Package ‘M2SMF’

October 12, 2022

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

Version 2.0

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

Depends R (>= 3.4.0)

License GPL (>= 2)

Encoding UTF-8

LazyData true

RoxygenNote 7.0.0

Suggests knitr, rmarkdown

VignetteBuilder knitr

NeedsCompilation no

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Repository CRAN

Date/Publication 2019-11-17 05:10:02 UTC

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affinityMatrix

To calculate the similarity matrix

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  

*calculate the normalized mutual information.*

**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**

```r
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**  

*Calculate the cost*

**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
dist2bin

**Value**

A number indicating the total cost of the objective function

**Author(s)**

Xiaoyao Yin

**Examples**

```r
WL <- simu_data_gen()
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

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

---

**dist2chi**

*Calculate the chi-squared distance*

**Description**

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

**Usage**

```r
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**

```r
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**

\[
\text{dist2eu}(X, C)
\]

**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**

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

---

**initialization**

*initialize the sub-matrix \( C_i \) into \( \alpha \)\( \times \)Li by SVD*

**Description**

\( Li \) takes the first \( k \) columns of matrix \( d \) in SVD, while \( \alpha \) is the mean of all the \( u \) of SVD result in each modality.

**Usage**

\[
\text{initialization}(WL, k)
\]
**initialize_WL**

**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**

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

---

**Description**

Initialize from the similarity matrix list

Factorize the each of the similarity matrix $S_i$ into $C_i^tC_i$ 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**

```r
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**

```r
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**

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

Calculate the modularity

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()
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  Generate simulated data

Description

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

Usage

simu_data_gen()
Standard_Normalization

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

the function to update alpha

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)
The function to update $L_i$, for $i = 1, 2, ..., N$

**Description**

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

**Usage**

```r
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**

```r
cir <- simu_data_gen()
cir[[1]] <- affinityMatrix(dist2eu(Standard_Normalization(cir[[1]]), Standard_Normalization(cir[[1]])))
cir[[2]] <- affinityMatrix(dist2eu(Standard_Normalization(cir[[2]]), Standard_Normalization(cir[[2]])))
new_cir_list <- initialize_cir(cir)
k <- 5
init_list <- initialization(new_cir_list, k)
update_cir_list <- update_cir(cir, init_list)
```
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