

Package ‘optimalFlow’

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costWasserMatchingEllipse
costWasserMatchinEllipse

Description

Calculates a similarity distance based on the 2-Wassertein distance between mixtures of multivariate normal distributions.

Usage

```
costWasserMatchingEllipse(  
  test.cytometry,  
  training.cytometries,  
  equal.weights = FALSE  
)
```

Arguments

`test.cytometry` A clusering represented as a list of clusters. Each cluster is a list with elements mean, cov, weight and type.

`training.cytometries`
A list of clusterings with the same format as `test.cytometry`.

`equal.weights` If True, weights assigned to every cluster in a partion are uniform (1/number of clusters) when calculating the similarity distance. If False, weights assigned to clusters are the proportions of points in every cluster compared to the total amount of points in the partition.

Value

A vector representing the similarity distance between `test.cytometry` and the elements in `training.cytometries`.

References

E del Barrio, H Inouzhe, JM Loubes, C Matran and A Mayo-Iscar. (2019) optimalFlow: Optimal-transport approach to flow cytometry gating and population matching. arXiv:1907.08006

Examples

```
partition1 <- list(list(mean = c(1, 1), cov = diag(1, 2), weight = 0.5, type = '1'),
                  list(mean = c(-1, -1), cov = diag(1, 2), weight = 0.5, type = '2'))
partition2 <- list(list(list(mean = c(1, -1), cov = diag(1, 2),
                             weight = 0.5, type = '1'), list(mean = c(-1, 1), cov = diag(1, 2), weight = 0.5, type = '2')))
costWasserMatchingEllipse(partition1, partition2)
```

cytoPlot

cytoPlot

Description

A plot wrapper for cytometries as a mixture of multivariate normals as used in `optimalFlowTemplates`.

Usage

```
cytoPlot(
  cytometry.as.mixture,
  dimensions = c(1, 2),
  xlim = NULL,
  ylim = NULL,
  xlab = NULL,
  ylab = NULL
)
```

Arguments

<code>cytometry.as.mixture</code>	A list, where each element contains the parameters of a component of the mixture as a list with entries: mean, cov, weight and type.
<code>dimensions</code>	A vector containing the two variables on which to perform the projection.
<code>xlim</code>	the x limits (<code>x1</code> , <code>x2</code>) of the plot. Note that <code>x1 > x2</code> is allowed and leads to a 'reversed axis'. The default value, <code>NULL</code> , indicates that the range of the finite values to be plotted should be used.
<code>ylim</code>	the y limits of the plot.
<code>xlab</code>	a label for the x axis, defaults to a description of x.
<code>ylab</code>	a label for the y axis, defaults to a description of y.

Value

A two dimensional plot of ellipses containing the 95

Examples

```

database <- buildDatabase(
  dataset_names = paste0('Cytometry', c(2:5, 7:9, 12:17, 19, 21)),
  population_ids = c('Monocytes', 'CD4+CD8-', 'Mature SIg Kappa', 'TCRgd-'))
templates.optimalFlow <-
  optimalFlowTemplates(
    database = database, templates.number = 5, cl.paral = 1
  )
cytoPlot(templates.optimalFlow$templates[[3]], dimensions = c(4, 3), xlim = c(0, 8000), ylim = c(0, 8000), xlab

```

 cytoPlot3d

cytoPlot3d

Description

A `rgl::plot3d` wrapper for cytometries as a mixture of multivariate normals as used in `optimalFlowTemplates`.

Usage

```

cytoPlot3d(
  cytometry.as.mixture,
  dimensions = c(1, 2),
  xlim = NULL,
  ylim = NULL,
  zlim = NULL,
  xlab = NULL,
  ylab = NULL,
  zlab = NULL
)

```

Arguments

<code>cytometry.as.mixture</code>	A list, where each element contains the parameters of a component of the mixture as a list with entries: mean, cov, weight and type.
<code>dimensions</code>	A vector containing the three variables on which to perform the projection.
<code>xlim</code>	the x limits (<code>x1</code> , <code>x2</code>) of the plot. Note that <code>x1 > x2</code> is allowed and leads to a 'reversed axis'. The default value, <code>NULL</code> , indicates that the range of the finite values to be plotted should be used.
<code>ylim</code>	the y limits of the plot.
<code>zlim</code>	the z limits of the plot.
<code>xlab</code>	a label for the x axis, defaults to a description of x.
<code>ylab</code>	a label for the y axis, defaults to a description of y.
<code>zlab</code>	a label for the z axis, defaults to a description of z.

