

# Package ‘omada’

December 20, 2024

**Type** Package

**Title** Machine learning tools for automated transcriptome clustering analysis

**Version** 1.9.0

**Description** Symptomatic heterogeneity in complex diseases reveals differences in molecular states that need to be investigated. However, selecting the numerous parameters of an exploratory clustering analysis in RNA profiling studies requires deep understanding of machine learning and extensive computational experimentation. Tools that assist with such decisions without prior field knowledge are nonexistent and further gene association analyses need to be performed independently. We have developed a suite of tools to automate these processes and make robust unsupervised clustering of transcriptomic data more accessible through automated machine learning based functions. The efficiency of each tool was tested with four datasets characterised by different expression signal strengths. Our toolkit’s decisions reflected the real number of stable partitions in datasets where the subgroups are discernible. Even in datasets with less clear biological distinctions, stable subgroups with different expression profiles and clinical associations were found.

**Depends** pdfCluster (>= 1.0-3), kernlab (>= 0.9-29), R (>= 4.2), fpc (>= 2.2-9), Rcpp (>= 1.0.7), diceR (>= 0.6.0), ggplot2 (>= 3.3.5), reshape (>= 0.8.8), genieclust (>= 1.1.3), clValid (>= 0.7), glmnet (>= 4.1.3), dplyr (>= 1.0.7), stats (>= 4.1.2), clValid (>= 0.7)

**Suggests** rmarkdown, knitr, testthat

**License** GPL-3

**Encoding** UTF-8

**RoxygenNote** 7.3.1

**VignetteBuilder** knitr

**biocViews** Software, Clustering, RNASeq, GeneExpression

**LazyData** true

**git\_url** <https://git.bioconductor.org/packages/omada>

**git\_branch** devel  
**git\_last\_commit** 5caa0b1  
**git\_last\_commit\_date** 2024-10-29  
**Repository** Bioconductor 3.21  
**Date/Publication** 2024-12-19  
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## Contents

clusteringMethodSelection . . . . .	3
clusterVoting . . . . .	4
feasibilityAnalysis . . . . .	4
feasibilityAnalysisDataBased . . . . .	5
featureSelection . . . . .	6
get_agreement_scores . . . . .	6
get_average_feature_k_stabilities . . . . .	7
get_average_stabilities_per_k . . . . .	8
get_average_stability . . . . .	8
get_cluster_memberships_k . . . . .	9
get_cluster_voting_k_votes . . . . .	9
get_cluster_voting_memberships . . . . .	10
get_cluster_voting_metric_votes . . . . .	10
get_cluster_voting_scores . . . . .	11
get_feature_selection_optimal_features . . . . .	11
get_feature_selection_optimal_number_of_features . . . . .	12
get_feature_selection_scores . . . . .	13
get_generated_dataset . . . . .	13
get_internal_metric_scores . . . . .	14
get_max_stability . . . . .	14
get_metric_votes_k . . . . .	15
get_optimal_features . . . . .	15
get_optimal_memberships . . . . .	16
get_optimal_number_of_features . . . . .	16
get_optimal_parameter_used . . . . .	17
get_optimal_stability_score . . . . .	17
get_partition_agreement_scores . . . . .	18
get_sample_memberships . . . . .	19
get_vote_frequencies_k . . . . .	19
omada . . . . .	20
optimalClustering . . . . .	20
partitionAgreement . . . . .	21
plot_average_stabilities . . . . .	22
plot_cluster_voting . . . . .	23
plot_feature_selection . . . . .	23

<i>clusteringMethodSelection</i>	3
plot_partition_agreement . . . . .	24
plot_vote_frequencies . . . . .	24
toy_genes . . . . .	25
toy_gene_memberships . . . . .	26
<b>Index</b>	<b>27</b>

---

clusteringMethodSelection  
*Method Selection through intra-method Consensus Partition Consistency*

---

### Description

Method Selection through intra-method Consensus Partition Consistency

### Usage

```
clusteringMethodSelection(data, method.upper.k = 5, number.of.comparisons = 3)
```

### Arguments

`data`            A dataframe, where columns are features and rows are data points

