

# Package ‘M2SMF’

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**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

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**License** GPL (>= 2)

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## R topics documented:

affinityMatrix . . . . .	2
Cal_NMI . . . . .	3
cost . . . . .	3
dist2bin . . . . .	4
dist2chi . . . . .	5
dist2eu . . . . .	6
initialization . . . . .	6

initialize_WL . . . . .	7
M2SMF . . . . .	8
new_modularity . . . . .	9
simu_data_gen . . . . .	9
Standard_Normalization . . . . .	10
update_alpha . . . . .	11
update_L . . . . .	12
<b>Index</b>	<b>13</b>

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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)
```

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CaI_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**

```
CaI_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 <- CaI_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  $\alpha$  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)
```

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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)
```



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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 <math>L_i</math>, for <math>i=1,2,\dots,N</math></i>
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---

**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)
```

# Index

affinityMatrix, [2](#)

Cal\_NMI, [3](#)

cost, [3](#)

dist2bin, [4](#)

dist2chi, [5](#)

dist2eu, [6](#)

initialization, [6](#)

initialize\_WL, [7](#)

M2SMF, [8](#)

new\_modularity, [9](#)

simu\_data\_gen, [9](#)

Standard\_Normalization, [10](#)

update\_alpha, [11](#)

update\_L, [12](#)