

# Package ‘imputeLCMD’

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**Type** Package

**Title** A Collection of Methods for Left-Censored Missing Data Imputation

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**Description** A collection of functions for left-censored missing data imputation. Left-censoring is a special case of missing not at random (MNAR) mechanism that generates non-responses in proteomics experiments. The package also contains functions to artificially generate peptide/protein expression data (log-transformed) as random draws from a multivariate Gaussian distribution as well as a function to generate missing data (both randomly and non-randomly). For comparison reasons, the package also contains several wrapper functions for the imputation of non-responses that are missing at random. \* New functionality has been added: a hybrid method that allows the imputation of missing values in a more complex scenario where the missing data are both MAR and MNAR.

**License** GPL (>= 2)

**Depends** R (>= 2.10), tmvtnorm, norm, pcaMethods, impute

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generate.ExpressionData

*Generate expression data*

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## Description

this function generates artificial peptide abundance data with DA proteins samples are drawn from a gaussian distribution

## Usage

```
generate.ExpressionData(
  nSamples1,
  nSamples2,
  meanSamples,
  sdSamples,
  nFeatures,
  nFeaturesUp,
  nFeaturesDown,
  meanDynRange,
  sdDynRange,
  meanDiffAbund,
  sdDiffAbund
)
```

## Arguments

nSamples1	number of samples in condition 1
nSamples2	number of samples in condition 2

meanSamples	xxx
sdSamples	xxx
nFeatures	number of total features
nFeaturesUp	number of features up regulated
nFeaturesDown	number of features down regulated
meanDynRange	mean value of the dynamic range
sdDynRange	sd of the dynamic range
meanDiffAbund	xxx
sdDiffAbund	xxx

**Value**

A list containing the data, the conditions label and the regulation label (up/down/no)

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<code>generate.RollUpMap</code>	<i>Generate roll up map</i>
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**Description**

This function generates a map for peptide to protein roll-up

**Usage**

```
generate.RollUpMap(nProt, pep.Expr.Data)
```

**Arguments**

nProt	number of proteins to map to the peptide expression data
pep.Expr.Data	matrix of peptide expression data

**Value**

the peptide to protein map (for each row in pep.prot.Map the corresponding value corresponds to the index of the protein that peptide is mapped to)

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impute.MAR	<i>imputation under MAR/MCAR hypothesis</i>
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### Description

This function performs missing values imputation under MAR/MCAR hypothesis. The imputation of MVs is performed for each protein containing MAR/MCAR missing values

### Usage

```
impute.MAR(dataSet.mvs, model.selector, method = "MLE")
```

### Arguments

dataSet.mvs	expression matrix containing abundances with MVs (either peptides or proteins)
model.selector	binary vector; "1" indicates MAR/MCAR proteins
method	the method to be used for MAR/MCAR missing values. Possible values: MLE (default), SVD, KNN

### Value

dataset containing only MNAR (assumed to be left-censored) missing data

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impute.MAR.MNAR	<i>Imputation under MCAR and MNAR hypothesis</i>
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### Description

this function performs missing values imputation under MCAR and MNAR hypothesis

### Usage

```
impute.MAR.MNAR(
  dataSet.mvs,
  model.selector,
  method.MAR = "KNN",
  method.MNAR = "QRILC"
)
```

### Arguments

dataSet.mvs	expression matrix containing abundances with MVs (either peptides or proteins)
model.selector	- binary vector; "1" indicates MCAR proteins
method.MAR	- the method to be used for MAR missing values - possible values: MLE (default), SVD, KNN
method.MNAR	- the method to be used for MAR missing values

**Value**

dataset containing complete abundances

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<code>impute.MinDet</code>	<i>Imputation with min value</i>
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**Description**

this function performs missing values imputation by the minimum value observed

**Usage**

```
impute.MinDet(dataSet.mvs, q = 0.01)
```

**Arguments**

<code>dataSet.mvs</code>	expression matrix with MVs (either peptides or proteins)
<code>q</code>	the q quantile used to estimate the minimum

