Package 'mmease'

Type Package

Version 1.0.0

Title enhanced analytical workflow for single-cell metabolomics

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Depends R (>= 4.3.3)

Imports multtest, mixOmics, e1071, adabag, C50, pROC, kknn, MASS, AUC, multiROC, caret, mlbench, dummies, randomForest, metabolomics, ropls, varSelRF, magrittr.

Description mmease provides entire analytical workflow of single-cell metabolomics. Specifically, mmease can (***a***) provide the most comprehensive workflow for enabling data processing and (***b***) realize systematical analytical functions for cellular heterogeneity.

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URL https://github.com/mmease2025/mmease

RoxygenNote 7.3.2

NeedsCompilation no

LazyData true

R topics documented:

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filtering	Data filtering for single-cell metabolomics data

Description

Data filtering for single-cell metabolomics data using the tolerable percentage of missing values in each metabolite.

Usage

filtering(data, percentage)

percentage of missing values must be between 0 and 1.

Arguments

data	Data frame of single-cell metabolomics, where cell name, cell class, cell type, and batch information are required in the first four columns of the input file. In the following columns, the raw peak intensities across all cells are further provided. Unique metabolite IDs or peaks are listed in the first row.
percentage	Percentage of missing values is an important parameter in single-cell metabolomics to assess data quality by quantifying missing values in data filtering.

Value

Filtered data is returned.

Examples

filted_data <− filtering(data, percentage = 0.2)

head(filted_data)

---

imputation	Data imputation of single-cell metabolomics data

Description

Imputation for missing values in single-cell metabolomics data.

Usage

imputation(data, method = "KNN")

Arguments

data	Data frame of single-cell metabolomics.
method	Imputation method for imputing missing values. The method can be 1/5 of minimum positive value or KNN.

Value

Imputed data is returned.

Examples

imputed_data <− imputation(data, method = "KNN")

head(imputed_data)

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transformation	Data transformation for single-cell metabolomics data

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Description

Data transformation of single-cell metabolomics data matrix.

Usage

transformation(data, method = "G-log")

Arguments

data	Data frame of single-cell metabolomics.
method	Data transformation method, which can be G-log, log2, or log10.

Value

Transformed data is returned.

Examples

```
transformed_data <− transformation(data, method = "G-log")
head(transformed_data)
```

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normalization — Data normalization for single-cell metabolomics data

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Description

Data normalization for single-cell metabolomics data

Usage

```
normalization(data, method = "Auto Scaling")
```

Arguments

data	Data frame of single-cell metabolomics.
method	The method for data normalization. The method can be Auto Scaling, Mean, Median, MSTUS or SIS. If SIS is selected, the internal standard name must be clearly specified in parameter IS.

Value

Normalized data is returned.

Examples

```
normalized_data <− normalization(data, method = "Auto Scaling")
head(normalized_data)
```

batch_correction	Remove batch effects for single-cell metabolomics data

Description

Batch correction for different analytical experiments of single-cell metabolomics data

Usage

batch_correction(data, method = "ComBat")

Arguments

data	Data frame of single-cell metabolomics.
method	The batch correction method can be ComBat or Limma.

Value

Corrected data is returned.

Examples

corrected_data <− batch_correction(data, method = "ComBat")

head(corrected_data)

differential	Identifying differential metabolites for single-cell metabolomics data

Description

Identifying differential metabolites for single-cell metabolomics data.

Usage

marker <− differential(data, label_col = 3, method = "t_test")

Arguments

data	Data frame of single-cell metabolomics.
label_col	label_col specifies the column of labels.
method	The method can be t_test, ANOVA, FC, PLS-DA, OPLS-DA, RF_RFE, Kruskal_Wallis or svmrfeFeatureRanking.

Value

Identified differential metabolites are returned.

Examples

table <− differential(data, label_col = 3, method = "t_test")

classification	Constructing classification models for identified differential metabolites

Description

Constructing classification models for identified differential metabolites

Usage

classification(data, label_col = 3, method = "AdaBoost")

classification_plots(class)

Arguments

data	Data frame of single-cell metabolomics.
label_col	label_col specifies the column of labels.
method	The method can be AdaBoost, Bagging, Decision Trees, K-Nearest Neighbor, Naive Bayes, Linear Discriminat Analysis, Random Forest or Support Vector Machine.
class	The result of classification model.

Value

Receiver operating characteristic (ROC) curve and area under the curve (AUC) value in classification model are returned.

Examples

class <− classification(data, label_col = 3, method = "AdaBoost")

classification_plots(class)