Value

A three dimensional plot of ellipsoids containing the 95

Examples

```

database <- buildDatabase(
  dataset_names = paste0('Cytometry', c(2:5, 7:9, 12:17, 19, 21)),
  population_ids = c('Monocytes', 'CD4+CD8-', 'Mature SIg Kappa', 'TCRgd-'))
templates.optimalFlow <-
  optimalFlowTemplates(
    database = database, templates.number = 5, cl.paral = 1
  )
# # To execute requires an actual monitor since it uses rgl.
# cytoPlot3d(templates.optimalFlow$templates[[3]], dimensions = c(4, 3, 9), xlim = c(0, 8000), ylim = c(0, 8000)

```

cytoPlotDatabase	<i>cytoPlotDatabase</i>
------------------	-------------------------

Description

A plot wrapper for a database (list) of cytometries as a mixture of multivariate normals as used in `optimalFlowTemplates`.

Usage

```

cytoPlotDatabase(
  database.cytometries.as.mixtures,
  dimensions = c(1, 2),
  xlim = c(0, 8000),
  ylim = c(0, 8000),
  xlab = "",
  ylab = "",
  colour = TRUE
)

```

Arguments

<code>database.cytometries.as.mixtures</code>	A list where each component is a mixture distribution. That is, each component is a list, where each element contains the parameters of a component of the mixture as a list with entries: mean, cov, weight and type.
<code>dimensions</code>	A vector containing the two variables on which to perform the projection.
<code>xlim</code>	the x limits (<code>x1</code> , <code>x2</code>) of the plot. Note that <code>x1 > x2</code> is allowed and leads to a 'reversed axis'. The default value, <code>NULL</code> , indicates that the range of the finite values to be plotted should be used.
<code>ylim</code>	the y limits of the plot.
<code>xlab</code>	a label for the x axis, defaults to a description of x.
<code>ylab</code>	a label for the y axis, defaults to a description of y.
<code>colour</code>	If <code>TRUE</code> plots elements of a mixture distribution in different colours. If <code>FALSE</code> plots them in black.

Value

A two dimensional plot of ellipses containing the 95

Examples

```

database <- buildDatabase(
  dataset_names = paste0('Cytometry', c(2:5, 7:9, 12:17, 19, 21)),
  population_ids = c('Monocytes', 'CD4+CD8-', 'Mature SIg Kappa', 'TCRgd-'))
templates.optimalFlow <-
  optimalFlowTemplates(
    database = database, templates.number = 5, cl.paral = 1
  )
cytoPlotDatabase(templates.optimalFlow$database.elliptical[which(templates.optimalFlow$clustering == 3)], d

```

cytoPlotDatabase3d *cytoPlotDatabase3d*

Description

A plot3d wrapper for a database (list) of cytometries as a mixture of multivariate normals as used in optimalFlowTemplates.

Usage

```

cytoPlotDatabase3d(
  database.cytometries.as.mixtures,
  dimensions = c(1, 2, 3),
  xlim = c(0, 8000),
  ylim = c(0, 8000),
  zlim = c(0, 8000),
  xlab = "",
  ylab = "",
  zlab = "",
  colour = TRUE
)

```

Arguments

database.cytometries.as.mixtures	A list where each component is a mixture distribution. That is, each component is a list, where each element contains the parameters of a component of the mixture as a list with entries: mean, cov, weight and type.
dimensions	A vector containing the two variables on which to perform the projection.
xlim	the x limits (x1, x2) of the plot. Note that x1 > x2 is allowed and leads to a 'reversed axis'. The default value, NULL, indicates that the range of the finite values to be plotted should be used.
ylim	the y limits of the plot.
zlim	the z limits of the plot.
xlab	a label for the x axis, defaults to a description of x.
ylab	a label for the y axis, defaults to a description of y.
zlab	a label for the z axis, defaults to a description of z.
colour	If TRUE plots elements of a mixture distribution in different colours. If FALSE plots them in black.