**Value**

dataset containing complete abundances

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<code>impute.MinProb</code>	<i>Imputation by random draws</i>
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**Description**

This function performs missing values imputation by random draws from a gaussian

**Usage**

```
impute.MinProb(dataSet.mvs, q = 0.01, tune.sigma = 1)
```

**Arguments**

<code>dataSet.mvs</code>	expression matrix containing abundances with MVs (either peptides or proteins)
<code>q</code>	the q-th quantile used to estimate the minimum value observed for each sample
<code>tune.sigma</code>	coefficient that controls the sd of the MNAR distribution

**Value**

dataset containing complete abundances

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<code>impute.QRILC</code>	<i>imputation based on quantile regression</i>
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**Description**

this function performs missing values imputation based quantile regression

**Usage**

```
impute.QRILC(dataSet.mvs, tune.sigma = 1)
```

**Arguments**

<code>dataSet.mvs</code>	expression matrix with MVs (either peptides or proteins)
<code>tune.sigma</code>	coefficient that controls the sd of the MNAR distribution

**Value**

a list containing: a matrix with the complete abundances, a list with the estimated parameters of the complete data distribution

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<code>impute.wrapper.KNN</code>	<i>Imputation with KNN</i>
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**Description**

This function performs missing values imputation based on KNN algorithm

**Usage**

```
impute.wrapper.KNN(dataSet.mvs, K)
```

**Arguments**

<code>dataSet.mvs</code>	expression matrix with MVs (either peptides or proteins)
<code>K</code>	the number of neighbors

**Value**

dataset containing complete abundances

---

`impute.wrapper.MLE`     *imputation using the EM algorithm*

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**Description**

This function performs missing values imputation using the EM algorithm

**Usage**

```
impute.wrapper.MLE(dataSet.mvs)
```

**Arguments**

`dataSet.mvs`     expression matrix with MVs (either peptides or proteins)

**Value**

expression matrix with MVs imputed

---

`impute.wrapper.SVD`     *imputation based on SVD algorithm*

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**Description**

this function performs missing values imputation based on SVD algorithm

**Usage**

```
impute.wrapper.SVD(dataSet.mvs, K)
```

**Arguments**

`dataSet.mvs`     expression matrix with MVs (either peptides or proteins)

`K`                the number of PCs

**Value**

expression matrix with MVs imputed

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impute.ZERO	<i>Imputation by 0.</i>
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**Description**

This function performs missing values imputation by 0.

**Usage**

```
impute.ZERO(dataSet.mvs)
```

**Arguments**

dataSet.mvs      expression matrix containing abundances with MVs (either peptides or proteins)

**Value**

dataset containing complete abundances

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insertMVs	<i>Generates missing values in data.</i>
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**Description**

this function generates missing data in a complete data matrix

**Usage**

```
insertMVs(original, mean.THR, sd.THR, MNAR.rate)
```

**Arguments**

original            complete data matrix containing all measurements  
 mean.THR, sd.THR

- parameters of the threshold distribution which controls the MVs rate (mean.THR should be initially set such that the result of the initial thresholding, in terms of no. of NAs, equals the desired total missing data rate) - example: if one wants to generate 30 mean.THR can be set as follows: mean.THR = quantile(pepExprsData, probs = 0.3) - sd.THR is usually set to a small value (e.g. 0.1)

MNAR.rate          percentage of MVs which are missing not at random

**Value**

A list that contains the original complete data matrix, the data matrix with missing data and the percentage of missing data

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intensity\_PXD000022     *Dataset PXD000022 from ProteomeXchange.*

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## Description

This dataset has been collected during a study designed to compare the protein content of the exosome-like vesicles (ELVs) released from C2C12 murine myoblasts during proliferation (ELV-MB), and after differentiation into myotubes (ELV-MT). The dataset within this package contains proteins intensity processed using MaxQuant. More information can be found on ProteomeExchange public repository (<http://proteomecentral.proteomexchange.org/cgi/GetDataset?ID=PXD000022>) or in the original paper (see reference).

