

Package ‘Cardinal’

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Description Implements statistical & computational tools for analyzing mass spectrometry imaging datasets, including methods for efficient pre-processing, spatial segmentation, and classification.

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Description

Implements statistical & computational tools for analyzing mass spectrometry imaging datasets, including methods for efficient pre-processing, spatial segmentation, and classification.

Details

Cardinal provides an abstracted interface to manipulating mass spectrometry imaging datasets, simplifying most of the basic programmatic tasks encountered during the statistical analysis of imaging data. These include image manipulation and processing of both images and mass spectra, and dynamic plotting of both.

While pre-processing steps including normalization, baseline correction, and peak-picking are provided, the core functionality of the package is statistical analysis. The package includes classification and clustering methods based on nearest shrunken centroids, as well as traditional tools like PCA and PLS.

Type `browseVignettes("Cardinal")` to view a user's guide and vignettes of common workflows.

Options

The following options can be set:

- `getCardinalBPPARAM()`, `setCardinalBPPARAM(BPPARAM=NULL)`: The default backend to use for parallel processing. By default, this is initially set to NULL (no parallelization). Otherwise, it must be a `BiocParallelParam` instance. See documentation for [bplapply](#).
- `getCardinalVerbose()`, `setCardinalVerbose(verbose=interactive())`: Should progress messages be printed?
- `getCardinalNChunks()`, `setCardinalNChunks(n=20L)`: The default number of data chunks used when iterating over large datasets. Used by many methods internally.

Additionally, graphical parameters can be set:

- `vizi_style()`: Set the default plotting style.
- `vizi_engine()`: Set the default plotting engine.
- `vizi_par()`: Set default graphical parameters.

Author(s)

Kylie A. Bemis

Maintainer: Kylie A. Bemis <k.bemis@northeastern.edu>

bin

*Bin spectra***Description**

Apply on-the-fly binning to spectra.

Usage

```
## S4 method for signature 'MSImagingExperiment'
bin(x, ref,
    spectra = "intensity", index = "mz",
    method = c("sum", "mean", "max", "min",
               "linear", "cubic", "gaussian", "lanczos"),
    resolution = NA, units = c("ppm", "mz"), ...)

## S4 method for signature 'MSImagingArrays'
bin(x, ref,
    spectra = "intensity", index = "mz",
    method = c("sum", "mean", "max", "min",
               "linear", "cubic", "gaussian", "lanczos"),
    resolution = NA, units = c("ppm", "mz"), ...)

## S4 method for signature 'SpectralImagingExperiment'
bin(x, ref,
    spectra = "intensity", index = NULL,
    method = c("sum", "mean", "max", "min",
               "linear", "cubic", "gaussian", "lanczos"),
    resolution = NA, units = c("relative", "absolute"),
    verbose = getCardinalVerbose(), ...)

## S4 method for signature 'SpectralImagingArrays'
bin(x, ref,
    spectra = "intensity", index = NULL,
    method = c("sum", "mean", "max", "min",
               "linear", "cubic", "gaussian", "lanczos"),
    resolution = NA, units = c("relative", "absolute"),
    verbose = getCardinalVerbose(), ...)
```

Arguments

| | |
|---------|--|
| x | A spectral imaging dataset. |
| ref | Optional. The bin centers, or their range if resolution is specified. Created from resolution if not provided. |
| spectra | The name of the array in spectraData() to bin. |

| | |
|------------|--|
| index | The name of the array in <code>spectraData()</code> (for <code>SpectralImagingArrays</code>) or column in <code>featureData()</code> (for <code>SpectralImagingExperiment</code>) to use for the bins. |
| method | The peak picking method to use. See approx1 for details. |
| resolution | The bin widths. |
| units | The units for the above resolution. |
| verbose | Should progress messages be printed? |
| ... | Ignored. |

Details

The binning is applied but not processed immediately. It is performed on-the-fly whenever the spectra are accessed.

Value

A new object derived from `SpectralImagingExperiment` with the binned spectra.

Author(s)

Kylie A. Bemis

See Also

[approx1](#), [estimateDomain](#), [estimateReferenceMz](#)

Examples

```
set.seed(1)
mse <- simulateImage(preset=1, npeaks=10, dim=c(3,3))

# bin to unit resolution
mse2 <- bin(mse, resolution=1, units="mz")

# bin to a specific range and resolution
mse3 <- bin(mse, ref=c(800, 1000), resolution=1, units="mz")
```

colocalized

Colocalized features

Description

Find colocalized features in an imaging dataset.

Usage

```
## S4 method for signature 'MSImagingExperiment'
colocalized(object, mz, ...)

## S4 method for signature 'SpectralImagingExperiment'
colocalized(object, i, ref,
  threshold = median, n = Inf,
  sort.by = c("cor", "MOC", "M1", "M2", "Dice", "none"),
  nchunks = getCardinalNChunks(),
  verbose = getCardinalVerbose(),
  BPPARAM = getCardinalBPPARAM(), ...)

## S4 method for signature 'SpatialDGMM'
colocalized(object, ref,
  threshold = median, n = Inf,
  sort.by = c("MOC", "M1", "M2", "Dice", "none"),
  nchunks = getCardinalNChunks(),
  verbose = getCardinalVerbose(),
  BPPARAM = getCardinalBPPARAM(), ...)
```

Arguments

| | |
|-----------|---|
| object | An imaging experiment. |
| mz | An m/z value of a feature in object to use as a reference. |
| i | The index of a feature in object to use as a reference. |
| ref | Either a flattened image (i.e., a numeric vector) or a logical mask of a region-of-interest to use as a reference. |
| threshold | Either a function that returns the cutoff to use for creating logical masks of numeric references, or a numeric threshold to use. |
| n | The number of top-ranked colocalized features to return. |
| sort.by | The colocalization measure used to rank colocalized features. Possible options include Pearson's correlation ("cor"), Manders overlap coefficient ("MOC"), Manders colocalization coefficients ("M1" and "M2"), and Dice similarity coefficient ("Dice"). |
| nchunks | The number of chunks to use for processing. |
| verbose | Should progress messages be printed? |
| BPPARAM | An optional instance of <code>BiocParallelParam</code> . See documentation for bplapply . |
| ... | Options passed to chunkApply . |

Value

A data frame with the colocalized features, or a list of data frames if multiple references are given.

Author(s)

Kylie A. Bemis

Examples

```

set.seed(1)
x <- simulateImage(preset=1, dim=c(10,10), representation="centroid")

# find features colocalized with first feature
colocalized(x, i=1)

```

 deprecated

Deprecated and defunct objects in Cardinal

Description

These functions are provided for compatibility with older versions of Cardinal, and will be removed in the future.

 estimateDomain

Estimate shared domain

Description

For unaligned spectral data, it is often necessary to estimate a suitable shared domain in order to calculate statistical summaries like the mean spectrum.

Usage

```

estimateDomain(xlist,
  units = c("relative", "absolute"),
  nchunks = getCardinalNChunks(),
  verbose = getCardinalVerbose(),
  BPPARAM = getCardinalBPPARAM(), ...)

estimateReferenceMz(object,
  units = c("ppm", "mz"),
  nchunks = getCardinalNChunks(),
  verbose = getCardinalVerbose(),
  BPPARAM = getCardinalBPPARAM(), ...)

estimateReferencePeaks(object, SNR = 2,
  method = c("diff", "sd", "mad", "quantile", "filter", "cwt"),
  nchunks = getCardinalNChunks(),
  verbose = getCardinalVerbose(),
  BPPARAM = getCardinalBPPARAM(), ...)

```

Arguments

| | |
|----------------------|---|
| <code>xlist</code> | A list of the domain values (e.g., m/z values) for each spectrum. |
| <code>object</code> | A mass spectral imaging dataset. |
| <code>units</code> | Should the spacing between domain values use absolute or relative units? |
| <code>method</code> | The peak picking method to use. See findpeaks for details. |
| <code>SNR</code> | The signal-to-noise threshold to use to determine a peak. |
| <code>nchunks</code> | The number of chunks to use for processing. |
| <code>verbose</code> | Should progress messages be printed? |
| <code>BPPARAM</code> | An optional instance of <code>BiocParallelParam</code> . See documentation for bplapply . |
| <code>...</code> | Options passed to chunkLapply . |

Details

For `estimateDomain`, the domain is estimated by first finding the resolution of each spectrum's individual domain values (e.g., the spacing between m/z values), and then creating a sequence of domain values using the median resolution of all spectra.

The `estimateReferenceMz` function simply calls `estimateDomain` on the appropriate components of a mass spectral imaging dataset to estimate profile m/z bins.

The `estimateReferencePeaks` function calculates the mean spectrum (or looks for a "mean" column in `featureData()`) and performs peak picking on the mean spectrum. It can be used to create a set of reference peaks if all relevant peaks appear in the mean spectrum.

Value

A vector of domain values, m/z values, or peaks.

Author(s)

Kylie A. Bemis

See Also

[summarizeFeatures](#), [recalibrate](#), [peakAlign](#), [peakProcess](#)

features

Find feature indices

Description

Search for the row indices of a spectral imaging dataset that correspond to specific features, based on a set of conditions.

Usage

```
## S4 method for signature 'MSImagingExperiment'
features(object, ..., mz, tolerance = NA, units = c("ppm", "mz"),
  env = NULL)

## S4 method for signature 'SpectralImagingExperiment'
features(object, ..., env = NULL)
```

Arguments

| | |
|-----------|---|
| object | A spectral imaging dataset. |
| ... | Expressions that evaluate to logical vectors in the environment of featureData(). |
| mz | The m/z values of features to include. |
| tolerance | The tolerance for matching features to m/z values. |
| units | The units for the above tolerance. |
| env | The enclosing environment for evaluating ... |

Author(s)

Kylie A. Bemis

Examples

```
set.seed(1)
mse <- simulateImage(preset=1, npeaks=10, dim=c(10,10))

features(mse, mz > 800, mz < 1800)
features(mse, mz=metadata(mse)$design$featureData$mz)
```

| | |
|---------------|-------------------------------|
| findNeighbors | <i>Find spatial neighbors</i> |
|---------------|-------------------------------|

Description

Find the indices of spatial neighbors for all observations in a dataset.

Usage

```
## S4 method for signature 'ANY'
findNeighbors(x, r = 1, groups = NULL,
  metric = "maximum", p = 2, matrix = FALSE, ...)

## S4 method for signature 'SpectralImagingData'
findNeighbors(x, r = 1, groups = run(x), ...)

## S4 method for signature 'PositionDataFrame'
findNeighbors(x, r = 1, groups = run(x), ...)
```

Arguments

| | |
|---------------------|---|
| <code>x</code> | An imaging dataset or data frame with spatial dimensions. |
| <code>r</code> | The spatial maximum distance for an observation to be considered a neighbor. |
| <code>groups</code> | A vector coercible to a factor giving which observations should be treated as spatially-independent. Observations in the same group are assumed to have a spatial relationship. |
| <code>metric</code> | Distance metric to use when finding the nearest neighbors. Supported metrics include "euclidean", "maximum", "manhattan", and "minkowski". |
| <code>p</code> | The power for the Minkowski distance. |
| <code>matrix</code> | Should the neighbors be returned as a sparse adjacency matrix instead of a list? |
| <code>...</code> | Additional arguments passed to the next call. |

Value

Either a list of indices of neighbors or a sparse adjacency matrix ([sparse_mat](#)).

Author(s)

Kylie A. Bemis

See Also

[spatialWeights](#)

Examples

```
pdata <- PositionDataFrame(coord=expand.grid(x=1:8, y=1:8))

# find spatial neighbors
findNeighbors(pdata, r=1)
```

MassDataFrame-class *MassDataFrame: Extended data frame with key columns*

Description

A data frame for mass spectrometry feature metadata with a required column for m/z values.

Usage

```
MassDataFrame(mz, ..., row.names = FALSE)
```

Arguments

| | |
|-----------|---|
| mz | A sorted vector of m/z values. |
| ... | Arguments passed to the <code>DataFrame()</code> . |
| row.names | Either a vector of row names or a logical value indicating whether row names should be generated automatically (from the m/z values). |

Methods

`mz(object, ...)`, `mz(object, ...) <- value`: Get or set the m/z values.

Author(s)

Kylie A. Bemis

See Also

[XDataFrame](#), [PositionDataFrame](#)

Examples

```
## Create an MassDataFrame object
MassDataFrame(mz=sort(500 * runif(10)), label=LETTERS[1:10])
```

MeansTest

Linear model-based testing for summarized imaging experiments

Description

Performs hypothesis testing for imaging experiments by fitting linear mixed models to summarizations or segmentations.

Usage

```
## S4 method for signature 'ANY'
meansTest(x, data, fixed, random, samples,
  response = "y", reduced = ~ 1, byrow = FALSE,
  nchunks = getCardinalNChunks(),
  verbose = getCardinalVerbose(),
  BPPARAM = getCardinalBPPARAM(), ...)

## S4 method for signature 'SpectralImagingExperiment'
meansTest(x, fixed, random, samples = run(x),
  response = "intensity", ...)

## S4 method for signature 'SpatialDGMM'
meansTest(x, fixed, random, class = 1L,
  response = "intensity", reduced = ~ 1,
```

```

nchunks = getCardinalNChunks(),
verbose = getCardinalVerbose(),
BPPARAM = getCardinalBPPARAM(), ...)

segmentationTest(x, fixed, random, samples = run(x),
  class = 1L, response = "intensity", reduced = ~ 1, ...)

## S4 method for signature 'MeansTest'
topFeatures(object, n = Inf, sort.by = "statistic", ...)

## S4 method for signature 'MeansTest,missing'
plot(x, i = 1L, type = "boxplot", show.obs = TRUE,
  fill = FALSE, layout = NULL, ...)

```

Arguments

| | |
|-------------------------|---|
| <code>x</code> | A dataset in $P \times N$ matrix format or a set of spatially segmented images. |
| <code>data</code> | A data frame of additional variables parallel to <code>x</code> . |
| <code>fixed</code> | A one-sided formula giving the fixed effects of the model on the RHS. The response will added to the LHS, and the formula will be passed to the underlying modeling function. |
| <code>random</code> | A one-sided formula giving the random effects of the model on the RHS. See lme for the allowed specifications. |
| <code>samples</code> | A vector coercible to a factor giving the observational unit (i.e., the samples and replicates). |
| <code>class</code> | For <code>SpatialDGMM</code> , the class (segment) from the Gaussian mixture models that should be used for the comparison. By default, compare the classes (segments) with the highest means in each sample. |
| <code>response</code> | The name of to assign the response variable in the fitted models. |
| <code>reduced</code> | A one-sided formula specifying the reduced model for the null hypothesis. The default is an intercept-only model. |
| <code>byrow</code> | For the default method, are the rows or the columns the <code>x</code> . |
| <code>nchunks</code> | The number of chunks to use for processing. |
| <code>verbose</code> | Should progress messages be printed? |
| <code>BPPARAM</code> | An optional instance of <code>BiocParallelParam</code> . See documentation for bplapply . |
| <code>...</code> | Passed to internal linear modeling methods. Either lm if only fixed effects are given or lme if random effects are given. |
| <code>object</code> | A fitted model object to summarize. |
| <code>n, sort.by</code> | For <code>topFeatures</code> , the number of top features to return and how to sort them. |
| <code>i</code> | The index of the model(s)/feature(s) to plot. |
| <code>type</code> | The type of plot to display. |
| <code>show.obs</code> | Should individual observations (i.e., the summarized mean for each sample) be plotted too? |

| | |
|--------|--|
| fill | Should the boxplots be filled? |
| layout | A vector of the form <code>c(nrow, ncol)</code> specifying the number of rows and columns in the facet grid. |

Value

An object of class `MeansTest` derived from `ResultsList`, where each element contains a linear model.

