Package 'batchCorr'

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Type Package

Title Within And Between Batch Correction Of LC-MS Metabolomics Data

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Description From the perspective of metabolites as the continuation of the central dogma of biology, metabolomics provides the closest link to many phenotypes of interest. This makes metabolomics research promising in teasing apart the complexities of living systems. However, due to experimental reasons, the data includes non-biological variation which limits quality and reproducibility, especially if the data is obtained from several batches. The batchCorr package reduces unwanted variation by way of between-batch alignment, within-batch drift correction and between-batch normalization using batch-specific quality control samples and long-term reference QC samples. Please see the associated article for more thorough descriptions of algorithms.

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biocViews BiomedicalInformatics, Metabolomics, MassSpectrometry, BatchEffect, Normalization, QualityControl

Depends R (>= 4.4.0), SummarizedExperiment

Imports reshape, mclust, BiocParallel, methods

Suggests BiocStyle, knitr, testthat

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Contents

alignBatches 2
correctDrift 4
getBatch 6
mergeBatches 7
normalizeBatches 8
peakInfo 10
ThreeBatchData 11

Index **12**

`alignBatches` *Between-batch alignment of features*

Description

Multi-batch alignment of features artificially split between batches.

Usage

```
alignBatches(PeakTabNoFill, PeakTabFilled, ...)

## S4 method for signature 'ANY,ANY'
alignBatches(
  peakInfo,
  PeakTabNoFill,
  PeakTabFilled,
  batches,
  sampleGroups,
  selectGroup = "QC",
  NAhard = 0.8,
  mzdiff = 0.002,
  rtdiff = 15,
  report = TRUE,
  reportPath = NULL
)

## S4 method for signature 'SummarizedExperiment,SummarizedExperiment'
alignBatches(
  PeakTabNoFill,
  PeakTabFilled,
  batches,
  sampleGroups,
  assay.type1 = NULL,
```

```
  assay.type2 = NULL,
  name = NULL,
  mz_col = "mz",
  rt_col = "rt",
  ...
)
```

Arguments

PeakTabNoFill	SummarizedExperiment object or matrix before gap-filling
PeakTabFilled	SummarizedExperiment object or matrix without missing values
...	parameters with same behavior across methods
peakInfo	matrix with mz and rt in columns 1:2 (see e.g. ?peakInfo)
batches	character scalar or factor, batch labels
sampleGroups	character scalar or character, group labels
selectGroup	character scalar, identifier of QC samples
NAhard	numeric scalar, proportion of NAs within batch for feature to be considered missing
mzdiff	numeric scalar, tolerance for difference in m/z
rtdiff	numeric scalar, tolerance for difference in retention time
report	boolean, whether to export diagnostic plots into your work directory (default: TRUE)
reportPath	character scalar, directory path for report
assay.type1	character scalar, assay of PeakTabNoFill to be used in case of multiple assays
assay.type2	character scalar, assay of PeakTabFilled to be used in case of multiple assays
name	character scalar, name of the resultant assay in case of multiple assays
mz_col	character scalar, name of column containing mass information
rt_col	character scalar, name of column for retention time

Details

A basic method with matrices (samples as rows) and SummarizedExperiment is supported. For grouping variables such as batches, the basic method expects vectors, while the SummarizedExperiment method expects the names of the respective columns in PeakTabFilled. The basic method returns a list with the aligned peak table and information about the process, whereas the SummarizedExperiment method assigns the aligned peak table to the object supplied to PeakTabFilled.

Value

a SummarizedExperiment object as PeakTabFill with the aligned matrix or a list of six:

- PTalign: the aligned peak table
- boolAveragedAlign: boolean vector of final features where alignment has been made using feature averaging
- PTfill: peaktable without missing values (indata)
- boolKeep: boolean vector of features kept after alignment
- boolAveragedFill boolean vector of original features where alignment has been made using feature averaging
- aI: alignIndex object (indata)

