Package 'mmease'

Type Package

Version 1.0.0

Title a unique online service of whole analytical workflow of single-cell metabolomics

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Depends R (>= 3.5)

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 from bulk metabolomics. Specifically, mmease can (a) provide the most comprehensive workflow for enabling data processing, (b) realize systematical analytical functions for both metabolic heterogeneity and functional heterogeneity

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

RoxygenNote 7.3.2

NeedsCompilation no

LazyData true

R topics documented:

filtering....2
imputation....3
transformation....3
normalization....4
batch_correction....4
differential....5
classification....6

Index

filtering	Data filtering for single-cell metabolomics data matrix

Description

Data filtering for single-cell metabolomics data matrix depend on the tolerable percent of missing values in each metabolite.

Usage

filtering(data,Percent of Missing Values)

#Percent of Missing Values must be between 0 and 1

Arguments

data	Single-cell metabolomics data matrix.
Percent of Missing Values	Percent of Missing Values is a key metric in single-cell metabolomics data analysis, used to assess data quality by quantifying the proportion of absent data points, which can influence decisions on data filtering and impact downstream analyses.

Value

Filtered single-cell metabolomics data matrix is returned.

Examples

```
filted_data <- filtering(data,0.2)

head(filted_data)
```

imputation	Data imputation for single-cell metabolomics data matrix

Description

Imputation fills missing values in single-cell metabolomics data matrix.

Usage

imputation(data, method = "KNN")

Arguments

data	Single-cell metabolomics data matrix.
method	The method for data imputation. The method can be 1/5 of minimum positive value or KNN.

Value

Imputed single-cell metabolomics data matrix is returned.

Examples

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

head(imputed_data)

transformation	Data transformation for single-cell metabolomics data matrix

Description

Transform data formats of single-cell metabolomics data matrix.

Usage

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

Arguments

data	Single-cell metabolomics data matrix.
method	The method for data transformation. The method can be G-log, log2, or log10.

Value

Transformed single-cell metabolomics data matrix is returned.

Examples

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

---

normalization	Data normalization for single-cell metabolomics data matrix

---

Description

Data normalization for single-cell metabolomics data matrix adjusts metabolite abundances across cells to a common scale

Usage

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

Arguments

data	Single-cell metabolomics data matrix.
method	The method for data normalization. The method can be Auto Scaling, Mean, Median, MSTUS or SIS.

Value

Normalized single-cell metabolomics data matrix is returned.

Examples

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

---

batch_correction	Remove batch effects for the integrated dataset

---

Description

Remove batch effects among different analytical experiments for the integrated dataset

Usage

```
batch_correction(data, method = "ComBat")
```

Arguments

data	Single-cell metabolomics data matrix.
method	The method used for Remove batch effects. The method can be ComBat or Limma.

Value

Corrected single-cell metabolomics data matrix is returned.

Examples

```
corrected_data <- batch_correction(data, method = "ComBat")
head(corrected_data)
```

---

differential Identifying differences between groups

Description

Identifying differences between groups defined by a label column.

Usage

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

Arguments

data	Single-cell metabolomics data matrix.
label_col	label_col specifies the column in the data matrix representing group labels.
method	The method used for identifying differences between groups. The method can be t_test, ANOVA, FC, PLS-DA, OPLS-DA, RF_RFE, Kruskal_Wallis or svmrfeFeatureRanking.

Value

Results such as feature rankings, statistical test values, or p-values in a formatted data frame are returned.

Examples

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

classification	Constructing classification models by classification methods

Description

Constructing classification models by classification methods

Usage

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

classification_plots(class)

Arguments

data	Single-cell metabolomics data matrix.
label_col	label_col specifies the column in the data matrix representing group labels.
method	The method used for constructing classification models. The method can be AdaBoost, Bagging, Decision Trees, K-Nearest Neighbor, Naive Bayes, Linear Discriminat Analysis, Random Forest or Support Vector Machine.

Value

Receiver Operating Characteristic (ROC) and Precision - Recall (PR) curves. It also outputs the Area Under the Curve (AUC) values for both the ROC and PR curves are returned.

Examples

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

plots <- classification_plots(class)