Author(s)

Dan Guo and Kylie A. Bemis

See Also

[lm](#), [lme](#), [spatialDGMM](#)

Examples

```
set.seed(1)
x <- simulateImage(preset=4, nrun=3, npeaks=10,
  dim=c(10,10), peakheight=5, peakdiff=2,
  representation="centroid")

samples <- replace(run(x), !(x$circleA | x$circleB), NA)

fit <- meansTest(x, ~condition, samples=samples)
print(fit)
```

MSImagingArrays-class *MSImagingArrays: MS imaging data with arbitrary m/z values*

Description

The `MSImagingArrays` class provides a list-like container for high-throughput mass spectrometry imaging data where every mass spectrum may have its own m/z values. It is designed for easy access to raw mass spectra for the purposes of pre-processing.

It can be converted to a [MSImagingExperiment](#) object for easier image slicing and for applying statistical models and machine learning methods.

Usage

```
## Instance creation
MSImagingArrays(spectraData = SimpleList(),
  pixelData = PositionDataFrame(), experimentData = NULL,
  centroided = NA, continuous = NA, metadata = list())

## Additional methods documented below
```

Arguments

| | |
|----------------|---|
| spectraData | Either a list-like object with lists of individual spectra and lists of their domain values, or a SpectraArrays instance. |
| pixelData | A PositionDataFrame with pixel metadata, with a row for each spectrum. |
| experimentData | Either NULL or a ImzMeta object with MS-specific experiment-level metadata. |
| centroided | A logical value indicated whether the spectra have been centroided. |
| continuous | A logical value indicated whether the spectra all have the same m/z values. |
| metadata | A list of arbitrary metadata. |

Slots

| | |
|------------------|---|
| spectraData: | A SpectraArrays object storing one or more array-like data elements with conformable dimensions. |
| elementMetadata: | A PositionDataFrame containing spectrum-level metadata, including each spectrum's pixel coordinates and experimental run information. |
| processing: | A list containing unexecuted ProcessingStep objects. |
| experimentData: | Either NULL or an ImzMeta object containing experiment-level metadata (necessary for writing the data to imzML). |
| centroided: | A logical value indicated whether the spectra have been centroided (if known). |
| continuous: | A logical value indicated whether the spectra all have the same m/z values (if known). |

Methods

All methods for [SpectralImagingData](#) and [SpectralImagingArrays](#) also work on [MSImagingArrays](#) objects. Additional methods are documented below:

| | |
|---|---|
| <code>mz(object, i = NULL, ...)</code> , <code>mz(object, i = NULL, ...) <- value</code> : | Get or set the m/z arrays in the <code>spectraData</code> slot. |
| <code>intensity(object, i = NULL, ...)</code> , <code>intensity(object, i = NULL, ...) <- value</code> : | Get or set the intensity arrays in the <code>spectraData</code> slot. |
| <code>centroided(object, ...)</code> , <code>centroided(object, ...) <- value</code> : | Get or set the <code>centroided</code> slot. |
| <code>isCentroided(object, ...)</code> : | Equivalent to <code>isTRUE(centroided(object))</code> . |
| <code>experimentData(object)</code> , <code>experimentData(object) <- value</code> : | Get or set the <code>experimentData</code> slot. |

Author(s)

Kylie A. Bemis

See Also

[SpectralImagingArrays](#), [MSImagingExperiment](#)

Examples

```

set.seed(1)
x <- replicate(9, rlnorm(10), simplify=FALSE)
mz <- replicate(9, 500 * sort(runif(10)), simplify=FALSE)
coord <- expand.grid(x=1:3, y=1:3)

msa <- MSImagingArrays(
  spectraData=list(intensity=x, mz=mz),
  pixelData=PositionDataFrame(coord))

print(msa)

```

MSImagingExperiment-class

MSImagingExperiment: MS imaging data with shared m/z values

Description

The MSImagingExperiment class provides a matrix-like container for high-throughput mass spectrometry imaging data where every mass spectrum shares the same m/z values. It is designed to provide easy access to both the spectra (as columns) and sliced images (as rows).

It can be converted from a [MSImagingArrays](#) object which is designed for representing raw mass spectra.

Usage

```

## Instance creation
MSImagingExperiment(spectraData = SimpleList(),
  featureData = MassDataFrame(), pixelData = PositionDataFrame(),
  experimentData = NULL, centroided = NA, metadata = list())

## Additional methods documented below

```

Arguments

| | |
|----------------|---|
| spectraData | Either a matrix-like object with number of rows equal to the number of features and number of columns equal to the number of pixels, a list of such objects, or a SpectraArrays instance. |
| featureData | A MassDataFrame with feature metadata, with a row for each feature. |
| pixelData | A PositionDataFrame with pixel metadata, with a row for each spectrum. |
| experimentData | Either NULL or a ImzMeta object with MS-specific experiment-level metadata. |
| centroided | A logical value indicated whether the spectra have been centroided. |
| metadata | A list of arbitrary metadata. |

Slots

spectraData: A [SpectraArrays](#) object storing one or more array-like data elements with conformable dimensions.

featureData: A [MassDataFrame](#) containing feature-level metadata.

elementMetadata: A [PositionDataFrame](#) containing spectrum-level metadata, including each spectrum's pixel coordinates and experimental run information.

processing: A list containing unexecuted [ProcessingStep](#) objects.

experimentData: Either NULL or an [ImzMeta](#) object containing experiment-level metadata (necessary for writing the data to imzML).

centroided: A logical value indicated whether the spectra have been centroided (if known).

Methods

All methods for [SpectralImagingData](#) and [SpectralImagingExperiment](#) also work on [MSImagingExperiment](#) objects. Additional methods are documented below:

mz(object, ...), mz(object, ...) <- value: Get or set the m/z column in the featureData slot.

intensity(object, ...), intensity(object, ...) <- value: Get or set the intensity matrix in the spectraData slot.

centroided(object, ...), centroided(object, ...) <- value: Get or set the centroided slot.

isCentroided(object, ...): Equivalent to isTRUE(centroided(object)).

experimentData(object), experimentData(object) <- value: Get or set the experimentData slot.

Author(s)

Kylie A. Bemis

See Also

[SpectralImagingExperiment](#), [MSImagingArrays](#)

Examples

```
set.seed(1)
x <- matrix(rlnorm(81), nrow=9, ncol=9)
mz <- sort(runif(9))
coord <- expand.grid(x=1:3, y=1:3)

mse <- MSImagingExperiment(
  spectraData=x,
  featureData=MassDataFrame(mz=mz),
  pixelData=PositionDataFrame(coord))

print(mse)
```

| | |
|-----------|--------------------------|
| normalize | <i>Normalize spectra</i> |
|-----------|--------------------------|

Description

Apply deferred normalization to spectra.

Usage

```
## S4 method for signature 'SpectralImagingData'  
normalize(object,  
          method = c("tic", "rms", "reference"), ...)
```

Arguments

| | |
|--------|---|
| object | A spectral imaging dataset. |
| method | The normalization method to use. See rescale for details. |
| ... | Additional arguments passed to the normalization function. |

Details

The supported normalization methods are:

- "tic": Total ion current normalization using [rescale_sum](#).
- "rms": Root-mean-squared normalization using [rescale_rms](#).
- "reference": Normalization according to a reference feature using [rescale_ref](#).

Value

An object of the same class with the processing step queued.

Note

The normalization is deferred until `process()` is called.

Author(s)

Kylie A. Bemis

See Also

[smooth](#), [recalibrate](#), [reduceBaseline](#), [peakPick](#), [process](#)

Examples

```

set.seed(1)
mse <- simulateImage(preset=1, npeaks=10, dim=c(3,3))

# queue normalization
mse2 <- normalize(mse, method="tic")

# apply normalization
mse2 <- process(mse2)

```

peakAlign

Align peaks across spectra

Description

Align peaks across spectra in a spectral imaging dataset.

Usage

```

## S4 method for signature 'MSImagingExperiment'
peakAlign(object, ref,
           spectra = "intensity", index = "mz",
           tolerance = NA, units = c("ppm", "mz"), ...)

## S4 method for signature 'MSImagingArrays'
peakAlign(object, ref,
           spectra = "intensity", index = "mz",
           tolerance = NA, units = c("ppm", "mz"), ...)

## S4 method for signature 'SpectralImagingExperiment'
peakAlign(object, ref,
           spectra = "intensity", index = NULL,
           tolerance = NA, units = c("relative", "absolute"),
           nchunks = getCardinalNChunks(),
           verbose = getCardinalVerbose(),
           BPPARAM = getCardinalBPPARAM(), ...)

## S4 method for signature 'SpectralImagingArrays'
peakAlign(object, ref,
           spectra = "intensity", index = NULL,
           tolerance = NA, units = c("relative", "absolute"),
           nchunks = getCardinalNChunks(),
           verbose = getCardinalVerbose(),
           BPPARAM = getCardinalBPPARAM(), ...)

```

Arguments

| | |
|-----------|---|
| object | A spectral imaging dataset. |
| ref | The locations of reference peaks to use for the alignment. |
| spectra | The name of the array in spectraData() to use for the peak intensities. |
| index | The name of the array in spectraData() (for SpectralImagingArrays) or column in featureData() (for SpectralImagingExperiment) to use for the peak locations. |
| tolerance | The tolerance for matching a detected peak to the reference. If NA, then the tolerance is automatically determined as half the minimum distance between locations in the estimated spectral domain (see "Details"). |
| units | The units for the above tolerance. |
| nchunks | The number of chunks to use for processing. |
| verbose | Should progress messages be printed? |
| BPPARAM | An optional instance of BiocParallelParam. See documentation for bplapply . |
| ... | Options passed to process(). |

Details

Before peak alignment, process() is called to apply any queued pre-processing steps. It is assumed that peakPick() has either been queued or already applied to the data.

If ref is provided, then the aligned peaks are returned immediately without additional processing. (Peaks are binned on-the-fly to the reference peak locations.)

If ref is not provided, then the shared peaks must be determined automatically. This starts with creation of a shared domain giving a list of possible peak locations.

For SpectralImagingArrays, estimateDomain() is used to create the shared domain from the index array. For SpectralImagingExperiment, the index column of featureData() is used directly.

Next, binpeaks is used to bin the observed peaks to the shared domain. Then, mergepeaks is used to merge peaks that are separated by a distance less than the given tolerance.

The averaged locations of the merged peaks in each bin are used as the shared peaks for the full dataset, and the aligned peaks are returned. (Peaks are binned on-the-fly to the shared peak locations.)

Value

A new object derived from SpectralImagingExperiment with the aligned peaks.

Author(s)

Kylie A. Bemis

See Also

[process](#) [peakPick](#), [peakProcess](#)

Examples

```

set.seed(1)
mse <- simulateImage(preset=1, npeaks=10, dim=c(3,3))

# queue peak picking
mse2 <- peakPick(mse, method="diff", SNR=6)

# align peaks
mse2 <- peakAlign(mse2)
plot(mse2, i=4)

```

peakPick

Peak pick spectra

Description

Apply deferred peak picking to spectra.

Usage

```

## S4 method for signature 'MSImagingExperiment'
peakPick(object, ref,
  method = c("diff", "sd", "mad", "quantile", "filter", "cwt"),
  SNR = 2, type = c("height", "area"),
  tolerance = NA, units = c("ppm", "mz"), ...)

## S4 method for signature 'MSImagingArrays'
peakPick(object, ref,
  method = c("diff", "sd", "mad", "quantile", "filter", "cwt"),
  SNR = 2, type = c("height", "area"),
  tolerance = NA, units = c("ppm", "mz"), ...)

## S4 method for signature 'SpectralImagingData'
peakPick(object, ref,
  method = c("diff", "sd", "mad", "quantile", "filter", "cwt"),
  SNR = 2, type = c("height", "area"),
  tolerance = NA, units = c("relative", "absolute"), ...)

```

Arguments

| | |
|--------|--|
| object | A spectral imaging dataset. |
| ref | Optional vector giving locations of reference peaks to extract from the dataset. |
| method | The peak picking method to use. See findpeaks for details. |
| SNR | The signal-to-noise threshold to use to determine a peak. |
| type | The type of value to use to summarize the peak. |

| | |
|-----------|--|
| tolerance | If ref is specified, the tolerance to use when deciding if a local peak in a spectrum matches a reference peak. If NA, then the tolerance is automatically determined as half the minimum distance between peaks in the reference. |
| units | The units for the above tolerance. |
| ... | Additional arguments passed to the peak picking function. |

Details

Unless otherwise specified, peaks are detected as local maxima which are then compared to the estimated noise level to determine a signal-to-noise ratio for each peak. Most of the peak detection methods below are differentiated by how they estimate the noise in the spectrum.

The supported peak picking methods are:

- "diff": Estimate noise based on the derivative of the signal using [estnoise_diff](#).
- "sd": Estimate noise from standard deviation using [estnoise_sd](#).
- "mad": Estimate noise from mean absolute deviation using [estnoise_mad](#).
- "quantile": Estimate noise from a rolling quantile of the difference between the raw signal and a smoothed signal using [estnoise_quant](#).
- "filter": Estimate noise using dynamic filtering of the local peaks using [estnoise_filt](#).
- "cwt": Detect peaks based on continuous wavelet transform (CWT) using [findpeaks_cwt](#).

If ref is provided, then the signal-to-noise ratio is not determined, and any detected local maxima are summarized as long as they match to a reference peak.

Value

An object of the same class with the processing step queued.

Note

The peak picking is deferred until `process()` is called.

Author(s)

Kylie A. Bemis

See Also

[process](#), [peakAlign](#), [peakProcess](#), [estimateReferencePeaks](#)

Examples

```
set.seed(1)
mse <- simulateImage(preset=1, npeaks=10, dim=c(3,3))

# queue peak picking
mse2 <- peakPick(mse, method="diff", SNR=6)
plot(mse2, i=4)
```

```
# apply peak picking
mse2 <- process(mse2)
```

peakProcess *Process peaks in mass spectra*

Description

Apply peak picking and alignment to a mass spectrometry imaging dataset.

