note

As mentioned in the *details* section the MS data is completely stored in Python and the backend only references to this data through the name of the variable in Python. Thus, each time MS data is requested from the backend, it is retrieved in its **current** state. If for example data was transformed or metadata added or removed in the Python object, it immediately affects the Spectra/backend.

Any replacement operation uses internally the spectraData()<- method, thus replacing/updating values for individual spectra variables or peaks variables will first load the current data from Python to R, update or replace the values and then store the full MS data again to the referenced Python attribute.

Author(s)

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Examples

```
## Loading an example MGF file provided by the SpectriPy package.
## As an alternative, the data could also be imported directly in Python
## using:
## import matchms
## from matchms.importing import load_from_mgf
## s_p = list(load_from_mgf(r.fl))
library(Spectra)
library(SpectriPy)
library(MsBackendMgf)

fl <- system.file("extdata", "mgf", "test.mgf", package = "SpectriPy")
s <- Spectra(fl, source = MsBackendMgf())
s

## Translating the MS data to Python and assigning it to a variable
## named "s_p" in the (*reticulate*'s) `py` Python environment. Assigning
## the variable to the Python environment has performance advantages, as
## any Python code applied to the MS data does not require any data
## conversions.
py_set_attr(py, "s_p", rspec_to_pyspec(s))

## Create a `MsBackendPy` representing an interface to the data in the
## "s_p" variable in Python:
be <- backendInitialize(MsBackendPy(), "s_p")
be

## Alternatively, by passing the full MS data with parameter `data`, the
## data is first converted to Python and the backend is initialized with
## that data. The `setBackend()` call from above internally uses this
## code to convert the data.
be <- backendInitialize(MsBackendPy(), "s_p3",
    data = spectraData(s, c(spectraVariables(s), "mz", "intensity")))

## Create a Spectra object which this backend:
s_2 <- Spectra(be)
s_2

## An easier way to change the data representation of a `Spectra` object
## from R to Python is to use the `Spectra`'s `setBackend()` method
## selecting a `MsBackendPy` as the target backend representation:
s_2 <- setBackend(s, MsBackendPy(), pythonVariableName = "s_p2")
s_2

## This moved the data from R to Python, storing it in a Python variable
## with the name `s_p2`. The resulting `s_2` is thus a `Spectra` object
## with all MS data however stored in Python.

## Note that by default only spectra variables that are part of
## `defaultSpectraVariableMapping()` are converted to Python
defaultSpectraVariableMapping()
```

```
## Thus, for example the precursor m/z is available in `s_2`, but other
## spectra variables from `s`, such as `"SMILES"` are not:
precursorMz(s)
precursorMz(s_2)

s$SMILES |> head()
## s_2$SMILES would throw an error.

## To also translate this spectra variable, it needs to be included and
## specified with the `spectraVariableMapping` parameter. The easiest
## approach is to use the `spectraVariableMapping()` function adding in
## addition to the default mapping for the Python library (`"matchms"`)
## also the mapping of additional spectra variables that should be converted:
s_2 <- setBackend(s, MsBackendPy(), pythonVariableName = "s_p2",
    spectraVariableMapping = spectraVariableMapping("matchms", c(SMILES = "smiles")))
s_2$SMILES |> head()

## Available spectra variables: these include, next to the *core* spectra
## variables, also the names of all metadata stored in the `matchms.Spectrum`
## objects.
spectraVariables(s_2)

## Get the full peaks data:
peaksData(s_2)

## Get the peaks from the first spectrum
peaksData(s_2)[[1L]]

## Get the full spectra data:
spectraData(s_2)

## Get the m/z values
mz(s_2)

## Plot the first spectrum
plotSpectra(s_2[1L])


########
## Using the spectrum_utils Python library

## Below we convert the data to a list of `MsmsSpectrum` object from the
## spectrum_utils library.
py_set_attr(py, "su_p", rspec_to_pyspec(s,
    spectraVariableMapping("spectrum_utils"), "spectrum_utils"))

## Create a MsBackendPy representing this data. Importantly, we need to
## specify the Python library using the `pythonLibrary` parameter and
## ideally also set the `spectraVariableMapping` to the one specific for
## that library.
be <- backendInitialize(MsBackendPy(), "su_p",
    spectraVariableMapping = spectraVariableMapping("spectrum_utils"),
    pythonLibrary = "spectrum_utils")
```

```
be

## Get the peaks data for the first 3 spectra
peaksData(be[1:3])

## Get the full spectraData
spectraData(be)

## Extract the precursor m/z
be$precursorMz
```

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