`method.upper.k` The number of clusters, k, up to which the average agreements will be calculated

`number.of.comparisons`  
                   The number of comparisons to average over per k

### Value

An object of class "methodSelection" containing a dataframe of partition agreement scores for a set of random parameters clustering runs across different methods and the corresponding plot

### Examples

```
clusteringMethodSelection(toy_genes, method.upper.k = 3,  
number.of.comparisons = 2)
```

---

clusterVoting	<i>Estimating number of clusters through internal exhaustive ensemble majority voting</i>
---------------	---

---

**Description**

Estimating number of clusters through internal exhaustive ensemble majority voting

**Usage**

```
clusterVoting(data, min.k, max.k, algorithm)
```

**Arguments**

data	A dataframe, where columns are features and rows are data points
min.k	Minimum number of clusters for which we calculate stabilities
max.k	Maximum number of clusters for which we calculate stabilities
algorithm	The clustering algorithm to use for the multiple clustering runs to be measured

**Value**

An object of class "clusterVoting" containing a matrix with metric scores for every k and internal index, cluster memberships for every k, a dataframe with the k votes for every index, k vote frequencies and the frequency barplot of the k votes

**Examples**

```
clusterVoting(toy_genes, 4,14,"sc")
```

---

feasibilityAnalysis	<i>Simulating dataset and calculate stabilities over different number of clusters</i>
---------------------	---

---

**Description**

Simulating dataset and calculate stabilities over different number of clusters

**Usage**

```
feasibilityAnalysis(classes = 3, samples = 320, features = 400)
```

**Arguments**

classes	The number of classes of samples to be reflected in the simulated dataset. Also determines the ks to be considered (classes-2, classes+2)
samples	The number of samples in the simulated dataset
features	The number of features in the simulated dataset

**Value**

An object of class "feasibilityAnalysis" containing the average stabilities for all number of clusters(k), the average (over all k) and maximum stabilities observed and the generated dataset

**Examples**

```
feasibilityAnalysis(classes = 2, samples = 20, features = 30)
```

---

```
feasibilityAnalysisDataBased
```

*Simulating dataset based on existing dataset's dimensions, mean and standard deviation*

---

**Description**

Simulating dataset based on existing dataset's dimensions, mean and standard deviation

**Usage**

```
feasibilityAnalysisDataBased(data, classes = 3)
```

**Arguments**

data	The dataset to base the simulation extracting the number of samples, features and numeric
classes	The number of classes of samples to be reflected in the simulated dataset. Also determines the ks to be considered (classes-2, classes+2)

**Value**

An object of class "feasibilityAnalysis" containing the average stabilities for all numbers of clusters(k), the average (over all k) and maximum stabilities observed and the generated dataset

**Examples**

```
feasibilityAnalysisDataBased(data = toy_genes, classes = 2)
```

---

featureSelection	<i>Predictor variable subsampling sets and bootstrapping stability set selection</i>
------------------	--

---

### Description

Predictor variable subsampling sets and bootstrapping stability set selection

### Usage

```
featureSelection(data, min.k = 2, max.k = 4, step = 5)
```

### Arguments

data	A dataframe, where columns are features and rows are data points
min.k	Minimum number of clusters for which we calculate stabilities
max.k	Maximum number of clusters for which we calculate stabilities
step	The number for additional features each feature set will contain

### Value

An object of class "featureSelection" containing the dataframe of average bootstrap stabilities, where rows represent feature sets and columns number of clusters, the corresponding line plot, the number and the names of the selected features

### Examples

```
featureSelection(toy_genes, min.k = 2, max.k = 4, step = 10)
```

---

get_agreement_scores	<i>Get a dataframe of partition agreement scores for a set of random parameters clustering runs across different methods</i>
----------------------	--

---

### Description

Get a dataframe of partition agreement scores for a set of random parameters clustering runs across different methods