Usage

```
## S4 method for signature 'MSImagingExperiment_OR_Arrays'
peakProcess(object, ref,
  spectra = "intensity", index = "mz",
  method = c("diff", "sd", "mad", "quantile", "filter", "cwt"),
  SNR = 2, type = c("height", "area"),
  tolerance = NA, units = c("ppm", "mz"),
  sampleSize = NA, filterFreq = TRUE, outfile = NULL,
  nchunks = getCardinalNChunks(),
  verbose = getCardinalVerbose(),
  BPPARAM = getCardinalBPPARAM(), ...)
```

Arguments

| | |
|------------|--|
| object | A spectral imaging dataset. |
| ref | The locations of reference peaks to use for the alignment. |
| spectra | The name of the array in <code>spectraData()</code> to use for the peak intensities. |
| index | The name of the array in <code>spectraData()</code> (for <code>MSImagingArrays</code>) or column in <code>featureData()</code> (for <code>MSImagingExperiment</code>) to use for the peak locations. |
| method | The peak picking method to use. See findpeaks for details. |
| SNR | The signal-to-noise threshold to use to determine a peak. |
| type | The type of value to use to summarize the peak. |
| tolerance | The tolerance for matching a detected peak to the reference peaks or the shared m/z values. Passed to peakPick and peakAlign . |
| units | The units for the above tolerance. |
| sampleSize | The count or proportion giving a subset of spectra to use to determine reference peaks. |
| filterFreq | Either a logical value indicating whether singleton peaks should be removed, or a count or frequency used as a threshold to filter the peaks. |
| outfile | Optional. The name of a file to write the resulting dataset as <code>imzML</code> . |
| nchunks | The number of chunks to use for processing. |
| verbose | Should progress messages be printed? |
| BPPARAM | An optional instance of <code>BiocParallelParam</code> . See documentation for bplapply . |
| ... | Options passed to <code>process()</code> . |

Details

This method provides a combined interface for [peakPick](#) and [peakAlign](#) for the most common approaches to peak processing.

If `peakPick()` has been queued already, then it will be applied. Otherwise, it will be called internally with the provided arguments.

There are two main paths depending on whether (1) peaks should be extracted based on a reference or (2) peak picking should be performed on the full dataset and then aligned.

If either `ref` is provided or `sampleSize` is finite, then (1) is chosen and peaks are extracted based on the reference. If the reference is not provided, then peak picking and alignment performed on a subset of spectra (according to `sampleSize`) to create the reference peaks. The reference peaks are then used to extract peaks from the full dataset.

Otherwise, (2) is chosen and peaks are picked and aligned across all spectra.

The advantage of (1) is that all reference peaks will be summarized even they would not have a high enough signal-to-noise ratio to be detected in some spectra. The disadvantage is that rare peaks that do not appear in the sampled subset of spectra will not be included in the process peaks.

The advantage of (2) is that rare peaks will be included because peak detection is performed on all spectra. The disadvantage is that some peaks may be missing from some spectra despite having nonzero intensities, because they did not have a high enough signal-to-noise ratio to be detected as peaks.

Setting `sampleSize` to 1 will balance these advantages and disadvantages because the reference will be based on all spectra. However, this means the full dataset must be processed at least twice (possibly more if intermediate calculations are necessary), so it will be more time-consuming.

Value

A new object derived from `MSImagingExperiment` with the processed peaks.

Author(s)

Kylie A. Bemis

See Also

[process](#) [peakPick](#), [peakAlign](#)

Examples

```
set.seed(1)
mse <- simulateImage(preset=1, npeaks=10, dim=c(3,3))

# process peaks
mse2 <- peakProcess(mse, method="diff", SNR=3)
plot(mse2, i=4)
```

`pixels`*Find pixel indices*

Description

Search for the column indices of a spectral imaging dataset that correspond to specific pixels, based on a set of conditions.

Usage

```
## S4 method for signature 'SpectralImagingExperiment'  
pixels(object, ..., coord, run, tolerance = NA,  
        env = NULL)  
  
## S4 method for signature 'SpectralImagingArrays'  
pixels(object, ..., coord, run, tolerance = NA,  
        env = NULL)  
  
## S4 method for signature 'SpectralImagingData'  
pixels(object, ..., env = NULL)
```

Arguments

| | |
|------------------------|---|
| <code>object</code> | A spectral imaging dataset. |
| <code>...</code> | Expressions that evaluate to logical vectors in the environment of <code>pixelData()</code> . |
| <code>coord</code> | The coordinates of the pixels to include. |
| <code>run</code> | The run of the pixels to include. |
| <code>tolerance</code> | The tolerance for matching pixels to coordinates. |
| <code>env</code> | The enclosing environment for evaluating ... |

Author(s)

Kylie A. Bemis

Examples

```
set.seed(1)  
mse <- simulateImage(preset=1, npeaks=10, dim=c(10,10))  
  
pixels(mse, x > 6, y > 6)  
pixels(mse, coord=expand.grid(x=1:3, y=1:3))
```

plot-image

Plot images from a spectral imaging dataset

Description

Create and display images from the spectra or pixel data of a spectral imaging dataset using a formula interface.

Usage

```
## S4 method for signature 'MSImagingExperiment'
image(x,
      formula = intensity ~ x * y,
      i = features(x, mz=mz),
      mz = NULL,
      tolerance = NA,
      units = c("ppm", "mz"),
      ...,
      xlab, ylab)

## S4 method for signature 'SpectralImagingExperiment'
image(x,
      formula,
      i = 1L,
      run = NULL,
      groups = NULL,
      superpose = FALSE,
      key = TRUE,
      ...,
      enhance = NULL,
      smooth = NULL,
      scale = NULL,
      subset = TRUE)
```

Arguments

| | |
|-----------|---|
| x | A spectral imaging dataset. |
| formula | A formula of the form $vals \sim x * y$ giving the image values and the pixel coordinates. The LHS is taken to be the name of an array in <code>spectraData()</code> and the RHS is taken to be columns of <code>pixelData()</code> . Alternatively, if <code>formula</code> is a string or if <code>i</code> is <code>NULL</code> , then the LHS is interpreted as the name of a column of <code>pixelData()</code> as well. |
| i | The index of the feature(s) to plot for the image(s). |
| mz | The m/z value(s) to plot for the image(s). |
| tolerance | If specified, the tolerance to consider a feature as being equal to the given mz value. |

| | |
|------------|---|
| units | The units for the above tolerance. |
| ... | Additional arguments passed to plot_image . |
| xlab, ylab | Plotting labels. |
| run | The names of experimental runs to include, or the index of the levels of the runs to include. |
| groups | A vector coercible to a factor indicating which of the specified features should be plotted with the same color. |
| superpose | If multiple images are plotted, should they be superposed on top of each other, or plotted separately? |
| key | Should a legend or colorkey be plotted? |
| enhance | The name of a contrast enhancement method, such as "hist" or "adapt" for <code>enhance_hist()</code> and <code>enhance_adapt()</code> , etc. See enhance for details. |
| smooth | The name of a smoothing method, such as "gauss" or "bi" for <code>filt2_gauss()</code> and <code>filt2_bi()</code> , etc. See filt2 for details. |
| scale | If multiple images are plotted, should they be scaled to the same intensity scale? |
| subset | A logical vector indicating which pixels to include in the image. |

Author(s)

Kylie A. Bemis

See Also

[image](#), [plot_image](#), [selectROI](#)

Examples

```
set.seed(1)
x <- simulateImage(preset=2, npeaks=10, dim=c(16,16))
peaks <- mz(metadata(x)$design$featureData)

image(x, mz=peaks[1L], tolerance=0.5, units="mz")
image(x, mz=peaks[1L], smooth="gaussian")
image(x, mz=peaks[1:9], smooth="adaptive")

x <- summarizePixels(x, stat=c(TIC="mean"))
image(x, "TIC")
```

plot-spectra

Plot spectra from a spectral imaging dataset

Description

Create and display sliced images from a spectral imaging dataset using a formula interface.

Usage

```
## S4 method for signature 'MSImagingExperiment,missing'
plot(x,
     formula = intensity ~ mz,
     i = pixels(x, coord=coord, run=run),
     coord = NULL,
     run = NULL,
     ...,
     xlab, ylab,
     isPeaks = isCentroided(x))

## S4 method for signature 'MSImagingArrays,missing'
plot(x,
     formula = intensity ~ mz,
     i = pixels(x, coord=coord, run=run),
     coord = NULL,
     run = NULL,
     ...,
     xlab, ylab,
     isPeaks = isCentroided(x))

## S4 method for signature 'SpectralImagingExperiment,missing'
plot(x,
     formula,
     i = 1L,
     groups = NULL,
     superpose = FALSE,
     key = TRUE,
     ...,
     n = Inf,
     downsampler = "lttb",
     isPeaks = FALSE,
     annPeaks = 0)

## S4 method for signature 'SpectralImagingArrays,missing'
plot(x,
     formula,
     i = 1L,
     groups = NULL,
```

```

superpose = FALSE,
key = TRUE,
...,
n = Inf,
downsampler = "lttb",
isPeaks = FALSE,
annPeaks = 0)

```

Arguments

| | |
|----------------|--|
| x | A spectral imaging dataset. |
| formula | A formula of the form <code>vals ~ t</code> giving the spectra values and their domain locations. The LHS is taken to be the name of an array in <code>spectraData()</code> and the RHS is either an array in <code>spectraData()</code> for <code>SpectralImagingArrays</code> -derived classes or a column of <code>featureData()</code> for <code>SpectralImagingExperiment</code> -derived classes. Alternatively, if <code>formula</code> is a string or if <code>i</code> is <code>NULL</code> , then the LHS is interpreted as the name of a column of <code>featureData()</code> for <code>SpectralImagingExperiment</code> as well. |
| i | The index of the spectrum to plot. |
| coord | The coordinates of the spectrum to plot. |
| run | The run of the spectrum to plot. |
| ... | Additional arguments passed to <code>plot_signal</code> . |
| xlab, ylab | Plotting labels. |
| isPeaks | Should the spectrum be plotted as peaks or as a continuous signal? |
| annPeaks | If <code>isPeaks</code> is <code>TRUE</code> , either an integer giving the number of peaks to annotate (i.e., label with their location), or a plotting symbol (e.g., "circle", "cross", etc.) to indicate the peak locations. |
| groups | A vector coercible to a factor indicating which of the specified spectra should be plotted with the same color. |
| superpose | If multiple spectra are plotted, should they be superposed on top of each other, or plotted separately? |
| key | Should a legend or colorkey be plotted? |
| n, downsampler | A spectrum can contain far more data points than are needed to visualize it, potentially making the plotting unnecessarily slow. Downsampling can be performed to improve plotting speed while maintaining the visual integrity of the spectrum. See <code>downsample</code> for details. |

Author(s)

Kylie A. Bemis

See Also

`plot`, `plot_signal`

Examples

```

set.seed(1)
x <- simulateImage(preset=1, npeaks=10, dim=c(3,3))

plot(x, i=4)
plot(x, coord=c(x=1, y=2))
plot(x, log2(intensity + 1) ~ mz, i=4,
      xlab=expression(italic("m/z")),
      ylab=expression(italic("Log Intensity")))

```

PositionDataFrame-class

PositionDataFrame: Extended data frame with key columns

Description

A data frame for metadata with spatial coordinates and multiple experimental runs.

Usage

```
PositionDataFrame(coord, run, ..., row.names = FALSE)
```

Arguments

| | |
|-----------|---|
| coord | A data frame or matrix of coordinates. |
| run | A factor giving the experimental runs. |
| ... | Arguments passed to the <code>DataFrame()</code> . |
| row.names | Either a vector of row names or a logical value indicating whether row names should be generated automatically (from the m/z values). |

Methods

`coord(object)`, `coord(object) <- value`: Get or set the coordinate columns.

`coordNames(object)`, `coordNames(object) <- value`: Get or set the names of the coordinate columns.

`run(object)`, `run(object) <- value`: Get or set the experimental run column.

`runNames(object)`, `runNames(object) <- value`: Get or set the experimental run levels.

`nrun(object)`: Get the number of experimental runs.

`is3D(object)`: Check if the number of spatial dimensions is greater than 2.

Author(s)

Kylie A. Bemis

See Also

[XDataFrame](#), [MassDataFrame](#)

Examples

```
## Create an PositionDataFrame object
coord <- expand.grid(x=1:3, y=1:3)
PositionDataFrame(coord=coord, label=LETTERS[1:9])
```

process

Apply queued processing to spectra

Description

Queue pre-processing steps on an imaging dataset and apply them, possibly writing out the processed data to a file.

Usage

```
## S4 method for signature 'MSImagingExperiment'
process(object, spectra = "intensity", index = "mz",
        domain = NULL, outfile = NULL, ...)

## S4 method for signature 'MSImagingArrays'
process(object, spectra = "intensity", index = "mz",
        domain = NULL, outfile = NULL, ...)

## S4 method for signature 'SpectralImagingExperiment'
process(object, spectra = "intensity", index = NULL,
        domain = NULL, outfile = NULL,
        nchunks = getCardinalNChunks(),
        verbose = getCardinalVerbose(),
        BPPARAM = getCardinalBPPARAM(), ...)

## S4 method for signature 'SpectralImagingArrays'
process(object, spectra = "intensity", index = NULL,
        domain = NULL, outfile = NULL,
        nchunks = getCardinalNChunks(),
        verbose = getCardinalVerbose(),
        BPPARAM = getCardinalBPPARAM(), ...)

## S4 method for signature 'SpectralImagingData'
addProcessing(object, FUN, label, verbose = getCardinalVerbose(), ...)

reset(object, ...)
```

Arguments

| | |
|---------|--|
| object | A spectral imaging dataset. |
| spectra | The name of the array in <code>spectraData()</code> to use for the peak intensities. |
| index | The name of the array in <code>spectraData()</code> (for <code>MSImagingArrays</code>) or column in <code>featureData()</code> (for <code>MSImagingExperiment</code>) to use for the peak locations. |
| domain | Optional. The name of the array in <code>spectraData()</code> (for <code>MSImagingArrays</code>) or column in <code>featureData()</code> (for <code>MSImagingExperiment</code>) to use for output domain (if known). |
| outfile | Optional. The name of a file to write the resulting dataset. Creates an imzML file for <code>MSImagingExperiment</code> or <code>MSImagingArrays</code> . The "continuous" format will be written if domain is specified; otherwise the "processed" format will be used in most cases. |
| nchunks | The number of chunks to use for processing. |
| verbose | Should progress messages be printed? |
| BPPARAM | An optional instance of <code>BiocParallelParam</code> . See documentation for bplapply . |
| ... | Options passed to chunk_mapply or chunk_colapply . |
| FUN | A user-specified processing function. |
| label | The name of the processing step. |

Details

This method allows queuing of delayed processing to an imaging dataset. All of the queued processing steps will be applied in sequence whenever `process()` is called next. Use `reset()` to remove all queued processing steps.

Typically, processing steps are queued using methods like `normalize`, `smooth`, `peakPick`, etc.

However, a processing step can be queued manually with `addProcessing`.

In this case, the user-specified function *must* accept (1) a first argument giving the spectral intensities as a numeric vector and (2) a second argument giving the intensity locations (e.g., *m/z* values) as a numeric vector.