Value

A three dimensional plot of ellipsoids containing the 95

Examples

```
database <- buildDatabase(
  dataset_names = paste0('Cytometry', c(2:5, 7:9, 12:17, 19, 21)),
  population_ids = c('Monocytes', 'CD4+CD8-', 'Mature SIg Kappa', 'TCRgd-'))
templates.optimalFlow <-
  optimalFlowTemplates(
    database = database, templates.number = 5, cl.paral = 1
  )
# # To execute requires an actual monitor since it uses rgl.
# cytoPlotDatabase3d(templates.optimalFlow$database.elliptical[which(templates.optimalFlow$clustering == 3)])
```

estimationCellBarycenter

estimationCellBarycenter

Description

Estimates a Wasserstein barycenter for a cluster type using a collection of partitions.

Usage

```
estimationCellBarycenter(cell, cytometries)
```

Arguments

cell Name of the cluster of interest.
cytometries List of clusterings.

Value

A list representing the (1-)barycenter:

mean Mean of the barycenter.

cov Covariance of the barycenter.

weight Weight associated to the barycenter.

type Type of the cluster.

Examples

```
partition1 <- list(list(mean = c(1, 1), cov = diag(1, 2), weight = 0.5, type = '1'),
  list(mean = c(-1, -1), cov = diag(1, 2), weight = 0.5, type = '2'))
partition2 <- list(list(mean = c(1, -1), cov = diag(1, 2), weight = 0.5, type = '1'),
  list(mean = c(-1, 1), cov = diag(1, 2), weight = 0.5, type = '2'))
cytometries <- list(partition1, partition2)
estimationCellBarycenter('1', cytometries)
```

estimCovCellGeneral	<i>estimCovCellGeneral</i>
---------------------	----------------------------

Description

Estimation of mean and covariance for a label in a partition.

Usage

```
estimCovCellGeneral(cell, cytometry, labels, type = "standard", alpha = 0.85)
```

Arguments

cell	Label of the cluster of interest.
cytometry	Data of the partition, without labels.
labels	Labels of the partition.
type	How to estimate covariance matrices of a cluster. 'standard' is for using cov(), while 'robust' is for using robustbase::covMcd.
alpha	Only when type = 'robust'. Indicates the value of alpha in robustbase::covMcd.

Value

A list containing:

mean Mean of the cluster.
cov Covariance of the cluster.
weight Weight associated to the cluster.
type Type of the cluster.

Examples

```
estimCovCellGeneral('Basophils', Cytometry1[,1:10], Cytometry1[,11])
```

f1Score	<i>f1Score</i>
---------	----------------

Description

Calculates the F1 score for each group in a partition.

Usage

```
f1Score(clustering, cytometry, noise.cells)
```

Arguments

clustering	The labels of the new classification.
cytometry	Data of the clustering, where the last variable contains the original labels.
noise.cells	An array of labels to be considered as noise.

Value

A matrix where the first row is the F1 score, the second row is the Precision and the third row is the Recall.

References

E del Barrio, H Inouzhe, JM Loubes, C Matran and A Mayo-Iscar. (2019) optimalFlow: Optimal-transport approach to flow cytometry gating and population matching. arXiv:1907.08006

Examples

```
f1Score(dplyr::pull(Cytometry3[c(sample(1:250,250),251:(dim(Cytometry3)[1])),],11),
  Cytometry3, noise.types)
```

f1ScoreVoting	<i>f1ScoreVoting</i>
---------------	----------------------

Description

Calculates the F1 score fore each group in a partition, when provided with a fuzzy classification.