### Usage

```
get_agreement_scores(object)
```

### Arguments

object	An object of class "partitionAgreement"
--------	---

**Value**

A dataframe of partition agreement scores for a set of random parameters clustering runs across different methods

**Examples**

```
pa.object <- partitionAgreement(toy_genes, algorithm.1 = "spectral",  
measure.1 = "rbfdot", algorithm.2 = "kmeans", measure.2 = "Lloyd",  
number.of.clusters = 3)  
get_agreement_scores(pa.object)
```

---

*get\_average\_feature\_k\_stabilities*

*Get a dataframe of average bootstrap stabilities*

---

**Description**

Get a dataframe of average bootstrap stabilities

**Usage**

```
get_average_feature_k_stabilities(object)
```

**Arguments**

object            An object of class "featureSelection"

**Value**

A dataframe of average bootstrap stabilities

**Examples**

```
fs.object <- featureSelection(toy_genes, min.k = 3, max.k = 4, step = 10)  
get_average_feature_k_stabilities(fs.object)
```

get\_average\_stabilities\_per\_k

*Get average stabilities for all numbers of clusters(k)*

---

**Description**

Get average stabilities for all numbers of clusters(k)

**Usage**

```
get_average_stabilities_per_k(object)
```

**Arguments**

object            An object of class "feasibilityAnalysis"

**Value**

Average stabilities for all numbers of clusters(k)

**Examples**

```
fa.object <- feasibilityAnalysis(classes = 2, samples = 10, features = 15)
average.sts.k <- get_average_stabilities_per_k(fa.object)
```

---

get\_average\_stability *Get the average stability(over all k)*

---

**Description**

Get the average stability(over all k)

**Usage**

```
get_average_stability(object)
```

**Arguments**

object            An object of class "feasibilityAnalysis"

**Value**

The average stability(over all k)

**Examples**

```
fa.object <- feasibilityAnalysis(classes = 2, samples = 10, features = 15)
average.st <- get_average_stability(fa.object)
```



---

`get_cluster_memberships_k`  
*Get cluster memberships for every k*

---

**Description**

Get cluster memberships for every k

**Usage**

```
get_cluster_memberships_k(object)
```

**Arguments**

object            An object of class "clusterVoting"

**Value**

Cluster memberships for every k

**Examples**

```
cv.object <- clusterVoting(toy_genes, 4,6,"sc")  
get_cluster_memberships_k(cv.object)
```

---

`get_cluster_voting_k_votes`  
*Get k vote frequencies*

---

**Description**

Get k vote frequencies

**Usage**

```
get_cluster_voting_k_votes(object)
```

**Arguments**

object            An object of class "clusterAnalysis"

**Value**

Matrix with k vote frequencies

**Examples**

```
oa.object <- omada(toy_genes, method.upper.k = 4)
get_cluster_voting_k_votes(oa.object)
```

---

```
get_cluster_voting_memberships
```

*Get cluster memberships for every k*

---

**Description**

Get cluster memberships for every k

**Usage**

```
get_cluster_voting_memberships(object)
```

**Arguments**

object            An object of class "clusterAnalysis"

**Value**

Cluster memberships for every k

**Examples**

```
oa.object <- omada(toy_genes, method.upper.k = 4)
get_cluster_voting_memberships(oa.object)
```

---

```
get_cluster_voting_metric_votes
```

*Get a dataframe with the k votes for every index*

---

**Description**

Get a dataframe with the k votes for every index

**Usage**

```
get_cluster_voting_metric_votes(object)
```

**Arguments**

object            An object of class "clusterAnalysis"

**Value**

Dataframe with the k votes for every index

**Examples**

```
oa.object <- omada(toy_genes, method.upper.k = 4)
get_cluster_voting_metric_votes(oa.object)
```

---

`get_cluster_voting_scores`

*Get a matrix with metric scores for every k and internal index*

---

**Description**

Get a matrix with metric scores for every k and internal index

**Usage**

```
get_cluster_voting_scores(object)
```

**Arguments**

object            An object of class "clusterAnalysis"