The value returned by a user-specified function must return either (1) a numeric vector of the same length as the input intensities or (2) a 2-column matrix where the first column is the new locations (e.g., *m/z* values of peaks) and the second column is the new intensities.

Value

An object of the same class as the original object, with all processing steps applied.

Author(s)

Kylie A. Bemis

See Also

[normalize](#), [smooth](#), [recalibrate](#), [reduceBaseline](#), [peakPick](#)

Examples

```
set.seed(1)
mse <- simulateImage(preset=1, dim=c(3,3), baseline=1)

mse2 <- smooth(mse, width=11)
mse2 <- reduceBaseline(mse2)
plot(mse2, i=4)

mse2 <- process(mse2)
```

readMSIData

Read mass spectrometry imaging data files

Description

Read supported mass spectrometry imaging data files, including imzML and Analyze 7.5.

Usage

```
## Read any supported MS imaging file
readMSIData(file, ...)

## Read imzML file
readImzML(file, memory = FALSE, check = FALSE,
mass.range = NULL, resolution = NA, units = c("ppm", "mz"),
guess.max = 1000L, as = "auto", parse.only=FALSE,
nchunks = getCardinalNChunks(),
verbose = getCardinalVerbose(),
BPPARAM = getCardinalBPPARAM(), ...)

## Read Analyze 7.5 file
readAnalyze(file, memory = FALSE, as = "auto",
verbose = getCardinalVerbose(), ...)

## Convert from MSImagingExperiment to MSImagingArrays
convertMSImagingExperiment2Arrays(object)

## Convert from MSImagingArrays to MSImagingExperiment
convertMSImagingArrays2Experiment(object, mz = NULL,
mass.range = NULL, resolution = NA, units = c("ppm", "mz"),
guess.max = 1000L, tolerance = 0.5 * resolution,
nchunks = getCardinalNChunks(),
verbose = getCardinalVerbose(),
BPPARAM = getCardinalBPPARAM(), ...)
```


Arguments

| | |
|------------|--|
| file | The absolute or relative file path. The file extension must be included for readMSIData. |
| memory | Should the spectra be loaded into memory? If FALSE, the spectra are attached as an out-of-memory matrix. |
| check | Should the UUID and checksum of the binary data file be checked against the corresponding imzML tags? |
| mass.range | The mass range to use when converting the data to an MSImagingExperiment. |
| resolution | The mass resolution to use when converting the data to an MSImagingExperiment. This is the <i>inverse</i> of the instrument resolution, if known. It is the width of the m/z bins when converting the data to an MSImagingExperiment. |
| units | The units for the above resolution. |
| guess.max | The number of spectra to use when guessing the mass range and resolution, if they are not provided. |
| as | After reading in the data, what class of object should be returned? The data is initially loaded as an MSImagingArrays object. It may be converted to an MSImagingExperiment object. Setting to "auto" means to determine whichever is more appropriate depending on whether the spectra appear to have been processed and centroided. |
| parse.only | If TRUE, return only the parsed imzML metadata without creating a new MSImagingArrays or MSImagingExperiment object. |
| nchunks | The number of chunks to use for processing. |
| verbose | Should progress messages be printed? |
| BPPARAM | An optional instance of BiocParallelParam. See documentation for bplapply . |
| ... | Additional arguments passed to parseImzML or parseAnalyze . |
| object | A mass spectrometry imaging dataset to convert from one class to another. |
| mz | A vector of shared m/z values for converting to MSImagingExperiment, if not to be determined automatically. |
| tolerance | If the spectra have been centroided but the peaks are unaligned, then this is passed to peakAlign . |

Details

The spectra are initially loaded into a MSImagingArrays object before conversion to MSImagingExperiment (if applicable).

This conversion can be sped up by specifying the mass.range and resolution so they do not have to be determined from the spectra directly. Using a larger value of guess.max can improve the accuracy of the m/z binning for downstream analysis at the expense of a longer conversion time.

If greater control is desired, spectra should be imported as MSImagingArrays, and processing to MSImagingExperiment can be performed manually.

If problems are encountered while trying to import imzML files, the files should be verified and fixed with imzMLValidator.

A Java version of imzML validator can be found at: <https://gitlab.com/imzML/imzMLValidator>.

A web-based version of imzML validator can be found at: <https://imzml.github.io>.

Value

A [MSImagingExperiment](#) or [MSImagingArrays](#) object.

Author(s)

Kylie A. Bemis

References

Schramm T, Hester A, Klinkert I, Both J-P, Heeren RMA, Brunelle A, Laprevote O, Desbenoit N, Robbe M-F, Stoeckli M, Spengler B, Rompp A (2012) imzML - A common data format for the flexible exchange and processing of mass spectrometry imaging data. *Journal of Proteomics* 75 (16):5106-5110. doi:10.1016/j.jprot.2012.07.026

See Also

[parseImzML](#), [parseAnalyze](#) [writeMSIData](#)

recalibrate

Recalibrate spectra

Description

Apply deferred recalibration to spectra.

Usage

```
## S4 method for signature 'MSImagingExperiment_OR_Arrays'
recalibrate(object, ref,
            method = c("locmax", "dtw", "cow"),
            tolerance = NA, units = c("ppm", "mz"), ...)

## S4 method for signature 'SpectralImagingData'
recalibrate(object, ref,
            method = c("locmax", "dtw", "cow"),
            tolerance = NA, units = c("relative", "absolute"), ...)
```

Arguments

| | |
|-----------|---|
| object | A spectral imaging dataset. |
| ref | The domain (m/z) values or indices of reference peaks to use for the recalibration. |
| method | The recalibration method to use. See warp1 for details. |
| tolerance | The tolerance for how much a peak can be shifted in either direction. |
| units | The units for the above tolerance. |
| ... | Additional arguments passed to the recalibration function. |

Details

The supported recalibration methods are:

- "locmax": Align to local maxima using [warp1_loc](#).
- "dtw": Dynamic time warping using [warp1_dtw](#).
- "cow": Correlation optimized warping using [warp1_cow](#).

Value

An object of the same class with the processing step queued.

Note

The recalibration is deferred until `process()` is called.

Author(s)

Kylie A. Bemis

See Also

[normalize](#), [smooth](#), [recalibrate](#), [peakPick](#), [process](#)

Examples

```
set.seed(1)
mse <- simulateImage(preset=1, npeaks=10, dim=c(3,3), sdmz=250)
plot(mse, i=c(2,4,5), superpose=TRUE, xlim=c(1260,1320))

# queue recalibration
peaks <- estimateReferencePeaks(mse)
mse2 <- recalibrate(mse, ref=peaks, method="locmax", tolerance=500)

# apply recalibration
mse2 <- process(mse2)
plot(mse2, i=c(2,4,5), superpose=TRUE, xlim=c(1260,1320))
```

reduceBaseline

Reduce baselines in spectra

Description

Apply deferred baseline reduction to spectra.

Usage

```
## S4 method for signature 'SpectralImagingData'
reduceBaseline(object,
  method = c("locmin", "hull", "snip", "median"), ...)
```

Arguments

| | |
|--------|---|
| object | A spectral imaging dataset. |
| method | The baseline estimation method to use. See estbase for details. |
| ... | Additional arguments passed to the baseline estimation function. |

Details

The supported baseline estimation methods are:

- "locmin": Interpolate from local minima using [estbase_loc](#).
- "hull": Convex hull estimation using [estbase_hull](#).
- "snip": Sensitive nonlinear iterative peak (SNIP) clipping using [estbase_snip](#).
- "median": Running medians using [estbase_med](#).

Value

An object of the same class with the processing step queued.

Note

The baseline reduction is deferred until `process()` is called.

Author(s)

Kylie A. Bemis

See Also

[normalize](#), [smooth](#), [reduceBaseline](#), [peakPick](#), [process](#)

Examples

```
set.seed(1)
mse <- simulateImage(preset=1, npeaks=10, dim=c(3,3), baseline=1)

# queue baseline reduction
mse2 <- reduceBaseline(mse, method="locmin")
plot(mse2, i=4)

# apply baseline reduction
mse2 <- process(mse2)
```

ResultsList-class *ResultsList: List of modeling results*

Description

The ResultsList class provides a container for modeling results with spatial metadata.

Usage

```
## Instance creation
ResultsList(..., mcols = NULL)

## Additional methods documented below
```

Arguments

| | |
|-------|-----------------------|
| ... | The modeling results. |
| mcols | The metadata columns. |

Methods

All methods for [SimpleList](#) also work on ResultsList objects. Additional methods are documented below:

`fitted(object, ...)`: Extract fitted values from each modeling results object in the list.

`predict(object, ...)`: Predict on each modeling results object in the list.

`topFeatures(object, ...)`: Rank top features for each modeling results object in the list.

`plot(x, i = 1L, ...)`: Plot the *i*th modeling results.

`image(x, i = 1L, ...)`: Display images for the *i*th modeling results.

Author(s)

Kylie A. Bemis

See Also

[SpatialResults](#)

`selectROI`*Select regions-of-interest in an image*

Description

Manually select regions-of-interest or pixels on an imaging dataset. The `selectROI` method uses the built-in `locator` function. It can be used with an existing image plot, or a new image will be plotted if `image` arguments are passed via `...`

The regions of interest are returned as logical vectors indicating which pixels have been selected. These logical vectors can be combined into factors using the `makeFactor` function.

Usage

```
## S4 method for signature 'SpectralImagingExperiment'  
selectROI(object, ..., mode = c("region", "pixels"))  
  
makeFactor(..., ordered = FALSE)
```

Arguments

| | |
|----------------------|---|
| <code>object</code> | A spectral imaging dataset. |
| <code>mode</code> | The mode of selection: "region" to select a region-of-interest as a polygon, or "pixels" to select individual pixels. |
| <code>...</code> | Additional arguments to be passed to <code>image</code> for <code>selectROI</code> , or name-value pairs of logical vectors to be combined by <code>makeFactor</code> . |
| <code>ordered</code> | Should the resulting factor be ordered or not? |

Value

A logical vector of length equal to the number of pixels for `selectROI`.

A factor of the same length as the logical vectors for `makeFactor`.

Author(s)

Kylie A. Bemis

See Also

[image](#)

| | |
|-----------------|--|
| simulateSpectra | <i>Simulate a mass spectrum or MS imaging experiment</i> |
|-----------------|--|

Description

Simulate mass spectra or complete MS imaging experiments, including a possible baseline, spatial and spectral noise, mass drift, mass resolution, and multiplicative variation, etc.

A number of preset imaging designs are available for quick-and-dirty simulation of images.

These functions are designed for small proof-of-concept examples and testing, and may not scale well to simulating larger datasets.

Usage

```
simulateSpectra(n = 1L, npeaks = 50L,
  mz = rlnorm(npeaks, 7, 0.3), intensity = rlnorm(npeaks, 1, 0.9),
  from = 0.9 * min(mz), to = 1.1 * max(mz), by = 400,
  sdpeaks = sdpeakmult * log1p(intensity), sdpeakmult = 0.2,
  sdnoise = 0.1, sdmz = 10, resolution = 1000, fmax = 0.5,
  baseline = 0, decay = 10, units=c("ppm", "mz"),
  representation = c("profile", "centroid"), ...)
```

```
simulateImage(pixelData, featureData, preset,
  from = 0.9 * min(mz), to = 1.1 * max(mz), by = 400,
  sdrun = 1, sdpixel = 1, spcorr = 0.3, units=c("ppm", "mz"),
  representation = c("profile", "centroid"),
  nchunks = getCardinalNChunks(),
  verbose = getCardinalVerbose(),
  BPPARAM = getCardinalBPPARAM(), ...)
```

```
addShape(pixelData, center, size, shape=c("circle", "square"), name=shape)
```

```
presetImageDef(preset = 1L, nrun = 1, npeaks = 30L,
  dim = c(20L, 20L), peakheight = 1, peakdiff = 1,
  sdsample = 0.2, jitter = TRUE, ...)
```

Arguments

| | |
|-----------|---|
| n | The number of spectra to simulate. |
| npeaks | The number of peaks to simulate. Not used if mz and intensity are provided. |
| mz | The theoretical m/z values of the simulated peaks. |
| intensity | The mean intensities of the simulated peaks. |
| from | The minimum m/z value used for the mass range. |
| to | The maximum m/z value used for the mass range. |
| by | The step-size used for the observed m/z-values of the profile spectrum. |

| | |
|----------------|--|
| sdpeaks | The standard deviation(s) for the distributions of observed peak intensities on the log scale. |
| sdpeakmult | A multiplier used to calculate sdpeaks based on the mean intensities of peaks; used to simulate multiplicative variance. Not used if sdpeaks is provided. |
| sdnoise | The standard deviation of the random noise in the spectrum on the log scale. |
| sdmz | The standard deviation of the mass error in the observed m/z values of peaks, in units indicated by units. |
| resolution | The mass resolution as defined by $m / \Delta m$, where m is the observed mass and Δm is the width of the peak at a proportion of its maximum height defined by f_{\max} (defaults to full-width-at-half-maximum – FWHM – definition). Note that this is NOT the same as the definition of resolution in the <code>readImzML</code> function. |
| fmax | The fraction of the maximum peak height to use when defining the mass resolution. |
| baseline | The maximum intensity of the baseline. Note that baseline=0 means there is no baseline. |
| decay | A constant used to calculate the exponential decay of the baseline. Larger values mean the baseline decays more sharply at the lower mass range of the spectrum. |
| units | The units for by and sdmz. Either parts-per-million or absolute m/z units. |
| representation | Should a profile spectrum be returned or only the centroided peaks? |
| nchunks | The number of chunks to use for processing. |
| verbose | Should progress messages be printed? |
| BPPARAM | An optional instance of <code>BiocParallelParam</code> . See documentation for <code>bplapply</code> . |
| pixelData | A <code>PositionDataFrame</code> giving the pixel design of the experiment. The names of the columns should match the names of columns in <code>featureData</code> . Each column should be a logical vector corresponding to a morphological substructure, indicate which pixels belong to that substructure. |
| featureData | A <code>MassDataFrame</code> giving the feature design of the experiment. Each row should correspond to an expected peak. The names of the columns should match the names of columns in <code>pixelData</code> . Each column should be a numeric vector corresponding to a morphological substructure, giving the mean intensity of that peak for that substructure. |
| preset | A number indicating a preset image definition to use. |
| nrun | The number of runs to simulate for each condition. |
| sdrun | A standard deviation giving the run-to-run variance. |
| sdpixel | A standard deviation giving the pixel-to-pixel variance. |
| spcorr | The spatial autocorrelation. Must be between 0 and 1, where <code>spcorr=0</code> indicates no spatial autocorrelation. |
| ... | Additional arguments to pass to <code>simulateSpectra</code> or <code>presetImageDef</code> . |
| dim | The dimensions of the preset image. |
| peakheight | Reference intensities used for peak heights by the preset. |
| peakdiff | A reference intensity difference used for the mean peak height difference between conditions, for presets that simulate multiple conditions. |

| | |
|----------|---|
| sdsample | A standard deviation giving the amount of variation from the true peak heights for this simulated sample. |
| jitter | Should random noise be added to the location and size of the shapes? |
| center | The center of the shape. |
| size | The size of the shape (from the center). |
| shape | What type of shape to add. |
| name | The name of the added column. |

Details

The `simulateSpectra()` and `simulateImage()` functions are used to simulate mass spectra and MS imaging experiments. They provide a great deal of control over the parameters of the simulation, including all sources of variation.