Usage

```
f1ScoreVoting(voting, clustering, cytometry, nivel_sup, noise.cells)
```

Arguments

voting	A list where each entry is a vote on the respective label.
clustering	Labels of the partition.
cytometry	Data of the clustering, where the last variable contains the original labels.
nivel_sup	level of tolerance for assigning a hard clustering. Should be greater or equal than 1. Class A is assigned if class A > nivel_sup * Class B.
noise.cells	An array of labels to be considered as noise.

Value

A matrix where the first row is the F1 score, the second row is the Precision and the third row is the Recall.

Examples

```

## We construct a simple database selecting only some of the Cytometries and some cell types for simplicity and
database <- buildDatabase(
  dataset_names = paste0('Cytometry', c(2:5, 7:9, 12:17, 19, 21)),
  population_ids = c('Monocytes', 'CD4+CD8-', 'Mature SIg Kappa', 'TCRgd-'))

templates.optimalFlow <- optimalFlowTemplates(database = database, templates.number = 5,
cl.paral = 1)

classification.optimalFlow <- optimalFlowClassification(as.data.frame(Cytometry1)[
  which(match(Cytometry1$`Population ID (name)`, c('Monocytes', 'CD4+CD8-',
    'Mature SIg Kappa', 'TCRgd-'), nomatch = 0) > 0), 1:10], database, templates.number = 5,
  cl.paral = 1,
  classif.method = 'matching', cost.function = 'ellipses', cl.paral = 1)

f1ScoreVoting(classification.optimalFlow$cluster.vote, classification.optimalFlow$cluster,
  as.data.frame(Cytometry1)[which(match(Cytometry1$`Population ID (name)`,
    c('Monocytes', 'CD4+CD8-', 'Mature SIg Kappa', 'TCRgd-'), nomatch = 0) > 0), 1:10])

```

labelTransfer

labelTransfer

Description

Label transfer between a test partition and a training set of partitions.

Usage

```

labelTransfer(
  training.cytometry,
  test.cytometry,
  test.partition,
  equal.weights = FALSE
)

```

Arguments

training.cytometry List of partitions, where each partition is a dataframe where the last column contains the labels of the partition.

test.cytometry Test data, a dataframe without labels.

test.partition Labels of a partition of the test data.

equal.weights If True, weights assigned to every cluster in a partition are uniform (1/number of clusters) when calculating the similarity distance. If False, weights assigned to clusters are the proportions of points in every cluster compared to the total amount of points in the partition.

Value

A fuzzy relabeling consistent of a transportation plan.

Examples

```
data.example <- data.frame(v1 = c(rnorm(50, 2, 1), rnorm(50, -2, 1)),
                           v2 = c(rnorm(50, 2, 1), rnorm(50, -2, 1)), id = c(rep(0, 50), rep(1, 50)))
test.labels <- c(rep('a', 50), rep('b', 50))
labelTransfer(data.example, data.example[, 1:2], test.labels)
```

labelTransferEllipse *labelTransferEllipse*

Description

Label transfer between a test partition and a training partitions viewed as a mixture of gaussians.

Usage

```
labelTransferEllipse(
  i,
  test.cytometry.ellipses,
  training.cytometries.barycenter,
  equal.weights = FALSE
)
```

Arguments

i A dummy variable, should be any integral. Ment for use with lapply.

test.cytometry.ellipses
A test clustering viewed as a mixture of multivariate normal distributions.

training.cytometries.barycenter
A training partition viewed as a mixture of multivariate normal distributions.

equal.weights If True, weights assigned to every cluster in a partition are uniform (1/number of clusters) when calculating the similarity distance. If False, weights assigned to clusters are the proportions of points in every cluster compared to the total amount of points in the partition.

Value

A fuzzy relabeling consistent of a transportation plan.