**Value**

A matrix with metric scores for every k and internal index

**Examples**

```
oa.object <- omada(toy_genes, method.upper.k = 4)
get_cluster_voting_scores(oa.object)
```

---

`get_feature_selection_optimal_features`

*Get the optimal features*

---

**Description**

Get the optimal features

**Usage**

```
get_feature_selection_optimal_features(object)
```

**Arguments**

object            An object of class "clusterAnalysis"

**Value**

The list of optimal features

**Examples**

```
oa.object <- omada(toy_genes, method.upper.k = 4)
get_feature_selection_optimal_features(oa.object)
```

---

`get_feature_selection_optimal_number_of_features`  
*Get the optimal number of features*

---

**Description**

Get the optimal number of features

**Usage**

```
get_feature_selection_optimal_number_of_features(object)
```

**Arguments**

object            An object of class "clusterAnalysis"

**Value**

The optimal number of features

**Examples**

```
oa.object <- omada(toy_genes, method.upper.k = 6)
get_feature_selection_optimal_number_of_features(oa.object)
```

---

`get_feature_selection_scores`*Get a dataframe of average bootstrap stabilities*

---

**Description**

Get a dataframe of average bootstrap stabilities

**Usage**

```
get_feature_selection_scores(object)
```

**Arguments**

object            An object of class "clusterAnalysis"

**Value**

A dataframe of average bootstrap stabilities

**Examples**

```
oa.object <- omada(toy_genes, method.upper.k = 6)
get_feature_selection_scores(oa.object)
```

---

`get_generated_dataset` *Get the simulated dataset*

---

**Description**

Get the simulated dataset

**Usage**

```
get_generated_dataset(object)
```

**Arguments**

object            An object of class "feasibilityAnalysis"

**Value**

Simulated dataset

**Examples**

```
fa.object <- feasibilityAnalysis(classes = 4, samples = 50, features = 15)
generated.ds <- get_generated_dataset(fa.object)
```

---

`get_internal_metric_scores`*Get a matrix with metric scores for every k and internal index*

---

**Description**

Get a matrix with metric scores for every k and internal index

**Usage**

```
get_internal_metric_scores(object)
```

**Arguments**

`object` An object of class "clusterVoting"

**Value**

A matrix with metric scores for every k and internal index

**Examples**

```
cv.object <- clusterVoting(toy_genes, 4,6,"sc")
get_internal_metric_scores(cv.object)
```

---

`get_max_stability`*Get the maximum stability*

---

**Description**

Get the maximum stability

**Usage**

```
get_max_stability(object)
```

**Arguments**

`object` An object of class "feasibilityAnalysis"

**Value**

The maximum stability

**Examples**

```
fa.object <- feasibilityAnalysis(classes = 2, samples = 10, features = 15)
maximum.st <- get_max_stability(fa.object)
```

---

get\_metric\_votes\_k     *Get a dataframe with the k votes for every index*

---

**Description**

Get a dataframe with the k votes for every index

**Usage**

```
get_metric_votes_k(object)
```

**Arguments**

object             An object of class "clusterVoting"

**Value**

Dataframe with the k votes for every index

**Examples**

```
cv.object <- clusterVoting(toy_genes, 4,6,"sc")
get_metric_votes_k(cv.object)
```

---

get\_optimal\_features     *Get the optimal features*

---

**Description**

Get the optimal features

**Usage**

```
get_optimal_features(object)
```

**Arguments**

object             An object of class "featureSelection"

**Value**

The list of optimal features

**Examples**

```
fs.object <- featureSelection(toy_genes, min.k = 3, max.k = 6, step = 10)
get_optimal_features(fs.object)
```

get\_optimal\_memberships

*Get a dataframe with the memberships of the samples found in the input data*

---

### **Description**

Get a dataframe with the memberships of the samples found in the input data

### **Usage**

```
get_optimal_memberships(object)
```

### **Arguments**

object            An object of class "optimalClustering"