For `simulateImage()`, the user should provide the design of the simulated experiment via matching columns in `pixelData` and `featureData`, where each column corresponds to different morphological substructures or differing conditions. These design data frames are returned in the `metadata()` of the returned object for later reference.

A number of presets are defined by `presetImageDef()`, which returns only the `pixelData` and `featureData` necessary to define the experiment for `simulateImage()`. These can be referenced for help in understanding how to define experiments for `simulateImage()`.

The preset images are:

- 1: a centered circle
- 2: a topleft circle and a bottomright square
- 3: two corner squares and a centered circle
- 4: a centered circle with conditions A and B in different runs
- 5: a topleft circle and a bottomright square with conditions A and B in different runs
- 6: two corner squares and a centered circle; the circle has conditions A and B in different runs
- 7: matched pairs of circles with conditions A and B within the same runs; includes reference peaks
- 8: matched pairs of circles inside squares with conditions A and B within the same runs; includes reference peaks
- 9: a small sphere inside a larger sphere (3D)

The `addShape()` function is provided for convenience when generating the `pixelData` for `simulateImage()`, as a simple way of adding morphological substructures using basic shapes such as squares and circles.

Value

For `simulateSpectra`, a list with elements:

- `mz`: a numeric vector of the observed `m/z` values
- `intensity`: a numeric vector or matrix of the intensities

For `simulateImage`, a `MSImagingExperiment` object.

For `addShape`, a new `PositionDataFrame` with a logical column added for the corresponding shape.

For `presetImageDef`, a list with two elements: the `pixelData` and `featureData` to be used as input to `simulateImage()`.

Author(s)

Kylie A. Bemis

See Also

[simspec](#)

Examples

```
set.seed(1)

# generate a spectrum
s <- simulateSpectra(1)
plot(s$intensity ~ s$mz, type="l")

# generate a noisy low-resolution spectrum with a baseline
s <- simulateSpectra(1, baseline=2, sdnoise=0.3, resolution=100)
plot(s$intensity ~ s$mz, type="l")

# generate a high-resolution spectrum
s <- simulateSpectra(1, npeaks=100, resolution=10000)
plot(s$intensity ~ s$mz, type="l")

# generate an image
mse <- simulateImage(preset=1, npeaks=10, dim=c(10,10))
peaks <- mz(metadata(mse)$design$featureData)

image(mse, mz=peaks[c(1,4,5,6)])
plot(mse, coord=c(x=3,y=3))
```

slice

Slice an image

Description

Slice a spectral imaging dataset as a "data cube".

Usage

```
slice(x, i = features(x, ...), ..., run = NULL,
      simplify = TRUE, drop = TRUE)
```

Arguments

| | |
|----------|---|
| x | A spectral imaging dataset. |
| i | The indices of features to slice for the images. |
| ... | Conditions describing features to slice, passed to features(). |
| run | The names of experimental runs to include, or the index of the levels of the runs to include. |
| simplify | The image slices be returned as a list, or simplified to an array? |
| drop | Should redundant array dimensions be dropped? If TRUE, dimensions with only one level are dropped using drop. |

Value

A list or array of the sliced image(s). If multiple images are sliced and simplify=TRUE, then the *last* dimension will be the features.

Author(s)

Kylie A. Bemis

Examples

```
set.seed(1)
mse <- simulateImage(preset=1, npeaks=10, dim=c(10,10), representation="centroid")
peaks <- mz(metadata(mse)$design$featureData)

# slice image for first feature
slice(mse, 1)

# slice by m/z-value
slice(mse, mz=peaks[1])

# slice multiple
slice(mse, mz=peaks[1:3])
```

smooth

Smooth spectra

Description

Apply deferred smoothing to spectra.

Usage

```
## S4 method for signature 'SpectralImagingData'
smooth(x,
  method = c("gaussian", "bilateral", "adaptive",
    "diff", "guide", "pag", "sgolay", "ma"), ...)
```

Arguments

| | |
|--------|---|
| x | A spectral imaging dataset. |
| method | The smoothing method to use. See filt1 for details. |
| ... | Additional arguments passed to the smoothing function. |

Details

The supported smoothing methods are:

- "gaussian": Gaussian smoothing using [filt1_gauss](#).
- "bilateral": Bilateral filter using [filt1_bi](#).
- "adaptive": Adaptive bilateral filter using [filt1_adapt](#).
- "diff": Nonlinear diffusion smoothing using [filt1_diff](#).
- "guide": Guided filter using [filt1_guide](#).
- "pag": Peak-aware guided filter using [filt1_pag](#).
- "sgolay": Savitzky-Golar filter using [filt1_sg](#).
- "ma": Moving average filter using [filt1_ma](#).

Value

An object of the same class with the processing step queued.

Note

The smoothing is deferred until `process()` is called.

Author(s)

Kylie A. Bemis

See Also

[normalize](#), [recalibrate](#), [reduceBaseline](#), [peakPick](#), [process](#)

Examples

```
set.seed(1)
mse <- simulateImage(preset=1, npeaks=10, dim=c(3,3))

# queue smoothing
mse2 <- smooth(mse, method="gaussian", width=11)
plot(mse2, i=4)

# apply smoothing
mse2 <- process(mse2)
```

Description

Apply cross-validation with an existing or a user-specified modeling function over folds of a spectral imaging dataset.

Usage

```
crossValidate(fit., x, y, folds = run(x), ...,
  predict. = predict, keep.models = FALSE,
  trainProcess = peakProcess, trainArgs = list(),
  testProcess = peakProcess, testArgs = list(),
  nchunks = getCardinalNChunks(),
  verbose = getCardinalVerbose(),
  BPPARAM = getCardinalBPPARAM())
```

```
## S4 method for signature 'SpatialCV'
fitted(object, type = c("response", "class"), ...)
```

```
## S4 method for signature 'SpatialCV'
image(x, i = 1L, type = c("response", "class"),
  layout = NULL, free = "", ...)
```

Arguments

| | |
|--------------------------------------|---|
| <code>fit.</code> | The function used to fit the model. |
| <code>x, y</code> | The data and response variable, where <code>x</code> is assumed to be an $P \times N$ dataset such as a <code>SpectralImagingExperiment</code> |
| <code>folds</code> | A vector coercible to a factor giving the fold for each row or column of <code>x</code> . |
| <code>...</code> | Additional arguments passed to <code>fit.</code> and <code>predict.</code> |
| <code>predict.</code> | The function used to predict on new data from the fitted model. The fitted model is passed as the 1st argument and the test data is passed as the 2nd argument. |
| <code>keep.models</code> | Should the models be kept and returned? |
| <code>trainProcess, trainArgs</code> | A function and arguments used for processing the training sets. The training set is passed as the 1st argument to <code>trainProcess</code> . |
| <code>testProcess, testArgs</code> | A function and arguments used for processing the test sets. The test set is passed as the 1st argument to <code>trainProcess</code> , and the processed training set is passed as the 2nd argument. |
| <code>verbose</code> | Should progress be printed for each iteration? |
| <code>nchunks</code> | The number of chunks to use. <i>Passed</i> to <code>fit.</code> , <code>predict.</code> , <code>trainProcess</code> and <code>testProcess</code> . |

| | |
|---------|--|
| BPPARAM | An optional instance of <code>BiocParallelParam</code> . See documentation for bplapply . Passed to <code>fit.</code> , <code>predict.</code> , <code>trainProcess</code> and <code>testProcess</code> . |
| object | An object inheriting from <code>SpatialCV</code> . |
| type | The type of prediction, where "response" means the fitted response matrix and "class" will be the vector of class predictions (only for classification). |
| i | If predictions are made for multiple sets of parameters, which set of parameters (i.e., which element of the <code>fitted.values</code> list) should be plotted? |
| layout | A vector of the form <code>c(nrow, ncol)</code> specifying the number of rows and columns in the facet grid. |
| free | A string specifying the free spatial dimensions during faceting. E.g., "", "x", "y", "xy", "yx". |

Details

This method is designed to be used with the provided classification methods, but can also be used with user-provided functions and methods as long as they conform to certain expectations. Internally, `cv_do` from the `matter` package is used to perform the cross-validation. See `?cv_do` for details.

Value

An object of class `SpatialCV` derived from `SpatialResults` and containing accuracies for each fold, the predictions for each fold, and (optionally) the fitted models.

Author(s)

Kylie A. Bemis

See Also

[cv_do](#), [spatialShrunkenCentroids](#), [PLS](#), [OPLS](#)

Description

Fit a spatially-aware Gaussian mixture models to each feature. The model uses Dirichlet prior is used to achieve spatial smoothing. The means and standard deviations of the Gaussian components are estimated using gradient descent. Simulated annealing is used to avoid local optima and achieve better parameter estimates.

Usage

```

## S4 method for signature 'ANY'
spatialDGMM(x, coord, i, r = 1, k = 2, groups = NULL,
  weights = c("gaussian", "adaptive"),
  neighbors = findNeighbors(coord, r=r, groups=groups),
  annealing = TRUE, compress = TRUE, byrow = FALSE,
  nchunks = getCardinalNChunks(),
  verbose = getCardinalVerbose(),
  BPPARAM = getCardinalBPPARAM(), ...)

## S4 method for signature 'SpectralImagingExperiment'
spatialDGMM(x, i, r = 1, k = 2, groups = run(x),
  weights = c("gaussian", "adaptive"),
  neighbors = findNeighbors(coord(x), r=r, groups=groups), ...)

## S4 method for signature 'SpatialDGMM'
logLik(object, ...)

## S4 method for signature 'SpatialDGMM,missing'
plot(x, i = 1L, type = "density",
  layout = NULL, free = "", ...)

## S4 method for signature 'SpatialDGMM'
image(x, i = 1L, type = "class",
  layout = NULL, free = "", ...)

```

Arguments

| | |
|-----------|--|
| x | A spatial dataset in P x N matrix format. |
| i | The rows/columns of x to segment (if not all of them). |
| coord | The spatial coordinates of the rows/columns of x. Ignored if neighbors is provided. |
| r | The spatial maximum distance for an observation to be considered a neighbor. Ignored if neighbors is provided. |
| k | The number of Gaussian components. |
| groups | Observations belonging to the different groups will be segmented independently. This should be set to the samples if statistic testing (via meansTest is to be performed.) |
| weights | The type of spatial weights to use for the smoothing. Gaussian weights are weighted only by distance, while adaptive weights also consider the dissimilarity between neighboring observations. |
| neighbors | A factor giving which observations should be treated as spatially-independent. Observations in the same group are assumed to have a spatial relationship. |
| annealing | Should simulated annealing be used? |
| compress | Should the results be compressed? The results can be larger than the original dataset, so compressing them is useful. If this option is used, then the class |

| | |
|---------|--|
| | probabilities are not returned, and the class assignments are compressed using drle . |
| byrow | Should the rows or columns of <code>x</code> be segmented? |
| nchunks | The number of chunks to use for processing. |
| verbose | Should progress messages be printed? |
| BPPARAM | An optional instance of <code>BiocParallelParam</code> . See documentation for bplapply . |
| ... | Additional arguments passed to the next method. |
| object | A <code>SpatialDGMM</code> object. |
| type | The type of plot to display. |
| layout | A vector of the form <code>c(nrow, ncol)</code> specifying the number of rows and columns in the facet grid. |
| free | A string specifying the free spatial dimensions during faceting. E.g., "", "x", "y", "xy", "yx". |

Value

An object of class `SpatialDGMM` derived from `SpatialResults`, containing the fitted [sgmixn](#) object and the spatial metadata.

Author(s)

Dan Guo and Kylie A. Bemis

References

Guo, D., Bemis, K., Rawlins, C., Agar, J., and Vitek, O. (2019.) Unsupervised segmentation of mass spectrometric ion images characterizes morphology of tissues. Proceedings of ISMB/ECCB, Basel, Switzerland, 2019.

Examples

```
set.seed(1)
mse <- simulateImage(preset=3, dim=c(10,10), npeaks=9,
  peakheight=c(3,6,9), representation="centroid")

gmm <- spatialDGMM(mse, r=1, k=4, weights="adaptive")

image(gmm, i=1:9)
```

SpatialFastmap *Spatially-aware FastMap projection*

Description

Compute spatially-aware FastMap projection.

Usage

```
## S4 method for signature 'ANY'
spatialFastmap(x, coord, r = 1, ncomp = 3,
  weights = c("gaussian", "adaptive"),
  neighbors = findNeighbors(coord, r=r),
  transpose = TRUE, niter = 3L,
  nchunks = getCardinalNChunks(),
  verbose = getCardinalVerbose(),
  BPPARAM = getCardinalBPPARAM(), ...)

## S4 method for signature 'SpectralImagingExperiment'
spatialFastmap(x, r = 1, ncomp = 3,
  weights = c("gaussian", "adaptive"),
  neighbors = findNeighbors(x, r=r), ...)

## S4 method for signature 'SpatialFastmap'
predict(object, newdata,
  neighbors = findNeighbors(newdata, r=object$r),
  nchunks = getCardinalNChunks(),
  BPPARAM = getCardinalBPPARAM(), ...)

## S4 method for signature 'SpatialFastmap,missing'
plot(x, type = c("scree", "x"), ..., xlab, ylab)

## S4 method for signature 'SpatialFastmap'
image(x, type = "x", ...)
```

Arguments

| | |
|---------|--|
| x | A spatial dataset in P x N matrix format. |
| coord | The spatial coordinates of the rows/columns of x. Ignored if neighbors is provided. |
| r | The spatial maximum distance for an observation to be considered a neighbor. Ignored if neighbors is provided. |
| ncomp | The number of FastMap components. |
| weights | The type of spatial weights to use for the smoothing. Gaussian weights are weighted only by distance, while adaptive weights also consider the dissimilarity between neighboring observations. |

| | |
|------------|---|
| neighbors | A factor giving which observations should be treated as spatially-independent. Observations in the same group are assumed to have a spatial relationship. |
| transpose | Should x be considered P x N? |
| niter | The number of iterations used to calculate the pivots for each FastMap component. |
| nchunks | The number of chunks to use for processing. |
| verbose | Should progress messages be printed? |
| BPPARAM | An optional instance of BiocParallelParam. See documentation for bplapply . |
| ... | Additional arguments passed to the next method. |
| object | A SpatialFastmap object. |
| newdata | A new SpectralImagingExperiment for which to calculate the scores. |
| type | The type of plot to display. |
| xlab, ylab | Plotting labels. |

Value

An object of class `SpatialFastmap` derived from `SpatialResults`, containing the fitted `fastmap` object and the spatial metadata.