Examples

```
data("ThreeBatchData")
# Basic method
## Extract peakinfo (i.e. m/z and rt of features).
peakIn <- peakInfo(PT = PTnofill, sep = "@", start = 3)
## Perform multi-batch alignment
alignBat <- alignBatches(
    peakInfo = peakIn, PeakTabNoFill = PTnofill,
    PeakTabFilled = PTfill, batches = meta$batch,
    sampleGroups = meta$grp, selectGroup = "QC",
    report = FALSE
)
## Extract new peak table
PT <- alignBat$PTalign

# SummarizedExperiment
## Construct SummarizedExperiment
peaks <- SimpleList(t(PTnofill), t(PTfill))
sampleData <- meta
featureData <- peakInfo(PT = PTnofill, sep = "@", start = 3)
rownames(featureData) <- rownames(peaks[[1]])
se <- SummarizedExperiment(assays = peaks, colData = sampleData,
                           rowData = featureData)
names(assays(se)) <- c("nofill", "fill")

se <- alignBatches(PeakTabNoFill = se, PeakTabFilled = se,
                   batches = "batch", sampleGroups = "grp", report = FALSE,
                   assay.type1 = "nofill", assay.type2 = "fill",
                   name = "aligned", rt_col = "rt", mz_col = "mz")
```

`correctDrift` *Within-batch signal intensity drift correction*

Description

Correct drift with cluster-based drift correction.

Usage

```
correctDrift(peakTable, ...)

## S4 method for signature 'ANY'
correctDrift(
  peakTable,
  injections,
  sampleGroups,
  QCID = "QC",
  RefID = "none",
  modelNames = c("VVV", "VVE", "VEV", "VEE", "VEI", "VVI", "VII"),
  G = seq(5, 35, by = 10),
  smoothFunc = "spline",
  spar = 0.2,
  CVlimit = 0.3,
```

```
  report = TRUE,
  reportPath = NULL
)

## S4 method for signature 'SummarizedExperiment'
correctDrift(peakTable, injections, sampleGroups, assay.type, name, ...)
```

Arguments

peakTable	SummarizedExperiment object or matrix
...	parameters with same behavior across methods
injections	character scalar or numeric, injection order
sampleGroups	character scalar or character, group labels
QCID	character scalar, identifier of QC samples
RefID	character scalar, identifier of external reference samples for unbiased assessment of drift correction
modelNames	character, Which mclust geometries to test
G	integer, numbers of clusters to test
smoothFunc	character scalar, choice of regression function: spline or loess (default: spline)
spar	numeric, smoothing parameter value (defaults to 0.2)
CVlimit	coefficient of variance threshold for filtering (default = 0.3)
report	boolean, whether to print pdf reports of drift models
reportPath	character scalar, directory path for report
assay.type	character scalar, assay of to be used in case of multiple assays
name	character scalar, name of the resultant assay in case of multiple assays

Details

A basic method for matrix (samples as rows) and SummarizedExperiment is supported. For grouping variables such as sampleGroups, the basic method expects vectors, while the SummarizedExperiment method expects the names of the respective columns. The basic method returns a list with the corrected peak table and information about the process, whereas the SummarizedExperiment method assigns the corrected peak table to the object supplied.

Value

A SummarizedExperiment object with the corrected and filtered matrix or a list, including the corrected and filtered matrix as well as processing information:

- actionInfo: see what happened to each cluster
- TestFeatsCorr: to extract drift-corrected data
- TestFeatsFinal: to extract drift-corrected data which pass the criterion QC CV < CVlimit

Examples

```
data("ThreeBatchData")
set.seed(2024)
# Get batches
batchB <- getBatch(
    peakTable = PTfill, meta = meta,
    batch = meta$batch, select = "B"
)
batchF <- getBatch(
    peakTable = PTfill, meta = meta,
    batch = meta$batch, select = "F"
)
# Drift correction using QCs
BCorr <- correctDrift(
    peakTable = batchB$peakTable,
    injections = batchB$meta$inj,
    sampleGroups = batchB$meta$grp, QCID = "QC",
    G = seq(5, 35, by = 3), modelNames = c("VVE", "VEE"),
    report = FALSE
)
# Using SummarizedExperiment, more unbiased drift correction using QCs &
# external reference samples
## Construct SummarizedExperiment
peaks <- SimpleList(t(PTnofill), t(PTfill))
sampleData <- meta
featureData <- peakInfo(PT = PTnofill, sep = "@", start = 3)
rownames(featureData) <- rownames(peaks[[1]])
se <- SummarizedExperiment(assays = peaks, colData = sampleData,
                           rowData = featureData)
names(assays(se)) <- c("nofill", "fill")

## Correct drift for single batch
se <- se[, colData(se)$batch == "F"]
se <- correctDrift(se,
  injections = "inj", sampleGroups = "grp", RefID = "Ref",
  G = seq(5, 35, by = 3), modelNames = c("VVE", "VEE"),
  report = FALSE, assay.type = "fill", name = "corrected")
```

