

# Package ‘SDAMS’

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**Type** Package

**Title** Differential Abundant/Expression Analysis for Metabolomics,  
Proteomics and single-cell RNA sequencing Data

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**Author** Yuntong Li <liyuntong0704@gmail.com>, Chi Wang <chi.wang@uky.edu>,  
Li Chen <lichenuky@uky.edu>

**Maintainer** Yuntong Li <liyuntong0704@gmail.com>

**Depends** R(>= 3.5), SummarizedExperiment

**Suggests** testthat

**Imports** trust, qvalue, methods, stats, utils

**Description** This Package utilizes a Semi-parametric Differential  
Abundance/expression analysis (SDA) method for metabolomics and proteomics  
data from mass spectrometry as well as single-cell RNA sequencing data. 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** ImmunoOncology, DifferentialExpression, Metabolomics,  
Proteomics, MassSpectrometry, SingleCell

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|               |                                                                                                                                     |
|---------------|-------------------------------------------------------------------------------------------------------------------------------------|
| SDAMS-package | <i>SDAMS package for differential abundance/expression analysis of Metabolomics, Proteomics and single-cell RNA sequencing data</i> |
|---------------|-------------------------------------------------------------------------------------------------------------------------------------|

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**Description**

SDAMS is an R package for differential abundance/expression analysis of metabolomics, proteomics and single-cell RNA sequencing data, and the main function for differential abundance/expression 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.

**Author(s)**

Yuntong Li <liyuntong0704@gmail.com>, Chi Wang <chi.wang@uky.edu>, Li Chen <lichenuky@uky.edu>

**References**

Li, Y., Fan, T.W., Lane, A.N. et al. SDA: a semi-parametric differential abundance analysis method for metabolomics and proteomics data. BMC Bioinformatics 20, 501 (2019).

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|           |                                     |
|-----------|-------------------------------------|
| dataInput | <i>Mass spectrometry data input</i> |
|-----------|-------------------------------------|

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**Description**

Two ways to input metabolomics or proteomics data from mass spectrometry or single-cell RNA sequencing data as SummarizedExperiment:

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

**Usage**

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

```
createSEFromMatrix(feature, colData)
```

**Arguments**

|             |                                                                                                   |
|-------------|---------------------------------------------------------------------------------------------------|
| featurePath | path for feature/gene data.                                                                       |
| colDataPath | path for colData.                                                                                 |
| rownames1   | indicator for feature/gene data with row names. If NULL, row numbers are automatically generated. |
| rownames2   | indicator for colData with row names. If NULL, row numbers are automatically generated.           |

|         |                                                                                                                                                     |
|---------|-----------------------------------------------------------------------------------------------------------------------------------------------------|
| header1 | a logical value indicating whether the first row of feature/gene is column names. The default value is TRUE.                                        |
| header2 | a logical value indicating whether the first row of colData is column names. The default value is TRUE. If colData input is a vector, set to False. |
| feature | a matrix with row being features/genes and column being subjects/cells.                                                                             |
| colData | a column type data containing information about the subjects/cells.                                                                                 |

**Value**

An object of SummarizedExperiment class.

**Author(s)**

Yuntong Li <yuntong.li@uky.edu>, Chi Wang <chi.wang@uky.edu>, Li Chen <lichenuky@uky.edu>

**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("gene", 1:20, sep = '')
colnames(featureInfo) <- paste('cell', 1:40, sep = '')
groupInfo <- data.frame(grouping=matrix(sample(0:1, 40, replace = TRUE),
                                       ncol = 1))
rownames(groupInfo) <- colnames(featureInfo)

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

---

exampleData

*Two example datasets for SDAMS package*

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**Description**

SDAMS package provides two types of example datasets: one is prostate cancer proteomics data from mass spectrometry and the other one is single-cell RNA sequencing data.

1. For prostate cancer proteomics data, it 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. SDAMS package provides two different kinds of data formats for prostate cancer proteomics data. `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.
2. For single cell RNA sequencing data, it is in the form of transcripts per kilobase million (TPM). The count data can be found at Gene Expression Omnibus (GEO) database with Accession No. GSE29087. There are 92 single cells (48 mouse embryonic stem (ES) cells and 44 mouse embryonic fibroblasts (MEF)) that were analyzed. The example data provided by SDAMS contains 10% of genes which are randomly sampled from the raw dataset. `exampleSingleCell.rda` is an object of `SummarizedExperiment` class which stores the information of both gene expression and cell information.

### Usage

```
data(exampleSumExp)
data(exampleSingleCell)
```

### 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.

Islam, S., Kjallquist, U., Moliner, A., Zajac, P., Fan, J. B., Lonnerberg, P., & Linnarsson, S. (2011). Characterization of the single-cell transcriptional landscape by highly multiplex RNA-seq. *Genome research*, 21(7), 1160-1167.