References

E del Barrio, H Inouzhe, JM Loubes, C Matran and A Mayo-Iscar. (2019) optimalFlow: Optimal-transport approach to flow cytometry gating and population matching. arXiv:1907.08006

Examples

```
partition1 <- list(list(mean = c(1, 1), cov = diag(1, 2), weight = 0.5, type = '1'),
                  list(mean = c(-1, -1), cov = diag(1, 2), weight = 0.5, type = '2'))
partition2 <- list(list(mean = c(1, 1), cov = diag(1, 2), weight = 0.5, type = 'a'),
                  list(mean = c(-1, -1), cov = diag(1, 2), weight = 0.5, type = 'b'))
labelTransferEllipse(1, partition2, partition1)
```

```
optimalFlowClassification
      optimalFlowClassification
```

Description

Performs a supervised classification of input data when a database and a partition of the database are provided.

Usage

```
optimalFlowClassification(
  X,
  database,
  templates,
  consensus.method = "pooling",
  cov. estimation = "standard",
  alpha.cov = 0.85,
  initial.method = "supervized",
  max.clusters = NA,
  alpha.tclust = 0,
  restr.factor.tclust = 1000,
  classif.method = "qda",
  qda.bar = TRUE,
  cost.function = "points",
  cl.paral = 1,
  equal.weights.voting = TRUE,
  equal.weights.template = TRUE
)
```

Arguments

X	Datasample to be classified.
database	A list where each entry is a partition (clustering) represented as dataframe, of the same dimensions, where the last variable represents the labels of the partition.
templates	List of the consensus clusterings for every group in the partition of the database obtained by optimalFlowTemplates
consensus.method	The consensus.method value that was used in optimalFlowTemplates.
cov. estimation	How to estimate covariance matrices in each cluster of a partition. "standard" is for using cov(), while "robust" is for using robustbase::covMcd.
alpha.cov	Only when cov. estimation = "robust". Indicates the value of alpha in robustbase::covMcd.
initial.method	Indicates how to obtain a partition of X. Takes values in c("supervized", "unsupervized"). Supervized uses tclust initialized by templates. Unsupervized uses flowMeans.
max.clusters	The maximum numbers of clusters for flowMeans. Only when initial.method = unsupervized.
alpha.tclust	Level of trimming allowed fo tclust. Only when initial.method = supervized.

<code>restr.factor.tclust</code>	Fixes the <code>restr.fact</code> parameter in <code>tclust</code> . Only when <code>initial.method = supervised</code> .
<code>classif.method</code>	Indicates what type of supervised learning we want to do. Takes values on <code>c("matching", "qda", "random forest")</code> .
<code>qda.bar</code>	Only if <code>classif.method = "qda"</code> . If <code>True</code> then the appropriate consensus clustering (template, prototype) is used for learning. If <code>False</code> , the closest partition in the appropriate group is used.
<code>cost.function</code>	Only if <code>classif.method = "matching"</code> . Indicates the cost function, distance between clusters, to be used for label matching.
<code>cl.paral</code>	Number of cores to be used in parallel procedures.
<code>equal.weights.voting</code>	only when <code>classif.method = "qda"</code> and <code>qda.bar = F</code> , or when <code>classif.method = "random forest"</code> . Indicates the weights structure when looking for the most similar partition in a group.
<code>equal.weights.template</code>	If <code>True</code> , weights assigned to every cluster in a partition are uniform ($1/\text{number of clusters}$). If <code>False</code> , weights assigned to clusters are the proportions of points in every cluster compared to the total amount of points in the partition.

Value

A list formed by:

cluster Labels assigned to the input data.

clusterings A list that contains the initial unsupervised or semi-supervised clusterings of the cytometry of interest. Can have as much entries as the number of templates in the semi-supervised case (`initial.method = "supervised"`), or only one entry in the case of `initial.method = "unsupervised"`. Each entry is a list where the most relevant argument for the clusterings is cluster.

assigned.template.index Label of the group for which the template is closer to the data. When classical qda or random forest are used for classification there is a second argument indicating the index of the cytometry in the cluster used for learning.

cluster.vote Only when `classif.method = "matching"` or when `consensus.method` in `c("hierarchical", "k-barycenter")`. Vote on the type of every label in the partition of the data. In essence, `cluster + cluster.vote` return a fuzzy clustering of the data of interest.