## Usage

```
data(intensity_PXD000022)
```

## Format

A data frame with 660 observations on the following 7 variables.

Protein.IDs    Peptides/Proteins names

Intensity.MB.1    a numeric vector

Intensity.MB.2    a numeric vector

Intensity.MB.3    a numeric vector

Intensity.MT.1    a numeric vector

Intensity.MT.2    a numeric vector

Intensity.MT.3    a numeric vector

## Source

Original MaxQuant data: <http://proteomecentral.proteomexchange.org/cgi/GetDataset?ID=PXD000022>

## References

Forterre A, Jalabert A, Berger E, Baudet M, Chikh K, et al. (2014) Proteomic Analysis of C2C12 Myoblast and Myotube Exosome-Like Vesicles: A New Paradigm for Myoblast-Myotube Cross Talk? PLoS ONE 9(1): e84153. doi:10.1371/journal.pone.0084153

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intensity\_PXD000052     *Dataset PXD000052 from ProteomeXchange.*

---

### Description

This dataset has been collected during a study designed to perform the proteomic analysis of the SLP76 interactome in resting and activated primary mast cells. Four SLP76 replicates (with two analytical replicates each) have been affinity-purified from both resting and activated primary mast cells. The dataset within this package contains proteins intensity processed using MaxQuant. More information can be found on ProteomeExchange public repository (<http://proteomecentral.proteomexchange.org/cgi/GetDataset>) or in the original paper (see reference).

### Usage

```
data(intensity_PXD000052)
```

### Format

A data frame with 1991 observations on the following 17 variables.

Protein.IDs	Peptides/Proteins names
iBAQ.stSLP_activ1	a numeric vector
iBAQ.stSLP_activ2	a numeric vector
iBAQ.stSLP_activ3	a numeric vector
iBAQ.stSLP_activ4	a numeric vector
iBAQ.stSLP_rest1	a numeric vector
iBAQ.stSLP_rest2	a numeric vector
iBAQ.stSLP_rest3	a numeric vector
iBAQ.stSLP_rest4	a numeric vector
iBAQ.WT_activ1	a numeric vector
iBAQ.WT_activ2	a numeric vector
iBAQ.WT_activ3	a numeric vector
iBAQ.WT_activ4	a numeric vector
iBAQ.WT_rest1	a numeric vector
iBAQ.WT_rest2	a numeric vector
iBAQ.WT_rest3	a numeric vector
iBAQ.WT_rest4	a numeric vector

### Source

Original MaxQuant data: <http://proteomecentral.proteomexchange.org/cgi/GetDataset?ID=PXD000052>

## References

Bounab Y, Hesse AM, Iannascoli B, Grieco L, Coute Y, Niarakis A, Roncagalli R, Lie E, Lam KP, Demangel C, Thieffry D, Garin J, Malissen B, Da?ron M, Proteomic analysis of the SH2 domain-containing leukocyte protein of 76 kDa (SLP76) interactome in resting and activated primary mast cells [corrected]. *Mol Cell Proteomics*, 12(10):2874-89(2013).

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intensity\_PXD000438     *Dataset PXD000438 from ProteomeXchange.*

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## Description

This dataset has been collected during a study designed to compare human primary tumor-derived xenograph proteomes of the two major histological non-small cell lung cancer subtypes: adenocarcinoma (ADC) and squamous cell carcinoma (SCC). The dataset within this package contains proteins intensity for 6 ADC and 6 SCC samples, processed using MaxQuant. More information can be found on ProteomeExchange public repository (<http://proteomecentral.proteomexchange.org/cgi/GetDataset?ID=PXD000438>) or in the original paper (see reference).

## Usage

```
data(intensity_PXD000438)
```

## Format

A data frame with 3709 observations on the following 13 variables.

