Package 'UNDO'

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Type Package

Title Unsupervised Deconvolution of Tumor-Stromal Mixed Expressions

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Depends R (>= 2.15.2), methods, BiocGenerics, Biobase

Imports MASS, boot, nnls, stats, utils

biocViews Software

Description UNDO is an R package for unsupervised deconvolution of tumor and stromal mixed expression data. It detects marker genes and deconvolutes the mixing expression data without any prior knowledge.

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Contents

UNDO-package *Implementation of UNDO (unsupervised deconvolution of tumor-stromal mixed expressions)*

Description

This package contains main function "two_source_deconv" to implement the deconvolution of mixed tumor-stromal expressions in a completely unsupervised way. The prior knowledge of mixing matrix or pure expression is not needed. The package detects marker genes and calculate the mixing matrix and pure expressions automatically.

Details

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two_source_deconv(ExpressionData,lowper=0.4,highper=0.1,epsilon1=0.01,epsilon2=0.01,A=NULL,S1=NULL,S2=N

Author(s)

Niya Wang <wangny@vt.edu>

Examples

```
data(NumericalMixMCF7HS27)
X <- NumericalMixMCF7HS27
deconvResult <- two_source_deconv(X, lowper = 0.4, highper = 0.1, epsilon1 = 0.1, epsilon2 = 0.1, A = NULL, S1=NU
```

BiologicalMixMCF7HS27 *MCF7 and HS27 biologically mixed*

Description

Expression data from MCF7 and HS27 biologically mixing

Usage

```
data(BiologicalMixMCF7HS27)
```

Format

The format is: Formal class 'ExpressionSet' [package "Biobase"] with 7 slots ..@ experimentData :Formal class 'MIAME' [package "Biobase"] with 13 slots .. .. ..@ name : chr "" .. .. ..@ lab : chr "" .. .. ..@ contact : chr "" .. .. ..@ title : chr "" .. .. ..@ abstract : chr "" .. .. ..@ url : chr "" .. .. ..@ pubMedIds : chr "" .. .. ..@ samples : list() .. .. ..@ hybridizations : list() .. .. ..@ normControls : list() .. .. ..@ preprocessing : list() .. .. ..@ other : list() .. .. ..@ .__classVersion__:Formal class 'Versions' [package "Biobase"] with 1 slots .. ..@ .Data:List of 2 .. ..$: int [1:3] 1 0 0 .. ..$: int [1:3] 1 1 0 ..@ assayData :<environment: 0x0000000008d92618> ..@ phenoData :Formal class 'AnnotatedDataFrame' [package "Biobase"] with 4 slots .. .. ..@ varMetadata :'data.frame': 0 obs. of 1 variable: .. ..$ labelDescription: chr(0) .. .. ..@ data :'data.frame': 2 obs. of 0 variables .. .. ..@ dimLabels : chr [1:2] "sampleNames" "sampleColumns" .. .. ..@ .__classVersion__:Formal class 'Versions' [package "Biobase"] with 1 slots .. ..@ .Data:List of 1 .. ..$: int [1:3] 1 1 0 ..@ featureData :Formal class 'AnnotatedDataFrame' [package "Biobase"] with 4 slots .. .. ..@ varMetadata :'data.frame': 0 obs. of 1 variable: .. ..$ labelDescription: chr(0) .. .. ..@ data :'data.frame': 22215 obs. of 0 variables .. .. ..@ dimLabels : chr [1:2] "featureNames" "featureColumns" .. .. ..@ .__classVersion__:Formal class 'Versions' [package "Biobase"] with 1 slots .. ..@ .Data:List of 1 .. ..$: int [1:3] 1 1 0 ..@ annotation : chr "HG-U133A" ..@ protocolData :Formal class 'AnnotatedDataFrame' [package "Biobase"] with 4 slots .. .. ..@ varMetadata :'data.frame': 0 obs. of 1 variable: .. ..$ labelDescription: chr(0) .. .. ..@ data :'data.frame': 2 obs. of 0 variables .. .. ..@ dimLabels : chr [1:2] "sampleNames" "sampleColumns" .. .. ..@ .__classVersion__:Formal class 'Versions' [package "Biobase"] with 1 slots .. ..@ .Data:List of 1 .. ..$: int [1:3] 1 1 0 ..@ .__classVersion__:Formal class 'Versions' [package "Biobase"] with 1 slots .. .. ..@ .Data:List of 4 .. ..$: int [1:3] 3 1 0 .. ..$: int [1:3] 2 23 6 .. ..$: int [1:3] 1 3 0 .. ..$: int [1:3] 1 0 0