Author(s)

Kylie A. Bemis

References

Alexandrov, T., & Kobarg, J. H. (2011). Efficient spatial segmentation of large imaging mass spectrometry datasets with spatially aware clustering. *Bioinformatics*, 27(13), i230-i238. doi:10.1093/bioinformatics/btr246

Faloutsos, C., & Lin, D. (1995). FastMap: A Fast Algorithm for Indexing, Data-Mining and Visualization of Traditional and Multimedia Datasets. Presented at the Proceedings of the 1995 ACM SIGMOD international conference on Management of data.

See Also

[PCA](#), [NMF](#), [spatialKMeans](#)

Examples

```
set.seed(1)
mse <- simulateImage(preset=2, npeaks=20, dim=c(10,10),
  representation="centroid")

# project to FastMap components
fm <- spatialFastmap(mse, r=1, ncomp=2, weights="adaptive")

# visualize first 2 components
image(fm)
```

SpatialKMeans *Spatially-aware K-means clustering*

Description

Perform spatially-aware k-means clustering. First the data is projected to a reduced dimension space using `spatialFastmap`. Then ordinary k-means clustering is applied to the projected data.

Usage

```
## S4 method for signature 'ANY'
spatialKMeans(x, coord, r = 1, k = 2, ncomp = max(k),
              weights = c("gaussian", "adaptive"),
              neighbors = findNeighbors(coord, r=r),
              transpose = TRUE, niter = 2L,
              centers = TRUE, correlation = TRUE,
              nchunks = getCardinalNChunks(),
              verbose = getCardinalVerbose(),
              BPPARAM = getCardinalBPPARAM(), ...)

## S4 method for signature 'SpectralImagingExperiment'
spatialKMeans(x, r = 1, k = 2, ncomp = max(k),
              weights = c("gaussian", "adaptive"),
              neighbors = findNeighbors(x, r=r), ...)

## S4 method for signature 'SpatialKMeans'
topFeatures(object, n = Inf, sort.by = "correlation", ...)

## S4 method for signature 'SpatialKMeans,missing'
plot(x, type = c("correlation", "centers"), ..., xlab, ylab)

## S4 method for signature 'SpatialKMeans'
image(x, type = "cluster", ...)
```

Arguments

| | |
|----------------------|--|
| <code>x</code> | A spatial dataset in P x N matrix format. |
| <code>coord</code> | The spatial coordinates of the rows/columns of <code>x</code> . Ignored if <code>neighbors</code> is provided. |
| <code>r</code> | The spatial maximum distance for an observation to be considered a neighbor. Ignored if <code>neighbors</code> is provided. |
| <code>k</code> | The number of clusters. |
| <code>ncomp</code> | The number of FastMap components. |
| <code>weights</code> | The type of spatial weights to use for the smoothing. Gaussian weights are weighted only by distance, while adaptive weights also consider the dissimilarity between neighboring observations. |

| | |
|-------------|---|
| neighbors | A factor giving which observations should be treated as spatially-independent. Observations in the same group are assumed to have a spatial relationship. |
| transpose | Should x be considered P x N? |
| niter | The number of iterations used to calculate the pivots for each FastMap component. |
| centers | Should the cluster centers be re-calculated on the original data? |
| correlation | Should the correlations between features and the clusters be calculated? |
| nchunks | The number of chunks to use for processing. |
| verbose | Should progress messages be printed? |
| BPPARAM | An optional instance of BiocParallelParam. See documentation for bplapply . |
| ... | Additional arguments passed to the next method. |
| object | A SpatialKMeans object. |
| n, sort.by | For topFeatures, the number of top features to return and how to sort them. |
| type | The type of plot to display. |
| xlab, ylab | Plotting labels. |

Value

An object of class SpatialKMeans derived from SpatialResults, containing the fitted [kmeans](#) object and the spatial metadata.

Author(s)

Kylie A. Bemis

References

- Alexandrov, T., & Kobarg, J. H. (2011). Efficient spatial segmentation of large imaging mass spectrometry datasets with spatially aware clustering. *Bioinformatics*, 27(13), i230-i238. doi:10.1093/bioinformatics/btr246
- Faloutsos, C., & Lin, D. (1995). FastMap: A Fast Algorithm for Indexing, Data-Mining and Visualization of Traditional and Multimedia Datasets. Presented at the Proceedings of the 1995 ACM SIGMOD international conference on Management of data.

See Also

[spatialKMeans](#) [spatialShrunkenCentroids](#)

Examples

```
set.seed(1)
mse <- simulateImage(preset=3, dim=c(10,10), npeaks=20,
  peakheight=c(3,6,9), representation="centroid")

# fit spatial k-means
skm <- spatialKMeans(mse, r=1, k=4, weights="adaptive")

# visualize clusters
image(skm)
```

| | |
|------------|--|
| SpatialNMF | <i>Non-negative matrix factorization</i> |
|------------|--|

Description

Compute nonnegative matrix factorization using alternating least squares or multiplicative updates.

Usage

```
## S4 method for signature 'ANY'
NMF(x, ncomp = 3, method = c("als", "mult"),
    verbose = getCardinalVerbose(), ...)

## S4 method for signature 'SpectralImagingExperiment'
NMF(x, ncomp = 3, method = c("als", "mult"), ...)

## S4 method for signature 'SpatialNMF'
predict(object, newdata, ...)

## S4 method for signature 'SpatialNMF,missing'
plot(x, type = c("activation", "x"), ..., xlab, ylab)

## S4 method for signature 'SpatialNMF'
image(x, type = "x", ...)
```

Arguments

| | |
|------------|---|
| x | A dataset in P x N matrix format. |
| ncomp | The number of components to calculate. |
| method | The method to use. Alternating least squares ("als") tends to be faster and potentially more accurate, but can be numerically unstable for data with high correlated features. Multiplicative updates ("mult") can be slower, but is more numerically stable. |
| verbose | Should progress messages be printed? |
| ... | Options passed to irlba . |
| object | A SpatialNMF object. |
| newdata | A new SpectralImagingExperiment for which to calculate the scores. |
| type | The type of plot to display. |
| xlab, ylab | Plotting labels. |

Value

An object of class `SpatialNMF` derived from `SpatialResults`, containing the fitted `nmmf` object and the spatial metadata.

Author(s)

Kylie A. Bemis

See Also

[nmmf_als](#), [nmmf_mult](#), [PCA](#), [spatialFastmap](#)

Examples

```
set.seed(1)
mse <- simulateImage(preset=2, npeaks=20, dim=c(10,10),
  representation="centroid")

# project to principal components
mf <- NMF(mse, ncomp=2)

# visualize first 2 components
image(mf, superpose=FALSE, scale=TRUE)
```

SpatialPCA

Principal components analysis

Description

Compute principal components efficiently using implicitly restarted Lanczos bi-diagonalization (IRLBA) algorithm for approximate singular value decomposition.

Usage

```
## S4 method for signature 'ANY'
PCA(x, ncomp = 3,
  center = TRUE, scale = FALSE,
  nchunks = getCardinalNChunks(),
  verbose = getCardinalVerbose(),
  BPPARAM = getCardinalBPPARAM(), ...)

## S4 method for signature 'SpectralImagingExperiment'
PCA(x, ncomp = 3,
  center = TRUE, scale = FALSE, ...)

## S4 method for signature 'SpatialPCA'
predict(object, newdata,
  nchunks = getCardinalNChunks(),
  BPPARAM = getCardinalBPPARAM(), ...)

## S4 method for signature 'SpatialPCA,missing'
plot(x, type = c("rotation", "scree", "x"), ..., xlab, ylab)
```

```
## S4 method for signature 'SpatialPCA'  
image(x, type = "x", ...)
```

Arguments

| | |
|------------|---|
| x | A dataset in P x N matrix format. |
| ncomp | The number of principal components to calculate. |
| center | Should the data be centered? |
| scale | Should the data be scaled? |
| nchunks | The number of chunks to use for processing. |
| verbose | Should progress messages be printed? |
| BPPARAM | An optional instance of BiocParallelParam. See documentation for bplapply . |
| ... | Options passed to irlba . |
| object | A SpatialPCA object. |
| newdata | A new SpectralImagingExperiment for which to calculate the scores. |
| type | The type of plot to display. |
| xlab, ylab | Plotting labels. |

Value

An object of class `SpatialPCA` derived from `SpatialResults`, containing the fitted `prcomp_lanczos` object and the spatial metadata.

Author(s)

Kylie A. Bemis

See Also

[prcomp_lanczos](#), [NMF](#), [spatialFastmap](#), [irlba](#), [svd](#)

Examples

```
set.seed(1)  
mse <- simulateImage(preset=2, npeaks=20, dim=c(10,10),  
  representation="centroid")  
  
# project to principal components  
pc <- PCA(mse, ncomp=2)  
  
# visualize first 2 components  
image(pc, superpose=FALSE, scale=TRUE)
```

Description

Compute partial least squares (also called projection to latent structures or PLS). This will also perform discriminant analysis (PLS-DA) if the response is a factor. Orthogonal partial least squares options (O-PLS and O-PLS-DA) is also supported; in this case, O-PLS step is a pre-processing step to remove noise orthogonal to the response, before fitting a PLS model with a single component.

Usage

```
## S4 method for signature 'ANY'
PLS(x, y, ncomp = 3,
    method = c("nipals", "simpls", "kernel1", "kernel2"),
    center = TRUE, scale = FALSE, bags = NULL,
    nchunks = getCardinalNChunks(),
    verbose = getCardinalVerbose(),
    BPPARAM = getCardinalBPPARAM(), ...)

## S4 method for signature 'SpectralImagingExperiment'
PLS(x, y, ncomp = 3,
    method = c("nipals", "simpls", "kernel1", "kernel2"),
    center = TRUE, scale = FALSE, ...)

## S4 method for signature 'SpatialPLS'
fitted(object, type = c("response", "class"), ...)

## S4 method for signature 'SpatialPLS'
predict(object, newdata, ncomp,
    type = c("response", "class"), simplify = TRUE, ...)

## S4 method for signature 'SpatialPLS'
topFeatures(object, n = Inf, sort.by = c("vip", "coefficients"), ...)

## S4 method for signature 'SpatialPLS,missing'
plot(x, type = c("coefficients", "vip", "scores"), ..., xlab, ylab)

## S4 method for signature 'SpatialPLS'
image(x, type = c("response", "class"), ...)

## S4 method for signature 'ANY'
OPLS(x, y, ncomp = 3, retx = TRUE,
    center = TRUE, scale = FALSE, bags = NULL,
    nchunks = getCardinalNChunks(),
    verbose = getCardinalVerbose(),
    BPPARAM = getCardinalBPPARAM(), ...)
```



```

## S4 method for signature 'SpectralImagingExperiment'
OPLS(x, y, ncomp = 3, retx = FALSE,
     center = TRUE, scale = FALSE, ...)

## S4 method for signature 'SpatialOPLS'
coef(object, ...)

## S4 method for signature 'SpatialOPLS'
residuals(object, ...)

## S4 method for signature 'SpatialOPLS'
fitted(object, type = c("response", "class"), ...)

## S4 method for signature 'SpatialOPLS'
predict(object, newdata, ncomp,
        type = c("response", "class"), simplify = TRUE, ...)

## S4 method for signature 'SpatialOPLS'
topFeatures(object, n = Inf, sort.by = c("vip", "coefficients"), ...)

## S4 method for signature 'SpatialOPLS,missing'
plot(x, type = c("coefficients", "vip", "scores"), ..., xlab, ylab)

## S4 method for signature 'SpatialOPLS'
image(x, type = c("response", "class"), ...)

```

Arguments

| | |
|----------------------|---|
| <code>x</code> | A dataset in P x N matrix format. |
| <code>y</code> | The response variable. |
| <code>ncomp</code> | The number of principal components to calculate. |
| <code>method</code> | The method used for calculating the principal components. See pls for details. |
| <code>center</code> | Should the data be centered? |
| <code>scale</code> | Should the data be scaled? |
| <code>bags</code> | Bags for multiple instance learning. If provided, then it is assumed all observations within a bag have the same label, and if a single observation is "positive" then all observations in the bag are "positive". Multiple instance learning is performed using mi_learn . |
| <code>retx</code> | Should the (potentially large) processed data matrix be included in the result? |
| <code>nchunks</code> | The number of chunks to use for processing. |
| <code>verbose</code> | Should progress messages be printed? |
| <code>BPPARAM</code> | An optional instance of <code>BiocParallelParam</code> . See documentation for bplapply . |
| <code>...</code> | Options passed to irlba . |
| <code>object</code> | A <code>SpatialPLS</code> or <code>SpatialOPLS</code> object. |

| | |
|------------|---|
| newdata | A new SpectralImagingExperiment for which to make predictions. |
| type | The type of fitted values to extract or the type of predictions to make. |
| simplify | If predictions are made using multiple numbers of components, should they be returned as a list, or simplified to an array? |
| n, sort.by | For topFeatures, the number of top features to return and how to sort them. |
| xlab, ylab | Plotting labels. |

Value

An object of class SpatialPLS or SpatialOPLS derived from SpatialResults, containing the fitted [pls](#) or [opls](#) model and the spatial metadata.

Author(s)

Kylie A. Bemis

References

Trygg, J., & Wold, S. (2002). Orthogonal projections to latent structures (O-PLS). *Journal of Chemometrics*, 16(3), 119-128. doi:10.1002/cem.695

See Also

[PCA](#), [spatialShrunkenCentroids](#),

Examples

```
set.seed(1)
mse <- simulateImage(preset=2, npeaks=20, dim=c(10,10), representation="centroid")
cls <- makeFactor(circle=pData(mse)$circle, square=pData(mse)$square)

# fit a PLS model with 3 components
pls <- PLS(mse, cls, ncomp=1:3)
plot(pls, type="coefficients", annPeaks="circle")

# visualize predictions
image(pls)
```

SpatialResults-class *SpatialResults: Modeling results with spatial metadata*

Description

The SpatialResults class provides a container for modeling results with spatial metadata. Most modeling functions applied to a [SpectralImagingExperiment](#) will return a SpatialResults-derived model object.

Usage

```
## Instance creation
SpatialResults(model, data,
  featureData = if (!missing(data)) fData(data) else NULL,
  pixelData = if (!missing(data)) pData(data) else NULL)

## S4 method for signature 'SpatialResults,ANY'
plot(x, y, ...,
  select = NULL, groups = NULL,
  superpose = TRUE, reducedDims = FALSE)

## S4 method for signature 'SpatialResults'
image(x, y, ...,
  select = NULL, subset = TRUE,
  superpose = TRUE)

## Additional methods documented below
```

Arguments

| | |
|-------------|--|
| model | The model object. |
| data | An object (typically the original dataset) with featureData and pixelData components. |
| featureData | A DataFrame with feature metadata, with a row for each feature. |
| pixelData | A PositionDataFrame with pixel metadata, with a row for each spectrum. |
| x, y | The model object and results to plot. (Not typically called directly.) |
| ... | Additional options passed to plotting methods. |
| select | Select elements of the results to plot. For example, this selects a subset of matrix columns or a subset of factor levels to plot. |
| subset | A logical vector indicating which pixels to include in the image. |
| groups | A vector coercible to a factor indicating which of the specified spectra should be plotted with the same color. |
| superpose | If multiple results are plotted, should they be superposed on top of each other, or plotted separately? |
| reducedDims | Does this results component represent reduced dimensions (e.g., from PCA)? |

Slots

model: The model.

featureData: A [DataFrame](#) containing feature-level metadata (e.g., a color channel, a molecular analyte, or a mass-to-charge ratio).

pixelData: A [PositionDataFrame](#) containing spatial metadata, including each observations's pixel coordinates and experimental run information.

