

Package ‘SDAMS’

October 16, 2018

Type Package

Title Differential Abundant Analysis for Metabolomics and Proteomics Data

Version 1.0.0

Date 2018-3-17

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Depends R(>= 3.5), SummarizedExperiment

Suggests testthat

Imports trust, qvalue, methods, stats, utils

Description This Package utilizes a Semi-parametric Differential Abundance analysis (SDA) method for metabolomics and proteomics data from mass spectrometry. SDA is able to robustly handle non-normally distributed data and provides a clear quantification of the effect size.

License GPL

LazyLoad no

NeedsCompilation no

biocViews DifferentialExpression, Metabolomics, Proteomics, MassSpectrometry

git_url <https://git.bioconductor.org/packages/SDAMS>

git_branch RELEASE_3_7

git_last_commit 5a0ce82

git_last_commit_date 2018-07-10

Date/Publication 2018-10-15

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SDAMS-package	<i>SDAMS package for differential abundance analysis of Metabolomics and Proteomics data from mass spectrometry</i>
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Description

SDAMS is an R package for differential abundance analysis of metabolomics and proteomics data, and the main function for differential abundance analysis is [SDA](#). See the examples at [SDA](#) for basic analysis steps. SDAMS considers a two-part model, a logistic regression for the zero proportion and a semi-parametric log-linear model for the non-zero values.

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References

Yuntong Li, Teresa W.M. Fan, Andrew N. Lane, Woo-Young Kang, Susanne M. Arnold, Arnold J. Stromberg, Chi Wang and Li Chen: A Two-Part Semi-Parametric Model for Metabolomics and Proteomics Data. (Manuscript)

dataInput	<i>Mass spectrometry data input</i>
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Description

Two ways to input metabolomics or proteomics data from mass spectrometry as SummarizedExperiment:

1. `createSEFromCSV` creates SummarizedExperiment object from csv files;
2. `createSEFromMatrix` creates SummarizedExperiment object from separate matrices: one for feature data and the other one for group.

Usage

```
createSEFromCSV(featurePath, groupPath, rownames1 = 1, rownames2 = 1,
                header1 = TRUE, header2 = TRUE)
```

```
createSEFromMatrix(feature, group)
```

Arguments

featurePath	path for feature data.
groupPath	path for subject grouping data.
rownames1	indicator for feature data with row names. If NULL, row numbers are automatically generated.
rownames2	indicator for group data with row names. If NULL, row numbers are automatically generated.

header1	a logical value indicating whether the first row of feature is column names. The default value is TRUE.
header2	a logical value indicating whether the first row of group is column names. The default value is TRUE. If group input is a vector, set to False.
feature	a matrix with row being features and column being subjects.
group	a one column matrix containing subject grouping information.

Value

An object of SummarizedExperiment class.

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See Also

[SDA](#) input requires an object of SummarizedExperiment class.

Examples

```
# ----- csv input -----
directory1 <- system.file("extdata", package = "SDAMS", mustWork = TRUE)
path1 <- file.path(directory1, "ProstateFeature.csv")
directory2 <- system.file("extdata", package = "SDAMS", mustWork = TRUE)
path2 <- file.path(directory2, "ProstateGroup.csv")

exampleSE <- createSEFromCSV(path1, path2)
exampleSE

# ----- matrix input -----
set.seed(100)
featureInfo <- matrix(runif(800, -2, 5), ncol = 40)
featureInfo[featureInfo<0] <- 0
rownames(featureInfo) <- paste("feature", 1:20, sep = '')
colnames(featureInfo) <- paste('subject', 1:40, sep = '')
groupInfo <- data.frame(grouping=matrix(sample(0:1, 40, replace = TRUE),
                                       ncol = 1))
rownames(groupInfo) <- colnames(featureInfo)

exampleSE <- createSEFromMatrix(feature = featureInfo, group = groupInfo)
exampleSE
```

exampleData

An example data for the SDAMS package

Description

SDAMS package provides two different data formats for prostate cancer proteomics data, which is from the human urinary proteome database(<http://mosaiques-diagnostics.de/mosaiques-diagnostics/human-urinary-proteom-database>). There are 526 prostate cancer subjects and 1503 healthy subjects. A total of 5605 proteomic features were measured for each subject. For illustration purpose, we took a 10% subsample randomly from this real data. This example data contains 560

proteomic features for 202 experimental subjects with 49 prostate cancer subjects and 153 healthy subjects. `exampleSumExp.rda` is an object of `SummarizedExperiment` class which stores the information of both proteomic features and experimental subjects. `ProstateFeature.csv` contains a matrix-like proteomic feature data and `ProstateGroup.csv` contains a single column of experimental subject group data.