### **Value**

A dataframe with the memberships of the samples found in the input data

### **Examples**

```
oc.object <- optimalClustering(toy_genes, 4, "spectral")
get_optimal_memberships(oc.object)
```

---

get\_optimal\_number\_of\_features

*Get the optimal number of features*

---

### **Description**

Get the optimal number of features

### **Usage**

```
get_optimal_number_of_features(object)
```

### **Arguments**

object            An object of class "featureSelection"

### **Value**

The optimal number of features



**Examples**

```
fs.object <- featureSelection(toy_genes, min.k = 3, max.k = 6, step = 10)
get_optimal_number_of_features(fs.object)
```

---

`get_optimal_parameter_used`  
*Get the optimal parameter used*

---

**Description**

Get the optimal parameter used

**Usage**

```
get_optimal_parameter_used(object)
```

**Arguments**

object            An object of class "optimalClustering"

**Value**

The optimal parameter used

**Examples**

```
oc.object <- optimalClustering(toy_genes, 4, "spectral")
get_optimal_parameter_used(oc.object)
```

---

`get_optimal_stability_score`  
*Get the optimal stability score*

---

**Description**

Get the optimal stability score

**Usage**

```
get_optimal_stability_score(object)
```

**Arguments**

object            An object of class "optimalClustering"

**Value**

The optimal stability score

**Examples**

```
oc.object <- optimalClustering(toy_genes, 4, "spectral")
get_optimal_stability_score(oc.object)
```

---

```
get_partition_agreement_scores
```

*Get a dataframe of partition agreement scores for a set of random parameters clustering runs across different methods*

---

**Description**

Get a dataframe of partition agreement scores for a set of random parameters clustering runs across different methods

Get a dataframe of partition agreement scores

**Usage**

```
get_partition_agreement_scores(object)
```

```
get_partition_agreement_scores(object)
```

**Arguments**

object            An object of class "clusterAnalysis"

**Value**

A dataframe of partition agreement scores for a set of random parameters clustering runs across different methods

A dataframe of partition agreement scores parameters clustering runs across different methods

**Examples**

```
ms.object <- clusteringMethodSelection(toy_genes, method.upper.k = 3,
number.of.comparisons = 2)
get_partition_agreement_scores(ms.object)
oa.object <- omada(toy_genes, method.upper.k = 4)
get_partition_agreement_scores(oa.object)
```

---

`get_sample_memberships`

*Get a dataframe with the memberships of the samples found in the input data*

---

**Description**

Get a dataframe with the memberships of the samples found in the input data

**Usage**

```
get_sample_memberships(object)
```

**Arguments**

`object`            An object of class "clusterAnalysis"

**Value**

A dataframe with the memberships of the samples found in the input data

**Examples**

```
oa.object <- omada(toy_genes, method.upper.k = 4)
get_sample_memberships(oa.object)
```

---

`get_vote_frequencies_k`

*Get k vote frequencies*

---

**Description**

Get k vote frequencies

**Usage**

```
get_vote_frequencies_k(object)
```

**Arguments**

`object`            An object of class "clusterVoting"

**Value**

Matrix with k vote frequencies

**Examples**

```
cv.object <- clusterVoting(toy_genes, 4,6,"sc")
get_vote_frequencies_k(cv.object)
```

---

omada	<i>A wrapper function that utilizes all tools to produce the optimal sample memberships</i>
-------	---

---

**Description**

A wrapper function that utilizes all tools to produce the optimal sample memberships

**Usage**

```
omada(data, method.upper.k = 5)
```

**Arguments**

data                    A dataframe, where columns are features and rows are data points  
method.upper.k        The upper limit of clusters, k, to be considered. Must be more than 2

**Value**

An object of class "clusterAnalysis" containing partition.agreement.scores,partition.agreement.plot,feature.selection.scores, feature.selection.plot, feature.selection.optimal.features, feature.selection.optimal.number.of.features, cluster.voting.scores, cluster.voting.cluster.memberships,cluster.voting.metric.votes,

**Examples**

```
omada(toy_genes, method.upper.k = 3)
```

---

optimalClustering	<i>Clustering with the optimal parameters estimated by these tools</i>
-------------------	--

