

Package ‘M2SMF’

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Title Multi-Modal Similarity Matrix Factorization for Integrative
Multi-Omics Data Analysis

Version 1.0

Description A new method to implement clustering from multiple modality data of certain samples, the function M2SMF() jointly factorizes multiple similarity matrices into a shared sub-matrix and several modality private sub-matrices, which is further used for clustering. Along with this method, we also provide function to calculate the similarity matrix and function to evaluate the best cluster number from the original data.

Imports dplyr, MASS, stats

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License GPL (>= 2)

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Suggests knitr, rmarkdown

VignetteBuilder knitr

NeedsCompilation no

Author Xiaoyao Yin [aut, cre]

Maintainer Xiaoyao Yin <yinxy1992@sina.com>

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affinityMatrix	<i>To calculate the similarity matrix</i>
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Description

calculate the affinity matrix from the diff matrix with 20 neighbors

Usage

```
affinityMatrix(Diff, K = 20, sigma = 0.5)
```

Arguments

Diff	A diff matrix
K	The number of neighbors in consideration
sigma	A parameter to determine the scale

Value

W The similarity matrix

Author(s)

Xiaoyao Yin

Examples

```
data_list <- simu_data_gen()
Diff <- dist2eu(Standard_Normalization(data_list[[1]]),Standard_Normalization(data_list[[1]]))
simi <- affinityMatrix(Diff,20,0.5)
```

Cal_NMI	<i>calculate the normalized mutual information.</i>
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Description

calculate the normalized mutual information of two vectors x and y.

Usage

```
Cal_NMI(x, y)
```

Arguments

x	A vector
y	A vector as long as x

Value

A number between 0 and 1 indicating the normalized mutual information

Author(s)

Xiaoyao Yin

Examples

```
x <- c(0.1,0.2,0.3,0.4)
y <- c(0.1,0.2,0.3,0.4)
NMI <- Cal_NMI(x,y)
```

cost	<i>Calculate the cost</i>
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Description

A function to calculate the cost of the objective function

Usage

```
cost(new_WL_list, init_list, lambda)
```

Arguments

new_WL_list	A list of matrices factorized from the similarity matrices list WL
init_list	A list containing the updated result in this iteration
lambda	A parameter to set the relative weight of the group sparsity constraints

Value

A number indicating the total cost of the objective function

Author(s)

Xiaoyao Yin

Examples

```
WL <- simu_data_gen()
WL[[1]] <- affinityMatrix(dist2eu(Standard_Normalization(WL[[1]]),Standard_Normalization(WL[[1]])))
WL[[2]] <- affinityMatrix(dist2eu(Standard_Normalization(WL[[2]]),Standard_Normalization(WL[[2]])))
new_WL_list <- initialize_WL(WL)
k <- 5
lambda <- 0.25
init_list <- initialization(new_WL_list,k)
update_L_list <- update_L(new_WL_list,init_list)
update_alpha_list <- update_alpha(new_WL_list,update_L_list,lambda)
init_list <- update_alpha_list
new_loss <- cost(new_WL_list,init_list,lambda)
```

dist2bin

Calculate the agreement-based measurement

Description

Calculate the agreement-based measurement of two any pair-wise samples x_i and x_j for binary variables

Usage

```
dist2bin(X, C)
```

Arguments

X A sample-feature matrix with rows as samples and columns as features
C The same as X

Value

A matrix whose elements at (i,j) is the agreement-based measurement of two any pair-wise samples x_i and x_j

Author(s)

Xiaoyao Yin

Examples

```
data_list <- simu_data_gen()
X <- data_list[[1]]
C <- X
Diff <- dist2bin(X,C)
```

dist2chi	<i>Calculate the chi-squared distance</i>
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Description

Calculate the chi-squared distance of two any pair-wise samples x_i and x_j for discrete variables

Usage

```
dist2chi(X, C)
```

Arguments

X	A sample-feature matrix with rows as samples and columns as features
C	The same as X

Value

A matrix whose elements at (i,j) is the chi-squared distance of two any pair-wise samples x_i and x_j

Author(s)

Xiaoyao Yin

Examples

```
data_list <- simu_data_gen()
X <- data_list[[1]]
C <- X
Diff <- dist2chi(X,C)
```

dist2eu *Calculate the Euclidean distance*

Description

Calculate the Euclidean distance of two any pair-wise samples x_i and x_j for continuous variables

Usage

```
dist2eu(X, C)
```

Arguments

X A sample-feature matrix with rows as samples and columns as features
C The same as X

Value

A matrix whose elements at (i,j) is the Euclidean distance of two any pair-wise samples x_i and x_j

Author(s)

Xiaoyao Yin

Examples

```
data_list <- simu_data_gen()
X <- data_list[[1]]
C <- X
Diff <- dist2eu(X,C)
```

initialization *initialize the sub-matrix C_i into $\alpha * L_i$ by SVD*

Description

L_i takes the first k columns of matrix d in SVD, while α is the mean of all the u of SVD result in each modality

Usage

```
initialization(WL, k)
```

Arguments

WL A list of similarity matrices
k A parameter to specify the cluster number

Value

A list with N+2 elements, the former N as modality private sub-matrices, the Nth as the shared sub-matrix and the last one as 1

Author(s)