`getBatch` *Extract specific batch from peaktable and metadata*

Description

Extract specific batch from peaktable and metadata

Usage

```
getBatch(peakTable, meta, batch, select)
```

Arguments

`peakTable`	Multi-batch peak table

meta	Multi-batch metadata (including e.g. batch, injection sequence, sample tye, sample name, ...)
batch	vector (length = nSamples) containing batch information (e.g. A, B, C)
select	which batch to extract

Value

list object

$peakTable: Single batch peak table

$meta: Single batch metadata

Examples

```
data("ThreeBatchData")
# Get batches for drift correction
batchB <- getBatch(
    peakTable = PTfill, meta = meta,
    batch = meta$batch, select = "B"
)
batchF <- getBatch(
    peakTable = PTfill, meta = meta,
    batch = meta$batch, select = "F"
)
```

---

mergeBatches *Merge batches after drift correction*

Description

The output of the within-batch drift correction is a correction object. This function merges peak tables from several batches by extracting information from the correction objects. The user must specify a minimum proportion of qualified batches per feature, i.e. such batches where the QC CV is < the specified limit. There is thus a risk that features with poor quality (in certain batches) are present, but the features are present in high quality in sufficient proportion of batches to anyway warrant inclusion.

Usage

```
mergeBatches(batchList, qualRatio = 0.5)
```

Arguments

batchList	A list of correction objects (after drift correction)
qualRatio	numeric scalar, features with QC CV < the

Value

A list object containing

‘peakTableOrg‘ A merged peak table of original data

‘peakTableCorr‘ A merged peak table of drift-corrected data

‘batch‘ Batch identifier (per sample)

‘injection‘ Injection number (per sample)

Examples

```
data("ThreeBatchData")
set.seed(2024)
# Get batches
batchB <- getBatch(
    peakTable = PTfill, meta = meta,
    batch = meta$batch, select = "B"
)
batchF <- getBatch(
    peakTable = PTfill, meta = meta,
    batch = meta$batch, select = "F"
)
# Drift correction using QCs
BCorr <- correctDrift(
    peakTable = batchB$peakTable,
    injections = batchB$meta$inj,
    sampleGroups = batchB$meta$grp, QCID = "QC",
    G = seq(5, 35, by = 3), modelNames = c("VVE", "VEE"),
    report = FALSE
)
# Using SummarizedExperiment, more unbiased drift correction using QCs &
# external reference samples
## Construct SummarizedExperiment
peaks <- SimpleList(t(PTnofill), t(PTfill))
sampleData <- meta
featureData <- peakInfo(PT = PTnofill, sep = "@", start = 3)
rownames(featureData) <- rownames(peaks[[1]])
se <- SummarizedExperiment(assays = peaks, colData = sampleData,
                           rowData = featureData)
names(assays(se)) <- c("nofill", "fill")

## Correct drift for single batch
se <- se[, colData(se)$batch == "F"]
se <- correctDrift(se,
  injections = "inj", sampleGroups = "grp", RefID = "Ref",
  G = seq(5, 35, by = 3), modelNames = c("VVE", "VEE"),
  report = FALSE, assay.type = "fill", name = "corrected")
```

`normalizeBatches` *Between-batch normalisation*

Description

Batches are feature-wise normalised by Ref samples if passing heuristic criteria (CV and fold change). Otherwise normalized by population median.

Usage

```
normalizeBatches(peakTableCorr, ...)

## S4 method for signature 'ANY'
normalizeBatches(
  peakTableCorr,
  batches,
  sampleGroup,
  refGroup = "QC",
  population = "all",
  CVlimit = 0.3,
  FCLimit = 5,
  medianZero = c("mean", "min")
)

## S4 method for signature 'SummarizedExperiment'
normalizeBatches(peakTableCorr, batches, sampleGroup, assay.type, name, ...)
```