References

E del Barrio, H Inouzhe, JM Loubes, C Matran and A Mayo-Iscar. (2019) optimalFlow: Optimal-transport approach to flow cytometry gating and population matching. arXiv:1907.08006

Examples

```
## We construct a simple database selecting only some of the Cytometries and some cell types for simplicity and
database <- buildDatabase(
  dataset_names = paste0('Cytometry', c(2:5, 7:9, 12:17, 19, 21)),
  population_ids = c('Monocytes', 'CD4+CD8-', 'Mature SIg Kappa', 'TCRgd-'))
## To select the appropriate number of templates, via hierarchical tree, in an interactive fashion and produce a
# templates.optimalFlow <- optimalFlowTemplates(database = database)
templates.optimalFlow <- optimalFlowTemplates(database = database, templates.number = 5,
  cl.paral = 1)
classification.optimalFlow <- optimalFlowClassification(Cytometry1[
```

```

which(match(Cytometry1$`Population ID (name)`, c("Monocytes", "CD4+CD8-", "Mature SIg Kappa",
"TCRgd-"), nomatch = 0) > 0), 1:10], database, templates.optimalFlow, cl.par
scoreF1.optimalFlow <- optimalFlow::f1Score(classification.optimalFlow$cluster,
Cytometry1[which(match(Cytometry1$`Population ID (name)`,
c("Monocytes", "CD4+CD8-", "Mature SIg Kappa", "TCRgd-

```

optimalFlowTemplates *optimalFlowTemplates*

Description

Returns a partition of the input clusterings with a respective consensus clustering for every group.

Usage

```

optimalFlowTemplates(
  database,
  database.names = NULL,
  cov. estimation = "standard",
  alpha.cov = 0.85,
  equal.weights.template = TRUE,
  hclust.method = "complete",
  trimm.template = FALSE,
  templates.number = NA,
  minPts = 2,
  eps = 1,
  consensus.method = "pooling",
  barycenters.number = NA,
  bar.repetitions = 40,
  alpha.bar = 0.05,
  bar.ini.method = "plus-plus",
  consensus.minPts = 3,
  cl.paral = 1
)

```

Arguments

database	A list where each entry is a partition (clustering) represented as dataframe, of the same dimensions, where the last variable represents the labels of the partition.
database.names	Names of the elements in the database.
cov. estimation	How to estimate covariance matrices in each cluster of a partition. 'standard' is for using cov(), while 'robust' is for using robustbase::covMcd.
alpha.cov	Only when cov. estimation = 'robust'. Indicates the value of alpha in robustbase::covMcd.
equal.weights.template	If True, weights assigned to every cluster in a partition are uniform (1/number of clusters). If False, weights assigned to clusters are the proportions of points in every cluster compared to the total amount of points in the partition.

<code>hclust.method</code>	Indicates what kind of hierarchical clustering to do with the similarity distances matrix of the partitions. Takes values in <code>c('complete', 'single', 'average', 'hdbscan', 'dbscan')</code> .
<code>trimm.template</code>	Logical value. Indicates if it is allowed to not take into account some of the entries of database. Default is <code>False</code> .
<code>templates.number</code>	Only if <code>hclust.method</code> in <code>c('complete', 'single', 'average')</code> . Indicates the number of clusters to use with <code>cutree</code> . If set to <code>NA</code> (default), plots the hierarchical tree and asks the user to introduce an appropriate number of clusters.
<code>minPts</code>	Only if <code>hclust.method</code> in <code>c('hdbscan', 'dbscan')</code> . Indicates the value of argument <code>minPts</code> in <code>dbscan::dbscan</code> and <code>dbscan::hdbscan</code> .
<code>eps</code>	Only if <code>hclust.method = 'dbscan'</code> . Indicates the value of <code>eps</code> in <code>dbscan::dbscan</code> .
<code>consensus.method</code>	Sets the way of doing consensus clustering when clusters are viewed as Multivariate Distributions. Can take values in <code>c('pooling', 'k-barycenter', 'hierarchical')</code> . See details.
<code>barycenters.number</code>	Only if <code>consensus.method = 'k-barycenter'</code> . Sets the number, <code>k</code> , of barycenters when using <code>k-barycenters</code> .
<code>bar.repetitions</code>	Only if <code>consensus.method = 'k-barycenter'</code> . How many times to repeat the <code>k-barycenters</code> procedure. Equivalent to <code>nstart</code> in <code>kmeans</code> .
<code>alpha.bar</code>	Only if <code>consensus.method = 'k-barycenter'</code> . The level of trimming allowed during the <code>k-barycenters</code> procedure.
<code>bar.ini.method</code>	Only if <code>consensus.method = 'k-barycenter'</code> . Takes values in <code>c('rnd', 'plus-plus')</code> . See details.
<code>consensus.minPts</code>	Only if <code>consensus.method = 'hierarchical'</code> . The value of argument <code>minPts</code> for <code>dbscan::hdbscan</code> .
<code>cl.paral</code>	Number of cores to be used in parallel procedures.