Examples

```
data(BiologicalMixMCF7HS27)
str(BiologicalMixMCF7HS27)
```

---

calc_E1 *function calculating the E1 measurement*

Description

A function used to calculate the E1 measurement when the real mixing matrix is provided

Usage

```
calc_E1(A, Aest)
```

Arguments

A	real mixing matrix
Aest	estimated mixing matrix

Value

E1 measurement (numeric)

Author(s)

Niya Wang <wangny@vt.edu>

Examples

```
A <- matrix(runif(4),2,2)
Aest <- matrix(runif(4),2,2)
E1 <- calc_E1(A,Aest)  # to calculate the similarity of two randowm 2*2 matrix
```

`dimension_reduction` *Dimension reduction function*

Description

When the number of input samples is larger than 2, this function is called to reduce the dimension to 2 by using PCA.

Usage

```
dimension_reduction(X)
```

Arguments

`X`	gene expression data matrix

Value

`X`

`dimenMatrix`	the dimension reduction matrix used to recover the mixing matrix for all the samples

Author(s)

Niya Wang (wangny@vt.edu)

Examples

```
X <- matrix(runif(5000),1000,5)
dimenResult <- dimension_reduction(X)
```

gene_expression_input *Detect whether the input gene expression data are valid*

Description

Check the input gene expression data to see whether they are nonempty, nonnegative, etc.

Usage

```
gene_expression_input(X)
```

Arguments

X	gene expression data matrix with row representing genes/probe sets, and column representing samples.

Value

If the input is valid, the output will be the same as the input; otherwise, if the input contains NA, the corresponding rows will be deleted. if the input contains negative value, the algorithm will stop and give error information.

Author(s)

Niya Wang (wangny@vt.edu)

Examples

```
gene_expression <- matrix(runif(2000),1000,2)
valid_gene_expression <- gene_expression_input(gene_expression)
```

marker_gene_selection *Select marker genes in two sources*

Description

Select the marker genes in tumor and stroma in an unsupervised way

Usage

```
marker_gene_selection(X, lowper, highper, epsilon1, epsilon2)
```

Arguments

X	gene expression data
lowper	The percentage of genes the user wants to remove with lowest norm. The range should be between 0 and 1.
highper	The percentage of genes the user wants to remove with highest norm.The range should be between 0 and 1.
epsilon1	Influence the number of marker genes. With increasing of epsilon1, the number marker genes in source 1 will increase. The value should be positive.
epsilon2	Influence the number of marker genes. With increasing of epsilon1, the number marker genes in source 2 will increase. The value should be positive.

Value

a1	The slope of marker genes in source 1
a2	The slope of marker genes in source 2
MG1	The gene list of marker genes in source 1
MG2	The gene list of marker genes in source 2
dimenMatrix	dimension reduction matrix

Author(s)

Niya Wang (wangny@vt.edu)

Examples

```
X <- matrix(runif(20000),10000,2)
MG_set <- marker_gene_selection(X, 0.4, 0.1, 0.1, 0.1)
```

---

mixing_matrix_computation

Calculate and scale the mixing matrix

Description

Calculate the mixing matrix based on the output from marker_gene_selection(), and scale the mixing matrix to make the sum of proportions from tumor and stroma equal to 1. The pure expression levels of tumor and stroma are also computed.

Usage

```
mixing_matrix_computation(X, a1, a2, dimenMatrix)
```

Arguments

X	Gene expression data matrix
a1	The slope of marker genes in source 1
a2	The slope of marker genes in source 2
dimenMatrix	The dimention reduction matrix used to recover mixing matrix for all the samples

Value

Aest	estimated mixing matrix
Sest	estimated pure gene expression of two sources

Author(s)

Niya Wang (wangny@vt.edu)

Examples

```
a1<- matrix(runif(2),2,1)
a2<- matrix(runif(2),2,1)
X <- 1000*matrix(runif(20000),10000,2)
dimenMatrix <- NULL
Deconv <- mixing_matrix_computation(X, a1, a2, dimenMatrix)
```