---

**Description**

Clustering with the optimal parameters estimated by these tools

**Usage**

```
optimalClustering(data, clusters, algorithm)
```

**Arguments**

data                    A dataframe, where columns are features and rows are data points  
clusters                Number of clusters to be generated by this clustering  
algorithm                The clustering algorithm to be used

**Value**

An object of class "optimalClustering" containing a dataframe with the memberships of the samples found in the input data, the optimal stability score and parameter used

**Examples**

```
optimalClustering(toy_genes, 2, "kmeans")
```

---

partitionAgreement	<i>Partition Agreement calculation between two clustering runs</i>
--------------------	--

---

**Description**

Calculate the agreement (0,1) between two partitioning generated by two clustering runs using the adjust Rand Index. We can use three clustering algorithms (spectral, kmeans and hierarchical) along with the following parameters for each:

**Usage**

```
partitionAgreement(
  data,
  algorithm.1 = "hierarchical",
  measure.1 = "canberra",
  hier.agglo.algorithm.1 = "average",
  algorithm.2 = "hierarchical",
  measure.2 = "manhattan",
  hier.agglo.algorithm.2 = "average",
  number.of.clusters = 5
)
```

**Arguments**

data	A dataframe, where columns are features and rows are data points
algorithm.1	Second algorithm to be used (spectral/kmeans/hierarchical)
measure.1	Concerns the first algorithm to be used and represents a kernel for Spectral/kmeans or a distance measure for hierarchical clustering
hier.agglo.algorithm.1	Concerns the first algorithm to be used and represents the agglomerative method for hierarchical clustering (not used in spectral/kmeans clustering)
algorithm.2	First algorithm to be used (spectral/kmeans/hierarchical)
measure.2	Concerns the second algorithm to be used and represents a kernel for Spectral/kmeans or a distance measure for hierarchical clustering
hier.agglo.algorithm.2	Concerns the second algorithm to be used and represents the agglomerative method for hierarchical clustering (not used in spectral/kmeans clustering)

number.of.clusters

The upper limit of clusters to form starting from 2

### Details

Spectral kernels: rbfdot, polydot, vanilladot, tanhdot, laplacedot, besseldot, anovadot, splinedot

K-means kernels: "Hartigan-Wong", Lloyd, Forgy, MacQueen

Hierarchical Agglomeration methods: average, ward.D, ward.D2, single, complete, mcquitty, median, centroid

Distance measures: euclidean, manhattan, canberra, minkowski, maximum

### Value

An object of class "partitionAgreement" containing agreements (Rand Indexes) from 1 cluster (ARI=0) up to the number of clusters requested

### Examples

```
partitionAgreement(toy_genes, algorithm.1 = "hierarchical",
  measure.1 = "canberra", hier.agglo.algorithm.1 = "average",
  algorithm.2 = "hierarchical", measure.2 = "manhattan",
  hier.agglo.algorithm.2 = "average", number.of.clusters = 3)
```

```
partitionAgreement(toy_genes, algorithm.1 = "spectral", measure.1 = "rbfdot",
  algorithm.2 = "kmeans", measure.2 = "Lloyd", number.of.clusters = 5)
```

---

plot\_average\_stabilities

*Plot the average bootstrap stabilities*

---

### Description

Plot the average bootstrap stabilities

### Usage

```
plot_average_stabilities(object)
```

### Arguments

object            An object of class "featureSelection"

### Value

Line plot of average bootstrap stabilities

### Examples

```
fs.object <- featureSelection(toy_genes, min.k = 3, max.k = 6, step = 10)
plot_average_stabilities(fs.object)
```

---

plot\_cluster\_voting    *Plot k vote frequencies*

---

**Description**

Plot k vote frequencies

**Usage**

```
plot_cluster_voting(object)
```

**Arguments**

object            An object of class "clusterAnalysis"