Arguments

peakTableCorr	SummarizedExperiment object or matrix
...	parameters with same behavior across methods
batches	character scalar or factor, batch labels
sampleGroup	character scalar or character, group labels
refGroup	character scalar, identifier of reference samples (default = "QC")
population	character scalar, identifier of population samples in sampleGroups (default: "all")
CVlimit	numeric scalar, coefficient of variance threshold for normalizing each batch by reference samples (default: 0.3)
FCLimit	numeric scalar, fold-change between average intensity in batches threshold for normalizing each batch by reference samples (default: 5)
medianZero	character scalar, strategy for substituting median value for population normalization when median is zero (-> Inf). Either 'mean' or 'min' (default: "min, i.e. lowest non-zero value)
assay.type	character scalar, assay to be used in case of multiple assays
name	character scalar, name of the resultant assay in case of multiple assays

Details

A basic method for matrix (samples as rows) and SummarizedExperiment is supported. For grouping variables such as sampleGroup, the basic method expects vectors, while the SummarizedExperiment method expects the names of the respective columns. The basic method returns a list with the normalized peak table and information about the process, whereas the SummarizedExperiment method assigns the normalized peak table to the object supplied.

Value

An list object containing: A SummarizedExperiment object with the normalized peak table or a list, including the normalized matrix and processing information:

- peakTable: normalised peak table

- refCorrected: boolean matrix with information on which batches were normalised by reference samples; else normalised by population median

Examples

```
# Note that the example data does not include any biological samples
data("ThreeBatchData")
normData <- normalizeBatches(
    peakTableCorr = PTfill, batches = meta$batch,
    sampleGroup = meta$grp, refGroup = "Ref",
    population = "all"
)

# With SummarizedExperiment
peaks <- SimpleList(t(PTnofill), t(PTfill))
sampleData <- meta
featureData <- peakInfo(PT = PTnofill, sep = "@", start = 3)
rownames(featureData) <- rownames(peaks[[1]])
se <- SummarizedExperiment(assays = peaks, colData = sampleData,
                           rowData = featureData)
names(assays(se)) <- c("nofill", "fill")

se <- normalizeBatches(
    peakTableCorr = se, batches = "batch", sampleGroup = "grp",
    refGroup = "Ref", population = "all", assay.type = "fill",
    name = "normalized"
)
```

`peakInfo` *Extract m/z and rt from peak table*

Description

Extract features from peak table and report their m/z and rt values

Usage

```
peakInfo(PT, sep = "_", timepos = 2, start = 1)
```

Arguments

`PT`	a peak table with variables as columns
`sep`	character separating mz from rt, e.g. "_"
`timepos`	Which position carries info about rt (1 for before separator; 2 for after separator)
`start`	character from which to start the read of peakInfo (from PT colnames)

Value

a matrix with m/z and rt of features as columns

Examples

```
data("ThreeBatchData")
# Extract peakinfo (i.e. m/z and rt of features). These column names have 2
# leading characters describing LC-MS mode -> start at 3
peakIn <- peakInfo(PT = PTnofill, sep = "@", start = 3)
```

ThreeBatchData *ThreeBatchData*

Description

The untargeted LC-MS metabolomics data was collected as per the associated publication. In brief, the data was preprocessed using the **xcms** package and biological samples were removed.

Format

A list with three objects encompassing three batches, 48 QC samples, 42 long-term reference samples and 5000 features

PTnofill matrix, peak table with missing values

PTfill matrix, peak table without missing values

meta data.frame, sample metadata including batch, group and injection order

Author(s)

Carl Brunius

References

Carl Brunius, Lin Shi, Rikard Landberg Large-scale untargeted LC-MS metabolomics data correction using between-batch feature alignment and cluster-based within-batch signal intensity drift correction. Metabolomics, 12:173. https://doi.org/10.3390/metabo10040135

Index

alignBatches, 2
alignBatches,ANY,ANY-method
        *(*alignBatches*)*, 2
alignBatches,SummarizedExperiment,SummarizedExperiment-method
        *(*alignBatches*)*, 2

correctDrift, 4
correctDrift,ANY-method *(*correctDrift*)*,
        4
correctDrift,SummarizedExperiment-method
        *(*correctDrift*)*, 4

getBatch, 6

mergeBatches, 7
meta *(*ThreeBatchData*)*, 11

normalizeBatches, 8
normalizeBatches,ANY-method
        *(*normalizeBatches*)*, 8
normalizeBatches,SummarizedExperiment-method
        *(*normalizeBatches*)*, 8

peakInfo, 10
PTfill *(*ThreeBatchData*)*, 11
PTnofill *(*ThreeBatchData*)*, 11

ThreeBatchData, 11