NumericalMixingMatrix *mixing matrix of data NumericalMixMCF7HS27*

Description

real mixing matrix of data NumericalMixMCF7HS27

Usage

```
data(NumericalMixingMatrix)
```

Format

The format is: num [1:2, 1:2] 0.775 0.15 0.225 0.85 - attr(*, "dimnames")=List of 2 ..$: NULL ..$: chr [1:2] "V1" "V2"

Examples

```
data(NumericalMixingMatrix)
str(NumericalMixingMatrix)
```

NumericalMixMCF7HS27 *MCF7 and HS27 numerically mixed*

Description

Expression data from MCF7 and HS27 numerically mixing

Usage

```
data(NumericalMixMCF7HS27)
```

Format

The format is: Formal class 'ExpressionSet' [package "Biobase"] with 7 slots ..@ experimentData :Formal class 'MIAME' [package "Biobase"] with 13 slots .. .. ..@ name : chr "" .. .. ..@ lab : chr "" .. .. ..@ contact : chr "" .. .. ..@ title : chr "" .. .. ..@ abstract : chr "" .. .. ..@ url : chr "" .. .. ..@ pubMedIds : chr "" .. .. ..@ samples : list() .. .. ..@ hybridizations : list() .. .. ..@ normControls : list() .. .. ..@ preprocessing : list() .. .. ..@ other : list() .. .. ..@ .__classVersion__:Formal class 'Versions' [package "Biobase"] with 1 slots .. ..@ .Data:List of 2 .. ..$: int [1:3] 1 0 0 .. ..$: int [1:3] 1 1 0 ..@ assayData :<environment: 0x000000000e86a5d0> ..@ phenoData :Formal class 'AnnotatedDataFrame' [package "Biobase"] with 4 slots .. .. ..@ varMetadata :'data.frame': 0 obs. of 1 variable: .. ..$ labelDescription: chr(0) .. .. ..@ data :'data.frame': 2 obs. of 0 variables .. .. ..@ dimLabels : chr [1:2] "sampleNames" "sampleColumns" .. .. ..@ .__classVersion__:Formal class 'Versions' [package "Biobase"] with 1 slots .. ..@ .Data:List of 1 .. ..$: int [1:3] 1 1 0 ..@ featureData :Formal class 'AnnotatedDataFrame' [package "Biobase"] with 4 slots .. .. ..@ varMetadata :'data.frame': 0 obs. of 1 variable: .. ..$ labelDescription: chr(0) .. .. ..@ data :'data.frame': 22215 obs. of 0 variables .. .. ..@ dimLabels : chr [1:2] "featureNames" "featureColumns" .. .. ..@ .__classVersion__:Formal class 'Versions' [package "Biobase"] with 1 slots .. ..@ .Data:List of 1 .. ..$: int [1:3] 1 1 0 ..@ annotation : chr "HG-U133A" ..@ protocolData :Formal class 'AnnotatedDataFrame' [package "Biobase"] with 4 slots .. .. ..@ varMetadata :'data.frame': 0 obs. of 1 variable: .. ..$ labelDescription: chr(0) .. .. ..@ data :'data.frame': 2 obs. of 0 variables .. .. ..@ dimLabels : chr [1:2] "sampleNames" "sampleColumns" .. .. ..@ .__classVersion__:Formal class 'Versions' [package "Biobase"] with 1 slots .. ..@ .Data:List of 1 .. ..$: int [1:3] 1 1 0 ..@ .__classVersion__:Formal class 'Versions' [package "Biobase"] with 1 slots .. .. ..@ .Data:List of 4 .. ..$: int [1:3] 3 1 0 .. ..$: int [1:3] 2 23 6 .. ..$: int [1:3] 1 3 0 .. ..$: int [1:3] 1 0 0

Examples

```
data(NumericalMixMCF7HS27)
str(NumericalMixMCF7HS27)
```

PureMCF7HS27 *pure MCF7 and HS27*

Description

pure MCF7 and HS27 expression data

Usage

```
data(PureMCF7HS27)
```

Format

The format is: Formal class 'ExpressionSet' [package "Biobase"] with 7 slots ..@ experimentData :Formal class 'MIAME' [package "Biobase"] with 13 slots .. .. ..@ name : chr "" .. .. ..@ lab : chr "" .. .. ..@ contact : chr "" .. .. ..@ title : chr "" .. .. ..@ abstract : chr "" .. .. ..@ url : chr "" .. .. ..@ pubMedIds : chr "" .. .. ..@ samples : list() .. .. ..@ hybridizations : list() .. .. ..@ normControls : list() .. .. ..@ preprocessing : list() .. .. ..@ other : list() .. .. ..@ .__classVersion__:Formal class 'Versions' [package "Biobase"] with 1 slots .. ..@ .Data:List of 2 .. ..$: int [1:3] 1 0 0 .. ..$: int [1:3] 1 1 0 ..@ assayData :<environment: 0x000000000e979d20>