**Value**

Plot k vote frequencies

**Examples**

```
oa.object <- omada(toy_genes, method.upper.k = 3)
plot_cluster_voting(oa.object)
```

---

plot\_feature\_selection            *Plot the average bootstrap stabilities*

---

**Description**

Plot the average bootstrap stabilities

**Usage**

```
plot_feature_selection(object)
```

**Arguments**

object            An object of class "clusterAnalysis"

**Value**

Line plot of average bootstrap stabilities

**Examples**

```
oa.object <- omada(toy_genes, method.upper.k = 4)
plot_feature_selection(oa.object)
```

plot\_partition\_agreement  
*Plot of partition agreement scores*

---

**Description**

Plot of partition agreement scores  
Plot of partition agreement scores

**Usage**

```
plot_partition_agreement(object)  
  
plot_partition_agreement(object)
```

**Arguments**

object            An object of class "clusterAnalysis"

**Value**

Plot of partition agreement scores  
Plot of partition agreement scores

**Examples**

```
ms.object <- clusteringMethodSelection(toy_genes, method.upper.k = 3,  
number.of.comparisons = 2)  
plot_partition_agreement(ms.object)  
oa.object <- omada(toy_genes, method.upper.k = 4)  
plot_partition_agreement(oa.object)
```

---

plot\_vote\_frequencies *Plot k vote frequencies*

---

**Description**

Plot k vote frequencies

**Usage**

```
plot_vote_frequencies(object)
```

**Arguments**

object            An object of class "clusterVoting"



**Value**

Plot k vote frequencies

**Examples**

```
cv.object <- clusterVoting(toy_genes, 4,6,"sc")
plot_vote_frequencies(cv.object)
```

---

toy\_genes

*Toy gene data for package examples*

---

**Description**

Columns are genes and rows are samples

**Usage**

```
data(toy_genes)
```

**Format**

An object of class "cross"; see [qtl::read.cross()].

**Source**

nope

**References**

nothing

**Examples**

```
data(toy_genes)
```

---

toy\_gene\_memberships *Cluster memberships for toy gene data for package examples*

---

**Description**

Column "id" represents genes and column "memberships" represents their respective clusters. Rows are samples

**Usage**

```
data(toy_gene_memberships)
```

**Format**

An object of class "cross"; see [qtl::read.cross()].

**Source**

nope

**References**

nothing

**Examples**

```
data(toy_gene_memberships)
```

# Index

## \* datasets

toy\_gene\_memberships, 26  
toy\_genes, 25

clusteringMethodSelection, 3  
clusterVoting, 4

feasibilityAnalysis, 4  
feasibilityAnalysisDataBased, 5  
featureSelection, 6

get\_agreement\_scores, 6  
get\_average\_feature\_k\_stabilities, 7  
get\_average\_stabilities\_per\_k, 8  
get\_average\_stability, 8  
get\_cluster\_memberships\_k, 9  
get\_cluster\_voting\_k\_votes, 9  
get\_cluster\_voting\_memberships, 10  
get\_cluster\_voting\_metric\_votes, 10  
get\_cluster\_voting\_scores, 11  
get\_feature\_selection\_optimal\_features,  
11  
get\_feature\_selection\_optimal\_number\_of\_features,  
12  
get\_feature\_selection\_scores, 13  
get\_generated\_dataset, 13  
get\_internal\_metric\_scores, 14  
get\_max\_stability, 14  
get\_metric\_votes\_k, 15  
get\_optimal\_features, 15  
get\_optimal\_memberships, 16  
get\_optimal\_number\_of\_features, 16  
get\_optimal\_parameter\_used, 17  
get\_optimal\_stability\_score, 17  
get\_partition\_agreement\_scores, 18  
get\_sample\_memberships, 19  
get\_vote\_frequencies\_k, 19

omada, 20  
optimalClustering, 20

partitionAgreement, 21  
plot\_average\_stabilities, 22  
plot\_cluster\_voting, 23  
plot\_feature\_selection, 23  
plot\_partition\_agreement, 24  
plot\_vote\_frequencies, 24

toy\_gene\_memberships, 26  
toy\_genes, 25