Value

A list containing:

templates A list representing the consensus clusterings for every group in the partition of the database. Each element of the list is a template partition. Hence it is a list itself, containing the cell types in the prototype, where each element has components: mean, cov, weight and type.

clustering Clustering of the input partitions.

database.elliptical A list containing each cytometry in the database viewed as a mixture distribution. Each element of the list is a cytometry viewed as a mixture. Hence it is a list itself, containing the cell types in the cytometry, where each element has components: mean, cov, weight and type.

References

E del Barrio, H Inouzhe, JM Loubes, C Matran and A Mayo-Iscar. (2019) optimalFlow: Optimal-transport approach to flow cytometry gating and population matching. arXiv:1907.08006

Examples

```
## We construct a simple database selecting only some of the Cytometries and some cell types for simplicity and
database <- buildDatabase(
  dataset_names = paste0('Cytometry', c(2:5, 7:9, 12:17, 19, 21)),
  population_ids = c('Monocytes', 'CD4+CD8-', 'Mature SIg Kappa', 'TCRgd-'))

## To select the appropriate number of templates, via hierarchical tree, in an interactive fashion and produce a
# templates.optimalFlow <- optimalFlowTemplates(database = database)

templates.optimalFlow <- optimalFlowTemplates(database = database, templates.number = 5,
                                              cl.paral = 1)
```

qdaClassification *qdaClassification*

Description

Gives quadratic discriminant scores to the points in data for a multivariate normal.

Usage

```
qdaClassification(normal, data)
```

Arguments

normal	A list with arguments mean, covaruance and weight.
data	Data frame or matrix on which to perform qda.

Value

A score for each point.

Examples

```
data.qda = cbind(rnorm(50), rnorm(50))
exp(qdaClassification(list(mean = c(0,0), cov = diag(1,2), weight = 1), data.qda))
```

tclustWithInitialization
tclustWithInitialization

Description

A wrapper for the function tclust_H.

Usage

```
tclustWithInitialization(
  initialization,
  cytometry,
  i.sol.type = "points",
  trimming = 0.05,
  restr.fact = 1000
)
```

Arguments

initialization Initial solution for parameters provided by the user. Can be a matrix of data containing observations and cluster assignments or can be a list specifying a multivariate mixture of gaussians.

cytometry A matrix or data.frame of dimension $n \times p$, containing the observations (row-wise).

i.sol.type Type of initial solutions in `c('points', 'barycenters')`. 'points' refers to a classified data matrix, while 'barycenters' to a multivariate mixture.

trimming The proportion of observations to be trimmed.

restr.fact The constant `restr.fact` ≥ 1 constrains the allowed differences among group scatters. Larger values imply larger differences of group scatters, a value of 1 specifies the strongest restriction.

Value

A list with entries:

cluster A numerical vector of size n containing the cluster assignment for each observation. Cluster names are integer numbers from 1 to k , 0 indicates trimmed observations.

n_clus Number of clusters actually found.

obj The value of the objective function of the best (returned) solution.