### See Also

[SDA](#)

### Examples

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

## Description

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

## Usage

```
SDA(sumExp, VOI = NULL, ...)
```

## Arguments

|        |                                                                                                                                   |
|--------|-----------------------------------------------------------------------------------------------------------------------------------|
| sumExp | An object of 'SummarizedExperiment' class.                                                                                        |
| VOI    | Variable of interest. Default is NULL, when there is only one covariate, otherwise it must be one of the column names in colData. |
| ...    | Additional arguments passed to <a href="#">qvalue</a> .                                                                           |

## Details

The differential abundance/expression analysis is to compare metabolomic or proteomic profiles or gene expression 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  $Y_i$  be the random variable and  $X_i$  is a vector of covariates. This two-part model has the following form:

$$\log\left(\frac{\pi_i}{1 - \pi_i}\right) = \gamma_0 + \gamma X_i$$

$$\log(Y_i) = \beta X_i + \varepsilon_i$$

where  $\pi_i = Pr(Y_i = 0)$ . The model parameters  $\gamma$  quantify the covariates effects on the fraction of zero values and  $\gamma_0$  is the intercept.  $\beta$  are the model parameters quantifying the covariates effects on the non-zero values,  $\varepsilon_i$  are independent error terms with a common but completely unspecified density function  $f$ .

For differential abundant analysis on data from mass spectrometry,  $Y_i$  represents the abundance of certain feature for subject  $i$ ,  $\pi_i$  is the probability of point mass.  $X_i = (X_{i1}, X_{i2}, \dots, X_{iQ})^T$  is a Q-vector of covariates that specifies the treatment conditions applied to subject  $i$ . The corresponding Q-vector of model parameters  $\gamma = (\gamma_1, \gamma_2, \dots, \gamma_Q)^T$  and  $\beta = (\beta_1, \beta_2, \dots, \beta_Q)^T$  quantify the covariates effects for certain feature. Hypothesis testing on the effect of the  $q$ th covariate on certain feature is performed by assessing  $\gamma_q$  and  $\beta_q$ . Consider the null hypothesis  $H_0: \gamma_q = 0$  and  $\beta_q = 0$  against alternative hypothesis  $H_1$ : at least one of the two parameters is non-zero. We also consider the hypotheses for testing  $\gamma_q = 0$  and  $\beta_q = 0$  individually.

For differential expression analysis on single-cell RNA sequencing data,  $Y_i$  represents the expression (TPM value) of certain gene in  $i$ th cell,  $\pi_i$  is the drop-out probability.  $X_i = (Z_i, W_i)^T$  is a vector of covariates with  $Z_i$  being a binary indicator of the cell population under comparison and  $W_i$  being a vector of other covariates, e.g. cell size, and  $\gamma = (\gamma_Z, \gamma_W)$  and  $\beta = (\beta_Z, \beta_W)$  are model parameters. Hypothesis testing on the effect of different cell subpopulations on certain gene is performed by assessing  $\gamma_Z$  and  $\beta_Z$ . For each gene, the likelihood ratio test is performed

on the null hypothesis  $H_0: \gamma_Z = 0$  and  $\beta_Z = 0$  against alternative hypothesis  $H_1$ : at least one of the two parameters is non-zero. We also consider the hypotheses for testing  $\gamma_Z = 0$  and  $\beta_Z = 0$  individually.

The p-value is calculated based on an asymptotic chi-squared distribution. 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:

|                         |                                                                                         |
|-------------------------|-----------------------------------------------------------------------------------------|
| <code>gamma</code>      | a matrix of point estimators for $\gamma_g$ in the logistic model (binary part)         |
| <code>beta</code>       | a matrix of point estimators for $\beta_g$ in the semi-parametric model (non-zero part) |
| <code>pv_gamma</code>   | a matrix of one-part p-values for $\gamma_g$                                            |
| <code>pv_beta</code>    | a matrix of one-part p-values for $\beta_g$                                             |
| <code>qv_gamma</code>   | a matrix of one-part q-values for $\gamma_g$                                            |
| <code>qv_beta</code>    | a matrix of one-part q-values for $\beta_g$                                             |
| <code>pv_2part</code>   | a matrix of two-part p-values for overall test                                          |
| <code>qv_2part</code>   | a matrix of two-part q-values for overall test                                          |
| <code>feat.names</code> | a vector of feature/gene names                                                          |

### Author(s)

Yuntong Li <yuntong.li@uky.edu>, Chi Wang <chi.wang@uky.edu>, Li Chen <lichenuky@uky.edu>

### Examples

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

results = SDA(exampleSumExp)

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

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