..@ phenoData :Formal class 'AnnotatedDataFrame' [package "Biobase"] with 4 slots .. .. ..@ varMetadata :'data.frame': 0 obs. of 1 variable: .. ..$ labelDescription: chr(0) .. .. ..@ data :'data.frame': 2 obs. of 0 variables .. .. ..@ dimLabels : chr [1:2] "sampleNames" "sampleColumns" .. .. ..@ .__classVersion__:Formal class 'Versions' [package "Biobase"] with 1 slots .. ..@ .Data:List of 1 .. ..$: int [1:3] 1 1 0 ..@ featureData :Formal class 'AnnotatedDataFrame' [package "Biobase"] with 4 slots .. .. ..@ varMetadata :'data.frame': 0 obs. of 1 variable: .. ..$ labelDescription: chr(0) .. .. ..@ data :'data.frame': 22215 obs. of 0 variables .. .. ..@ dimLabels : chr [1:2] "featureNames" "featureColumns" .. .. ..@ .__classVersion__:Formal class 'Versions' [package "Biobase"] with 1 slots .. ..@ .Data:List of 1 .. ..$: int [1:3] 1 1 0 ..@ annotation : chr "HG-U133A" ..@ protocolData :Formal class 'AnnotatedDataFrame' [package "Biobase"] with 4 slots .. .. ..@ varMetadata :'data.frame': 0 obs. of 1 variable: .. ..$ labelDescription: chr(0) .. .. ..@ data :'data.frame': 2 obs. of 0 variables .. .. ..@ dimLabels : chr [1:2] "sampleNames" "sampleColumns" .. .. ..@ .__classVersion__:Formal class 'Versions' [package "Biobase"] with 1 slots .. ..@ .Data:List of 1 .. ..$: int [1:3] 1 1 0 ..@ .__classVersion__:Formal class 'Versions' [package "Biobase"] with 1 slots .. .. ..@ .Data:List of 4 .. ..$: int [1:3] 3 1 0 .. ..$: int [1:3] 2 23 6 .. ..$: int [1:3] 1 3 0 .. ..$: int [1:3] 1 0 0

Examples

```
data(PureMCF7HS27)
str(PureMCF7HS27)
```

`two_source_deconv` *Main function to call other subfunction to deconvolute the mixed expression data.*

Description

This is the main function that is to call all the other subfunctions and realize the deconvolution of mixed expression data. When the real mixing matrix exist, it will also compare the estimated mixing matrix and real mixing matrix and give the E1 measurement.

Usage

```
two_source_deconv(ExpressionData, lowper = 0.4, highper = 0.1, epsilon1 = 0.01, epsilon2 = 0.01, A =
```

Arguments

`ExpressionData`	gene expression data matrix/ExpressionSet object
`lowper`	The percentage of genes the user wants to remove with lowest norm. The range should be between 0 and 1.
`highper`	The percentage of genes the user wants to remove with highest norm.The range should be between 0 and 1.
`epsilon1`	Influence the number of marker genes. With increasing of epsilon1, the number marker genes in source 1 will increase. The value should be positive.
`epsilon2`	Influence the number of marker genes. With increasing of epsilon1, the number marker genes in source 2 will increase. The value should be positive.
`A`	real mixing matrix if existing
`S1`	Pure expression profile of first source if existing
`S2`	Pure expression profile of second source if existing
`return`	if it is equal to 0, do not return estimated S; otherwise, return the estimated S.

Value

Aest	estimated mixing matrix
E1	E1 measurement between real and estimated mixing matrix

Author(s)

Niya Wang (wangny@vt.edu)

Examples

```
data(NumericalMixMCF7HS27)
X <- NumericalMixMCF7HS27
deconvResult <- two_source_deconv(X, lowper = 0.4, highper = 0.1, epsilon1 = 0.1, epsilon2 = 0.1, A = NULL, S1=NU
```

Index