Usage

```
data(exampleSumExp)
```

Value

An object of `SummarizedExperiment` class.

References

Siwy, J., Mullen, W., Golovko, I., Franke, J., and Zurbig, P. (2011). Human urinary peptide database for multiple disease biomarker discovery. *PROTEOMICS-Clinical Applications* 5, 367-374.

See Also

[SDA](#)

Examples

```
#----- load data -----  
data(exampleSumExp)  
exampleSumExp  
feature = assay(exampleSumExp) # access feature data  
group = colData(exampleSumExp)$grouping # access grouping information  
SDA(exampleSumExp)
```

SDA

Semi-parametric differential abundance analysis

Description

This function considers a two-part semi-parametric model for metabolomics and proteomics data. A kernel-smoothed method is applied to estimate the regression coefficients. And likelihood ratio test is constructed for differential abundance analysis.

Usage

```
SDA(sumExp)
```

Arguments

`sumExp` An object of 'SummarizedExperiment' class.

Details

The differential abundance analysis is to compare metabolomic or proteomic profiles between different experimental groups, which utilizes a two-part model: a logistic regression model to characterize the zero proportion and a semi-parametric model to characterize non-zero values. Let Y_{ig} be the random variable representing the abundance of feature g in subject i . This two-part model has the following form:

$$\log\left(\frac{\pi_{ig}}{1 - \pi_{ig}}\right) = \gamma_{0g} + \gamma_g \mathbf{X}_i$$

$$\log(Y_{ig}) = \beta_g \mathbf{X}_i + \varepsilon_{ig}$$

where $\pi_{ig} = Pr(Y_{ig} = 0)$ be the probability of point mass, $\mathbf{X}_i = (X_{i1}, X_{i2}, \dots, X_{iQ})^T$ is a Q-vector covariates that specifies the treatment conditions applied to subject i . The corresponding Q-vector of model parameters $\gamma_g = (\gamma_{1g}, \gamma_{2g}, \dots, \gamma_{Qg})^T$ quantify the covariates effects on the fraction of zero values for feature g and γ_{0g} is the intercept. $\beta_g = (\beta_{1g}, \beta_{2g}, \dots, \beta_{Qg})^T$ is a Q-vector of model parameters quantifying the covariates effects on the non-zero values for the feature. And ε_{ig} are independent error terms with a common but completely unspecified density function f_g .

Hypothesis testing on the effect of the q th covariate on the g th feature is performed by assessing γ_{qg} and β_{qg} . Consider the null hypothesis H_0 : γ_{qg} and β_{qg} against alternative hypothesis H_1 : at least one of the two parameters is non-zero. The p-value is calculated based on a chi-square distribution with 2 degrees of freedom. To adjust for multiple comparisons across features, the false discovery rate (FDR) q-value is calculated based on the [qvalue](#) function in R/Bioconductor.

Value

A list containing the following components:

gamma	a vector of point estimators for γ_g in the logistic model (binary part)
beta	a vector of point estimators for β_g in the semi-parametric model (non-zero part)
pv_gamma	a vector of one-part p-values for γ_g
pv_beta	a vector of one-part p-values for β_g
qv_gamma	a vector of one-part q-values for γ_g
qv_beta	a vector of one-part q-values for β_g
pv_2part	a vector of two-part p-values for overall test
qv_2part	a vector of two-part q-values for overall test
feat.names	a vector of feature names

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Examples

```
##----- load data -----
data(exampleSumExp)

results = SDA(exampleSumExp)

##----- two part q-values -----
results$qv_2part
```

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