Xiaoyao Yin

Examples

```
WL <- simu_data_gen()
new_WL_list <- initialize_WL(WL)
k <- 5
init_list <- initialization(new_WL_list,k)
```

initialize_WL *Initialize from the simlairty matrix list*

Description

Factorize the each of the simlairty matrix S_i into $C_i * t(C_i)$ by SVD

Usage

```
initialize_WL(WL)
```

Arguments

WL A list of similarity matrices

Value

A list as long as WL with elements satisfying `res[[i]]`

Author(s)

Xiaoyao Yin

Examples

```
WL <- simu_data_gen()
new_WL_list <- initialize_WL(WL)
```

M2SMF

the main part for M2SMF and clustering result

Description

jointly factorize multiple matrices into a shared sub-matrix and multiple private sub-matrices

Usage

```
M2SMF(WL, lambda = 0.25, theta = 10-4, k)
```

Arguments

WL	A list of similarity matrices
lambda	A parameter to set the relative weight of the group sparsity constraints
theta	A parameter to determine the convergence
k	A parameter to specify the cluster number

Value

A list containing the clustering result

sub_matrices a list containing all the sub-matrices

cluster_res the clustering result which is as long as the number of samples

Author(s)

Xiaoyao Yin

Examples

```
WL <- simu_data_gen()  
res <- M2SMF(WL, 0.25, 10-4, 5)
```

new_modularity	<i>Calculate the modularity</i>
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Description

A function to calculate the modularity for weighted graph

Usage

```
new_modularity(init_list, WL)
```

Arguments

init_list	A list with N+2 elements, the former N as modality private sub-matrices, the Nth as the shared sub-matrix and the last one as the current loss
WL	A list of similarity matrices

Value

A single value indicating the modularity of current factorization and clustering

Author(s)

Xiaoyao Yin

Examples

```
WL <- simu_data_gen()
WL[[1]] <- affinityMatrix(dist2eu(Standard_Normalization(WL[[1]]),Standard_Normalization(WL[[1]])))
WL[[2]] <- affinityMatrix(dist2eu(Standard_Normalization(WL[[2]]),Standard_Normalization(WL[[2]])))
new_WL_list <- initialize_WL(WL)
init_list <- initialization(new_WL_list,5)
res <- M2SMF(WL,0.25,10^-4,5)
init_list <- res[[1]]
modularity <- new_modularity(init_list,WL)
```

simu_data_gen	<i>Generate simulated data</i>
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Description

A function to generate simulated data with two modularities and five clusters

Usage

```
simu_data_gen()
```

Value

A list with two elements, which are the sample-feature matrices from different modality

Author(s)

Xiaoyao Yin

Examples

```
data_list <- simu_data_gen()
```

Standard_Normalization

Normalize the input matrix by column

Description

Normalize each column of x to have mean 0 and standard deviation 1.

Usage

```
Standard_Normalization(x)
```

Arguments

x A sample-feature matrix with rows as samples and columns as features

Value

A sample-feature matrix with rows as samples and columns as features, each column of the matrix have mean 0 and standard deviation 1

Author(s)

Xiaoyao Yin

Examples

```
data_list <- simu_data_gen()
x <- data_list[[1]]
data_matrix <- Standard_Normalization(x)
```

update_alpha	<i>the function to update alpha</i>
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Description

update the sub-matrix alpha to convergence to its local minimum gradually

Usage

```
update_alpha(WL, update_L_list, lambda)
```

Arguments

WL	A list of similarity matrices
update_L_list	A list with N+2 elements, the former N as modality private sub-matrices, the Nth as the shared sub-matrix and the last one as the current loss
lambda	A parameter to set the relative weight of the group sparsity constraints

Value

A list containing the updated result in this iteration

Author(s)

Xiaoyao Yin

Examples

```
WL <- simu_data_gen()
WL[[1]] <- affinityMatrix(dist2eu(Standard_Normalization(WL[[1]]),Standard_Normalization(WL[[1]])))
WL[[2]] <- affinityMatrix(dist2eu(Standard_Normalization(WL[[2]]),Standard_Normalization(WL[[2]])))
new_WL_list <- initialize_WL(WL)
k <- 5
lambda <- 0.25
init_list <- initialization(new_WL_list,k)
update_L_list <- update_L(new_WL_list,init_list)
update_alpha_list <- update_alpha(WL,update_L_list,lambda)
```

update_L	<i>the function to update L_i, for $i=1,2,\dots,N$</i>
----------	--

Description

update the sub-matrix L_i , for $i=1,2,\dots,N$ to convergence to its local minimum gradually

Usage

```
update_L(WL, init_list)
```

Arguments

WL	A list of similarity matrices
init_list	A list with $N+2$ elements, the former N as modality private sub-matrices, the N th as the shared sub-matrix and the last one as 1

Value

A list containing the updated result in this iteration

Author(s)

Xiaoyao Yin

Examples

```
WL <- simu_data_gen()
WL[[1]] <- affinityMatrix(dist2eu(Standard_Normalization(WL[[1]]),Standard_Normalization(WL[[1]])))
WL[[2]] <- affinityMatrix(dist2eu(Standard_Normalization(WL[[2]]),Standard_Normalization(WL[[2]])))
new_WL_list <- initialize_WL(WL)
k <- 5
init_list <- initialization(new_WL_list,k)
update_L_list <- update_L(WL,init_list)
```

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