Methods

`modelData(object), modelData(object) <- value`: Get or set the model slot.
`featureData(object), featureData(object) <- value`: Get or set the featureData slot.
`fData(object), fData(object) <- value`: Get or set the featureData slot.
`featureNames(object), featureNames(object) <- value`: Get or set the feature names (i.e., the row names of the featureData slot).
`pixelData(object), pixelData(object) <- value`: Get or set the elementMetadata slot.
`pData(object), pData(object) <- value`: Get or set the elementMetadata slot.
`pixelNames(object), pixelNames(object) <- value`: Get or set the pixel names (i.e., the row names of the elementMetadata slot).
`coord(object), coord(object) <- value`: Get or set the pixel coordinate columns in pixelData.
`coordNames(object), coordNames(object) <- value`: Get or set the names of the pixel coordinate columns in pixelData.
`run(object), run(object) <- value`: Get or set the experimental run column from pixelData.
`runNames(object), runNames(object) <- value`: Get or set the experimental run levels from pixelData.
`nrun(object)`: Get the number of experimental runs.

Author(s)

Kylie A. Bemis

See Also

[ResultsList](#)

SpatialShrunkenCentroids

Spatially-aware shrunken centroid clustering and classification

Description

Perform spatially-aware nearest shrunken centroid clustering or classification. These methods use statistical regularization to shrink the t-statistics of the features toward 0 so that unimportant features are removed from the model. The dissimilarity to class centroids are spatially smoothed.

Usage

```
## S4 method for signature 'ANY,ANY'
spatialShrunkenCentroids(x, y, coord, r = 1, s = 0,
  weights = c("gaussian", "adaptive"),
  neighbors = findNeighbors(coord, r=r), bags = NULL,
  priors = table(y), center = NULL, transpose = TRUE,
```

```

nchunks = getCardinalNChunks(),
verbose = getCardinalVerbose(),
BPPARAM = getCardinalBPPARAM(), ...)

## S4 method for signature 'SpectralImagingExperiment,ANY'
spatialShrunkenCentroids(x, y, r = 1, s = 0,
  weights = c("gaussian", "adaptive"),
  neighbors = findNeighbors(x, r=r), ...)

## S4 method for signature 'ANY,missing'
spatialShrunkenCentroids(x, coord, r = 1, k = 2, s = 0,
  weights = c("gaussian", "adaptive"),
  neighbors = findNeighbors(coord, r=r),
  init = NULL, threshold = 0.01, niter = 10L,
  center = NULL, transpose = FALSE,
  nchunks = getCardinalNChunks(),
  verbose = getCardinalVerbose(),
  BPPARAM = getCardinalBPPARAM(), ...)

## S4 method for signature 'SpectralImagingExperiment,missing'
spatialShrunkenCentroids(x, r = 1, k = 2, s = 0,
  weights = c("gaussian", "adaptive"),
  neighbors = findNeighbors(x, r=r), ...)

## S4 method for signature 'SpatialShrunkenCentroids'
fitted(object, type = c("response", "class"), ...)

## S4 method for signature 'SpatialShrunkenCentroids'
predict(object, newdata,
  type = c("response", "class"),
  neighbors = findNeighbors(newdata, r=object$r),
  nchunks = getCardinalNChunks(),
  BPPARAM = getCardinalBPPARAM(), ...)

## S4 method for signature 'SpatialShrunkenCentroids'
logLik(object, ...)

## S4 method for signature 'SpatialShrunkenCentroids'
topFeatures(object, n = Inf, sort.by = c("statistic", "centers"), ...)

## S4 method for signature 'SpatialShrunkenCentroids,missing'
plot(x, type = c("statistic", "centers"), ..., xlab, ylab)

## S4 method for signature 'SpatialShrunkenCentroids'
image(x, type = c("probability", "class"), ...)

```

Arguments

x A spatial dataset in P x N matrix format.

| | |
|------------|---|
| y | The response variable. |
| coord | The spatial coordinates of the rows/columns of x. Ignored if neighbors is provided. |
| r | The spatial maximum distance for an observation to be considered a neighbor. Ignored if neighbors is provided. |
| k | The number of classes for clustering. |
| s | The sparsity parameter. |
| weights | The type of spatial weights to use for the smoothing. Gaussian weights are weighted only by distance, while adaptive weights also consider the dissimilarity between neighboring observations. |
| neighbors | A factor giving which observations should be treated as spatially-independent. Observations in the same group are assumed to have a spatial relationship. |
| bags | Bags for multiple instance learning. If provided, then it is assumed all observations within a bag have the same label, and if a single observation is "positive" then all observations in the bag are "positive". Multiple instance learning is performed using mi_learn . |
| priors | The (unnormalized) prior probabilities for each class. |
| center | The global centroid (if known). |
| transpose | Should x be considered P x N? |
| init | A list of initial cluster configurations. (Should resemble the output of kmeans.) |
| threshold | Stop iteration when the proportion of cluster assignment updates is less than this threshold. |
| niter | The maximum number of iterations. |
| nchunks | The number of chunks to use for processing. |
| verbose | Should progress messages be printed? |
| BPPARAM | An optional instance of BiocParallelParam. See documentation for bplapply . |
| ... | Additional arguments passed to the next method. |
| object | A SpatialShrunkenCentroids object. |
| newdata | A new SpectralImagingExperiment for which to make predictions. |
| type | The type of fitted values to extract or the type of predictions to make. |
| n, sort.by | For topFeatures, the number of top features to return and how to sort them. |
| xlab, ylab | Plotting labels. |

Value

An object of class `SpatialShrunkenCentroids` derived from `SpatialResults`, containing the fitted `nscenroids` object and the spatial metadata.

Author(s)

Kylie A. Bemis

References

Bemis, K., Harry, A., Eberlin, L. S., Ferreira, C., van de Ven, S. M., Mallick, P., Stolowitz, M., and Vitek, O. (2016.) Probabilistic segmentation of mass spectrometry images helps select important ions and characterize confidence in the resulting segments. *Molecular & Cellular Proteomics*. doi:10.1074/mcp.O115.053918

Tibshirani, R., Hastie, T., Narasimhan, B., & Chu, G. (2003). Class Prediction by Nearest Shrunken Centroids, with Applications to DNA Microarrays. *Statistical Science*, 18, 104-117.

Alexandrov, T., & Kobarg, J. H. (2011). Efficient spatial segmentation of large imaging mass spectrometry datasets with spatially aware clustering. *Bioinformatics*, 27(13), i230-i238. doi:10.1093/bioinformatics/btr246

See Also

[spatialKMeans](#)

Examples

```
set.seed(1)
mse <- simulateImage(preset=3, dim=c(10,10), npeaks=20,
  peakheight=c(3,6,9), representation="centroid")

# fit spatial shrunken centroids
ssc <- spatialShrunkenCentroids(mse, r=1, k=4, s=c(0,3,6,9), weights="adaptive")

# visualize classes
image(ssc, i=1:4)

# visualize t-statistics
plot(ssc, i=1:4)
```

spatialWeights

Calculate spatial weights

Description

Calculate weights for neighboring observations based on either the spatial distance between the neighbors or the dissimilarity between the observations.

Usage

```
## S4 method for signature 'ANY'
spatialWeights(x, coord = x, r = 1, byrow = TRUE,
  neighbors = findNeighbors(coord, r=r),
  weights = c("gaussian", "adaptive"),
  sd = ((2 * r) + 1) / 4, matrix = FALSE,
  nchunks = getCardinalNChunks(),
  verbose = getCardinalVerbose(),
  BPPARAM = getCardinalBPPARAM(), ...)
```

```
## S4 method for signature 'SpectralImagingExperiment'
spatialWeights(x, r = 1,
               neighbors = findNeighbors(x, r=r), ...)

## S4 method for signature 'PositionDataFrame'
spatialWeights(x, r = 1,
               neighbors = findNeighbors(x, r=r),
               sd = ((2 * r) + 1) / 4, ...)
```

Arguments

| | |
|-----------|--|
| x | Either matrix or data frame of spatial coordinates, or a data matrix with rows or columns located at the coordinates given by coord. |
| coord | The spatial coordinates of the rows/columns of x. Ignored if neighbors is provided. |
| r | The spatial maximum distance for an observation to be considered a neighbor. Ignored if neighbors is provided. |
| byrow | If x is a data matrix, then are the weights calculated based on the dissimilarity between the rows (TRUE) or the columns (FALSE). |
| neighbors | A factor giving which observations should be treated as spatially-independent. Observations in the same group are assumed to have a spatial relationship. |
| weights | The type of weights to calculate. Either Gaussian weights with a constant standard deviation, or adaptive weights with a standard deviation based on the dissimilarity between the neighboring observations. |
| sd | The standard deviation for the Gaussian weights. Ignored with weights="adaptive". |
| matrix | Should the weights be returned as a sparse adjacency matrix instead of a list? |
| nchunks | The number of chunks to use for processing. |
| verbose | Should progress messages be printed? |
| BPPARAM | An optional instance of BiocParallelParam. See documentation for bplapply . |
| ... | Additional arguments passed to the next method. |

Value

Either a list of weights of neighbors or a sparse adjacency matrix ([sparse_mat](#)).

Author(s)

Kylie A. Bemis

See Also

[findNeighbors](#)

Examples

```

set.seed(1)
mse <- simulateImage(preset=1, dim=c(10,10))

# calculate weights based on distance
spatialWeights(pixelData(mse), r=1)

# calculate weights based on spectral dissimilarity
spatialWeights(mse, r=1)

```

SpectraArrays-class *SpectraArrays: List of spectra arrays*

Description

The SpectraArrays class provides a list-like container for spectra arrays of conformable dimensions.

Usage

```

## Instance creation
SpectraArrays(arrays = SimpleList())

## Additional methods documented below

```

Arguments

arrays A list of arrays.

Details

The SpectraArrays class is intended to be flexible and the arrays do not need to be "array-like" (i.e., have non-NULL dim(.)) One dimensional arrays and lists are allowed. Every array must have the same NROW() and NCOL().

It supports lossless coercion to and from [SimpleList](#).

Methods

All methods for [SpectralImagingData](#) also work on SpectraArrays objects. Additional methods are documented below:

length(object): Get the number of spectra in the object.
names(object), names(object) <- value: Get or set the names of spectra arrays in the object.
object[[i]], object[[i]] <- value: Get or set an array in the object.
object[i, j, ..., drop]: Subset as a list or array, depending on the number of dimensions of the stored spectra arrays. The result is the same class as the original object.
rbind(...), cbind(...): Combine SpectraArrays objects by row or column.
c(...): Combine SpectraArrays objects as lists.

Author(s)

Kylie A. Bemis

See Also[SpectralImagingData](#), [MSImagingArrays](#)**Examples**

```
set.seed(1)
x <- matrix(rlnorm(128), nrow=16, ncol=8)
y <- matrix(rlnorm(128), nrow=16, ncol=8)

s <- SpectraArrays(list(x=x, y=y))

print(s)
```

SpectralImagingArrays-class

SpectralImagingArrays: Spectral imaging data with arbitrary domain

Description

The `SpectralImagingArrays` class provides a list-like container for high-dimensional spectral imaging data where every spectrum may have its own domain values. It is designed to provide easy access to raw individual spectra, but images cannot be easily reconstructed.

The `MSImagingArrays` class extends `SpectralImagingArrays` for mass spectrometry-based imaging experiments with unaligned mass features.

Usage

```
## Instance creation
SpectralImagingArrays(spectraData = SimpleList(),
  pixelData = PositionDataFrame(), metadata = list())

## Additional methods documented below
```

Arguments

| | |
|--------------------------|---|
| <code>spectraData</code> | Either a list-like object with lists of individual spectra and lists of their domain values, or a SpectraArrays instance. |
| <code>pixelData</code> | A PositionDataFrame with pixel metadata, with a row for each spectrum. |
| <code>metadata</code> | A list with experimental-level metadata. |

Slots

spectraData: A [SpectraArrays](#) object storing one or more array-like data elements with conformable dimensions.

elementMetadata: A [PositionDataFrame](#) containing spectrum-level metadata, including each spectrum's pixel coordinates and experimental run information.

processing: A list containing unexecuted [ProcessingStep](#) objects.

Methods

All methods for [SpectralImagingData](#) also work on [SpectralImagingArrays](#) objects. Additional methods are documented below:

length(object): Get the number of spectra in the object.

object[i, ..., drop]: Subset as a list based on the spectra. The result is the same class as the original object.

rbind(...), cbind(...): Combine [SpectralImagingArrays](#) objects by row or column.

Author(s)

Kylie A. Bemis

See Also

[SpectralImagingData](#), [MSImagingArrays](#)

Examples

```
set.seed(1)
x <- replicate(9, rlnorm(10), simplify=FALSE)
t <- replicate(9, sort(runif(10)), simplify=FALSE)
coord <- expand.grid(x=1:3, y=1:3)

sa <- SpectralImagingArrays(
  spectraData=list(intensity=x, wavelength=t),
  pixelData=PositionDataFrame(coord))

print(sa)
```

SpectralImagingData-class

SpectralImagingData: Abstract class for spectral imaging data

Description

The `SpectralImagingData` class is an abstract container for high-dimensional spectral imaging data. Every spectrum is associated with spatial coordinates so that an image can be constructed from the spectral intensities.

The `SpectralImagingArrays` and `SpectralImagingExperiment` classes directly extend this class, where `SpectralImagingArrays` is primarily intended for unprocessed spectra with unaligned features, and `SpectralImagingExperiment` is intended for processed spectra with aligned features.

The `MSImagingArrays` and `MSImagingExperiment` classes further extend these classes for mass spectrometry imaging data.

Slots

`spectraData`: A `SpectraArrays` object storing one or more array-like data elements with conformable dimensions.

`elementMetadata`: A `PositionDataFrame` containing spectrum-level metadata, including each spectrum's pixel coordinates and experimental run information.

`processing`: A list containing unexecuted `ProcessingStep` objects.

Methods

`spectraData(object, ...)`, `spectraData(object, ...) <- value`: Get or set the `spectraData` slot.

`spectraNames(object, ...)`, `spectraNames(object, ...) <- value`: Get or set the names of the spectra in the `spectraData` slot.