Protein.IDs Peptides/Proteins names

Intensity.092.1 a numeric vector

Intensity.092.2 a numeric vector

Intensity.092.3 a numeric vector

Intensity.441.1 a numeric vector

Intensity.441.2 a numeric vector

Intensity.441.3 a numeric vector

Intensity.561.1 a numeric vector

Intensity.561.2 a numeric vector

Intensity.561.3 a numeric vector

Intensity.691.1 a numeric vector

Intensity.691.2 a numeric vector

Intensity.691.3 a numeric vector

## Source

Original MaxQuant data: <http://proteomecentral.proteomexchange.org/cgi/GetDataset?ID=PXD000438>

## References

Zhang W, Wei Y, Ignatchenko V, Li L, Sakashita S, Pham NA, Taylor P, Tsao MS, Kislinger T, Moran MF, Proteomic profiles of human lung adeno and squamous cell carcinoma using super-SILAC and label-free quantification approaches. *Proteomics*, 14(6):795-803(2014).

## Examples

```
data(intensity_PXD000438)
```

---

intensity\_PXD000501     *Dataset PXD000501 from ProteomeXchange.*

---

## Description

This dataset contains three biological replicates with three technical replicates each for the conditions media (CM) and the whole cell lysates (WCL) of C8-D1A cell lines. The dataset within this package contains proteins iBAQ intensity processed using MaxQuant. More information can be found on ProteomeExchange public repository (<http://proteomecentral.proteomexchange.org/cgi/GetDataset?ID=PX000501>) or in the original paper (see reference).

## Usage

```
data(intensity_PXD000501)
```

## Format

A data frame with 7363 observations on the following 19 variables.

Protein.IDs	Peptides/Proteins names
iBAQ.secretome_set1_tech1	a numeric vector
iBAQ.secretome_set1_tech2	a numeric vector
iBAQ.secretome_set1_tech3	a numeric vector
iBAQ.secretome_set2_tech1	a numeric vector
iBAQ.secretome_set2_tech2	a numeric vector
iBAQ.secretome_set2_tech3	a numeric vector
iBAQ.secretome_set3_tech1	a numeric vector
iBAQ.secretome_set3_tech2	a numeric vector
iBAQ.secretome_set3_tech3	a numeric vector
iBAQ.whole_set1_tech1	a numeric vector
iBAQ.whole_set1_tech2	a numeric vector
iBAQ.whole_set1_tech3	a numeric vector
iBAQ.whole_set2_tech1	a numeric vector
iBAQ.whole_set2_tech2	a numeric vector

iBAQ.whole\_set2\_tech3 a numeric vector  
 iBAQ.whole\_set3\_tech1 a numeric vector  
 iBAQ.whole\_set3\_tech2 a numeric vector  
 iBAQ.whole\_set3\_tech3 a numeric vector

### Source

Original MaxQuant data: <http://proteomecentral.proteomexchange.org/cgi/GetDataset?ID=PXD000501>

### References

Han D, Jin J, Woo J, Min H, Kim Y, Proteomic analysis of mouse astrocytes and their secretome by a combination of FASP and StageTip-based, high pH, reversed-phase fractionation. *Proteomics*, ();(2014).

### Examples

```
data(intensity_PXD000501)
```

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model.Selector	<i>Identifies row in the data matrix affected by a MNAR missingness mechanism</i>
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### Description

- this function determines row in the data matrix affected by a MNAR missingness mechanism - it is based on the assumption that the distributions of the mean values of proteins follows a normal distribution - the method makes use of a decision function defined as a tradeoff between the empirical CDF of the proteins' means and the theoretical CDF assuming that no MVs are present

### Usage

```
model.Selector(dataSet.mvs)
```

### Arguments

dataSet.mvs expression matrix containing abundances with MVs (either peptides or proteins)

### Value

flags vector; "1" denotes rows containing random missing values; "0" denotes rows containing left-censored missing values

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pep2prot

*peptide to protein roll-up*

---

**Description**

this function performs peptide to protein roll-up

**Usage**

```
pep2prot(pep.Expr.Data, rollout.map)
```

**Arguments**

pep.Expr.Data    matrix of peptide expression data  
rollout.map     the map to peptide to protein mapping

**Value**

matrix of peptide expression data

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