`spectra(object, i = 1L, ...)`, `spectra(object, i = 1L, ...) <- value`: Get or set a specific spectra array in the `spectraData` slot.

`pixelData(object)`, `pixelData(object) <- value`: Get or set the `elementMetadata` slot.

`pData(object)`, `pData(object) <- value`: Get or set the `elementMetadata` slot.

`pixelNames(object)`, `pixelNames(object) <- value`: Get or set the pixel names (i.e., the row names of the `elementMetadata` slot).

`spectraVariables(object, ...)`: Get the names of the spectrum-level variables (i.e., the columns of the `elementMetadata` slot).

`coord(object)`, `coord(object) <- value`: Get or set the pixel coordinate columns in `pixelData`.

`coordNames(object)`, `coordNames(object) <- value`: Get or set the names of the pixel coordinate columns in `pixelData`.

`run(object)`, `run(object) <- value`: Get or set the experimental run column from `pixelData`.

`runNames(object)`, `runNames(object) <- value`: Get or set the experimental run levels from `pixelData`.

`nrun(object)`: Get the number of experimental runs.

`is3D(object)`: Check if the number of spatial dimensions is greater than 2.

`processingData(object, ...)`, `processingData(object, ...) <- value`: Get or set the `processing` slot.

Author(s)

Kylie A. Bemis

See Also[SpectralImagingExperiment](#), [SpectralImagingArrays](#), [MSImagingExperiment](#), [MSImagingArrays](#)

SpectralImagingExperiment-class*SpectralImagingExperiment: Spectral imaging data with shared domain*

Description

The `SpectralImagingExperiment` class provides a matrix-like container for high-dimensional spectral imaging data where every spectrum shares the same domain values. It is designed to provide easy access to both the spectra (as columns) and sliced images (as rows).

The `MSImagingExperiment` class extends `SpectralImagingExperiment` for mass spectrometry-based imaging experiments with aligned mass features.

Usage

```
## Instance creation
SpectralImagingExperiment(spectraData = SimpleList(),
  featureData = DataFrame(), pixelData = PositionDataFrame(),
  metadata = list())

## Additional methods documented below
```

Arguments

| | |
|--------------------------|---|
| <code>spectraData</code> | Either a matrix-like object with number of rows equal to the number of features and number of columns equal to the number of pixels, a list of such objects, or a SpectraArrays instance. |
| <code>featureData</code> | A DataFrame with feature metadata, with a row for each feature. |
| <code>pixelData</code> | A PositionDataFrame with pixel metadata, with a row for each spectrum. |
| <code>metadata</code> | A list with experimental-level metadata. |

Slots

`spectraData`: A [SpectraArrays](#) object storing one or more array-like data elements with conformable dimensions.

`featureData`: A [DataFrame](#) containing feature-level metadata (e.g., a color channel, a molecular analyte, or a mass-to-charge ratio).

`elementMetadata`: A [PositionDataFrame](#) containing spectrum-level metadata, including each spectrum's pixel coordinates and experimental run information.

`processing`: A list containing unexecuted [ProcessingStep](#) objects.

Methods

All methods for [SpectralImagingData](#) also work on `SpectralImagingExperiment` objects. Additional methods are documented below:

`featureData(object)`, `featureData(object) <- value`: Get or set the `featureData` slot.

`fData(object)`, `fData(object) <- value`: Get or set the `featureData` slot.

`featureNames(object)`, `featureNames(object) <- value`: Get or set the feature names (i.e., the row names of the `featureData` slot).

`length(object)`: Get the number of spectra in the object.

`nrow(object)`, `ncol(object)`: Get the number of rows (features) or the number of columns (pixels) in the object.

`object[i, j, ..., drop]`: Subset based on the rows (`featureData`) and the columns (`pixelData`). The result is the same class as the original object.

`rbind(...)`, `cbind(...)`: Combine `SpectralImagingExperiment` objects by row or column.

Author(s)

Kylie A. Bemis

See Also

[SpectralImagingData](#), [MSImagingExperiment](#)

Examples

```
set.seed(1)
x <- matrix(rlnorm(81), nrow=9, ncol=9)
index <- 1:9
coord <- expand.grid(x=1:3, y=1:3)

se <- SpectralImagingExperiment(
  spectraData=x,
  featureData=DataFrame(index=1:9),
  pixelData=PositionDataFrame(coord))

print(se)
```

spectrapply

Apply functions over spectra

Description

Apply a user-specified function over all spectra in a spectral imaging dataset.

Usage

```
## S4 method for signature 'MSImagingExperiment'
spectrapply(object, FUN, ...,
            spectra = "intensity", index = "mz")

## S4 method for signature 'MSImagingArrays'
spectrapply(object, FUN, ...,
            spectra = "intensity", index = "mz")

## S4 method for signature 'SpectralImagingExperiment'
spectrapply(object, FUN, ...,
            spectra = "intensity", index = NULL,
            simplify = TRUE, outpath = NULL,
            nchunks = getCardinalNChunks(),
            verbose = getCardinalVerbose(),
            BPPARAM = getCardinalBPPARAM())

## S4 method for signature 'SpectralImagingArrays'
spectrapply(object, FUN, ...,
            spectra = "intensity", index = NULL,
            simplify = TRUE, outpath = NULL,
            nchunks = getCardinalNChunks(),
            verbose = getCardinalVerbose(),
            BPPARAM = getCardinalBPPARAM())
```

Arguments

| | |
|----------|---|
| object | A spectral imaging dataset. |
| FUN | A function to be applied. The function <i>must</i> accept (1) a first argument giving the spectral intensities as a numeric vector and (2) a second argument giving the intensity locations (e.g., m/z values) as a numeric vector. |
| ... | Options passed to chunkMapply or chunkApply . |
| spectra | The name of the array in <code>spectraData()</code> to use for the spectral intensities. |
| index | The name of the array in <code>spectraData()</code> (for <code>SpectralImagingArrays</code>) or column in <code>featureData()</code> (for <code>SpectralImagingExperiment</code>) to use for the spectral locations. |
| simplify | Should the result be simplified to an array if possible? |
| outpath | Optional. The name of a file to write the resulting data. |
| nchunks | The number of chunks to use for processing. |
| verbose | Should progress messages be printed? |
| BPPARAM | An optional instance of <code>BiocParallelParam</code> . See documentation for bplapply . |

Value

A list if `simplify=FALSE`. Otherwise, a vector or matrix, or a higher-dimensional array if the attempted simplification is successful.

Author(s)

Kylie A. Bemis

See Also[summarizeFeatures](#), [summarizePixels](#)**Examples**

```
set.seed(1)
mse <- simulateImage(preset=1, npeaks=10, dim=c(10,10))

# find m/z locations of peaks in each spectrum
peaks <- spectrapply(mse, function(x, mz) mz[matter::findpeaks(x)])

head(peaks[[1L]])
head(peaks[[2L]])
```

| | |
|----------------|--|
| subsetFeatures | <i>Subset a spectral imaging dataset</i> |
|----------------|--|

Description

Returns a subset of the dataset that meets the conditions.

Usage

```
## S4 method for signature 'SpectralImagingArrays'
subset(x, subset, ...)

## S4 method for signature 'SpectralImagingExperiment'
subset(x, select, subset, ...)

subsetFeatures(x, ...)

subsetPixels(x, ...)
```

Arguments

| | |
|--------|---|
| x | A spectral imaging dataset. |
| select | Logical expression to be evaluated in the object's <code>featureData()</code> indicating which rows (features) to keep. |
| subset | Logical expression to be evaluated in the object's <code>pixelData()</code> indicating which columns (pixels) to keep. |
| ... | Conditions describing rows (features) or columns (pixels) to be retained. Passed to <code>features()</code> and <code>pixels()</code> methods to obtain the subset indices. |

Value

An object of the same class as `x` with the appropriate subsetting applied to it.

Author(s)

Kylie A. Bemis

Examples

```
set.seed(1)
mse <- simulateImage(preset=1, npeaks=10, dim=c(10,10))

# subset features to mass range 1000 - 1500
subsetFeatures(mse, 1000 < mz, mz < 1500)

# select pixels to coordinates x = 1..3, y = 1..3
subsetPixels(mse, x <= 3, y <= 3)

# subset both features + pixels
subset(mse, 1000 < mz & mz < 1500, x <= 3 & y <= 3)
```

| | |
|-------------------|---|
| summarizeFeatures | <i>Summarize a spectral imaging dataset</i> |
|-------------------|---|

Description

Summarizes over the rows or columns of the dataset.

Usage

```
summarizeFeatures(x, stat = "mean", groups = NULL,
  nchunks = getCardinalNChunks(),
  verbose = getCardinalVerbose(),
  BPPARAM = getCardinalBPPARAM(), ...)

summarizePixels(x, stat = c(tic="sum"), groups = NULL,
  nchunks = getCardinalNChunks(),
  verbose = getCardinalVerbose(),
  BPPARAM = getCardinalBPPARAM(), ...)

## S4 method for signature 'SpectralImagingExperiment'
rowStats(x, stat, ...,
  nchunks = getCardinalNChunks(),
  verbose = getCardinalVerbose(),
  BPPARAM = getCardinalBPPARAM())

## S4 method for signature 'SpectralImagingExperiment'
colStats(x, stat, ...,
```

```

nchunks = getCardinalNChunks(),
verbose = getCardinalVerbose(),
BPPARAM = getCardinalBPPARAM()

## S4 method for signature 'SpectralImagingExperiment'
rowSums(x, na.rm = FALSE, dims = 1, ...)

## S4 method for signature 'SpectralImagingExperiment'
colSums(x, na.rm = FALSE, dims = 1, ...)

## S4 method for signature 'SpectralImagingExperiment'
rowMeans(x, na.rm = FALSE, dims = 1, ...)

## S4 method for signature 'SpectralImagingExperiment'
colMeans(x, na.rm = FALSE, dims = 1, ...)

```

Arguments

| | |
|---------|---|
| x | A spectral imaging dataset. |
| stat | The name of summary statistics to compute over the rows or columns of a matrix. Allowable values include: "min", "max", "prod", "sum", "mean", "var", "sd", "any", "all", and "nnzero". |
| groups | A vector coercible to a factor giving groups to summarize. |
| na.rm | If TRUE, remove NA values before summarizing. |
| dims | Ignored. |
| nchunks | The number of chunks to use for processing. |
| verbose | Should progress messages be printed? |
| BPPARAM | An optional instance of BiocParallelParam. See documentation for bplapply . |
| ... | Additional arguments passed to rowStats or colStats , such as the number of chunks. |

Value

For `summarizeFeatures` and `summarizePixels`, an object of the same class as `x` with the statistical summaries added as columns in the `featureData()` or `pixelData()`, respectively.

For `rowStats`, `colStats`, etc., a vector, matrix, or array with the summary statistics.

Author(s)

Kylie A. Bemis

Examples

```

set.seed(1)
mse <- simulateImage(preset=1, npeaks=10, dim=c(10,10))

# summarize mean spectrum

```

```
mse <- summarizeFeatures(mse, stat="mean")
plot(mse, "mean")

# summarize total ion current
mse <- summarizePixels(mse, stat=c(TIC="sum"))
image(mse, "TIC")
```

`writeMSIData`*Write mass spectrometry imaging data files*

Description

Write supported mass spectrometry imaging data files, including imzML and Analyze 7.5.

Usage

```
writeMSIData(object, file, ...)

## S4 method for signature 'MSImagingExperiment_OR_Arrays'
writeImzML(object, file, bundle = TRUE,
  verbose = getCardinalVerbose(), ...)

## S4 method for signature 'MSImagingExperiment'
writeAnalyze(object, file, verbose = getCardinalVerbose(), ...)

## S4 method for signature 'SpectralImagingExperiment'
writeAnalyze(object, file, verbose = getCardinalVerbose(), ...)
```

Arguments

| | |
|----------------------|---|
| <code>object</code> | A spectral imaging dataset. |
| <code>file</code> | The absolute or relative file path. The file extension must be included for <code>writeMSIData</code> . |
| <code>bundle</code> | Should the ".imzML" and ".ibd" files be bundled into a new directory of the same name? |
| <code>verbose</code> | Should progress messages be printed? |
| <code>...</code> | Additional arguments passed to <code>writeImzML</code> or <code>writeAnalyze</code> . |

Details

The `writeImzML` function supports writing both the "continuous" and "processed" formats.

Exporting the experimental metadata to `cvParam` tags is lossy, and not all metadata will be preserved. If exporting an object that was originally imported from an imzML file, only metadata that appears in `experimentData()` will be preserved when writing.

Datasets with multiple experimental runs will be merged into a single file. The object's `pixelData()` and `featureData()` will also be written to tab-delimited files if appropriate. These will be read back in by `readImzML()`.

The imzML files can be modified after writing (such as to add additional experimental metadata) using the Java-based imzMLValidator application: <https://gitlab.com/imzML/imzMLValidator/>.

Value

TRUE if the file was written successfully, with the output file paths attached as an attribute.

Author(s)

Kylie A. Bemis

References

Schramm T, Hester A, Klinkert I, Both J-P, Heeren RMA, Brunelle A, Laprevote O, Desbenoit N, Robbe M-F, Stoeckli M, Spengler B, Rompp A (2012) imzML - A common data format for the flexible exchange and processing of mass spectrometry imaging data. *Journal of Proteomics* 75 (16):5106-5110. doi:10.1016/j.jprot.2012.07.026

See Also

[readMSIData](#)

XDataFrame-class

XDataFrame: Extended data frame with key columns

Description

The XDataFrame extends the [DataFrame](#) class from the S4Vectors package with support for columns (or sets of columns) designated as keys.

Usage

```
XDataFrame(..., keys = list())
```

Arguments

| | |
|------|--|
| ... | Arguments passed to the <code>DataFrame()</code> . |
| keys | A named list of character vectors giving the names of key columns. The names of the list become the names of the keys (which may be different from the columns). The character vectors specify the names of columns that compose that key. |

Details

For the most part, XDataFrame behaves identically to DataFrame, and key columns can be get or set as usual. The XDataFrame class is primarily intended as a way to enforce additional requirements or constraints on specific sets of columns in a structured way. It provides an abstracted way of manipulating sets of columns that are expected to follow certain rules. The keys remain consistent and accessible even if the columns of the data frame are renamed.

The base class currently has only minimal requirements for keys (i.e., that they are valid columns in the data frame). Additionally, keys are checked for compatibility when combining data frames. Uniqueness is *not* checked.

Subclasses can enforce additional constraints on key columns. For example, the [PositionDataFrame](#) and [MassDataFrame](#) classes.

Methods

`keys(object, i = NULL, ..., drop = TRUE)`, `keys(object, i = NULL, ...) <- value`: Get or set the key columns. By default, this gets or sets the keys slot. Provide `i` to get or set specific keys.

Author(s)

Kylie A. Bemis

See Also

[DataFrame](#), [MassDataFrame](#), [PositionDataFrame](#)

Examples

```
## Create an XDataFrame object
XDataFrame(id=1:10, letter=LETTERS[1:10], keys=list(index="id"))
```

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