Examples

```
x <- rbind(matrix(rnorm(100), ncol = 2), matrix(rnorm(100) + 2, ncol = 2),
           matrix(rnorm(100) + 4, ncol = 2))
## robust cluster obtention from a sample x asking for 3 clusters,
## trimming level 0.05 and constrain level 12
k <- 3; alpha <- 0.05; restr.fact <- 12
output = tclust_H(x = x, k = k, alpha = alpha, nstart = 50, iter.max = 20,
                 restr = 'eigen', restr.fact = restr.fact, sol_ini_p = FALSE, sol_ini = NA,
                 equal.weights = FALSE, trace = 0, zero.tol = 1e-16)
## cluster assignment
output2 <- tclustWithInitialization(data.frame(x, output$cluster), x, 'points', 0.05, 10)
```

tclust_H

*tclust_H***Description**

A wrapper for the internal function `tclust_`. Performs robust non spherical clustering, `tclust`, where initial solutions are allowed.

Usage

```
tclust_H(
  x,
  k = 3,
  alpha = 0.05,
  nstart = 50,
  iter.max = 20,
  restr = "eigen",
  restr.fact = 12,
  sol_ini_p = FALSE,
  sol_ini = NA,
  equal.weights = FALSE,
  trace = 0,
  zero.tol = 1e-16
)
```

Arguments

<code>x</code>	A matrix or data.frame of dimension $n \times p$, containing the observations (row-wise).
<code>k</code>	The number of clusters initially searched for.
<code>alpha</code>	The proportion of observations to be trimmed.
<code>nstart</code>	The number of random initializations to be performed. Only when <code>sol_ini_p = FALSE</code> .
<code>iter.max</code>	The maximum number of concentration steps to be performed. The concentration steps are stopped, whenever two consecutive steps lead to the same data partition.
<code>restr</code>	The type of restriction to be applied on the cluster scatter matrices. Valid values are "eigen" (default).
<code>restr.fact</code>	The constant <code>restr.fact</code> ≥ 1 constrains the allowed differences among group scatters. Larger values imply larger differences of group scatters, a value of 1 specifies the strongest restriction.
<code>sol_ini_p</code>	Initial solution for parameters provided by the user TRUE/FALSE, if TRUE is stored in <code>sol_ini</code> .
<code>sol_ini</code>	Initial solution for parameters provided by the user.
<code>equal.weights</code>	A logical value, specifying whether equal cluster weights (TRUE) or not (FALSE) shall be considered in the concentration and assignment steps.
<code>trace</code>	Defines the tracing level, which is set to 0 by default. Tracing level 2 gives additional information on the iteratively decreasing objective function's value.
<code>zero.tol</code>	The zero tolerance used. By default set to $1e-16$.

Details

This iterative algorithm initializes k clusters randomly and performs "concentration steps" in order to improve the current cluster assignment. The number of maximum concentration steps to be performed is given by `iter.max`. For approximately obtaining the global optimum, the system is initialized `nstart` times and concentration steps are performed until convergence or `iter.max` is reached. When processing more complex data sets higher values of `nstart` and `iter.max` have to be specified (obviously implying extra computation time). However, if more than half of the iterations would not converge, a warning message is issued, indicating that `nstart` has to be increased.

The parameter `restr` defines the cluster's shape restrictions, which are applied on all clusters during each iteration. Options "eigen"/"deter" restrict the ratio between the maximum and minimum eigenvalue/determinant of all cluster's covariance structures to parameter `restr.fact`. Setting `restr.fact` to 1, yields the strongest restriction, forcing all eigenvalues/determinants to be equal and so the method looks for similarly scattered (respectively spherical) clusters. Option "sigma" is a simpler restriction, which averages the covariance structures during each iteration (weighted by cluster sizes) in order to get similar (equal) cluster scatters.

Value

A list with values:

centers A matrix of size $p \times k$ containing the centers (column-wise) of each cluster.

cov An array of size $p \times p \times k$ containing the covariance matrices of each cluster.

cluster A numerical vector of size n containing the cluster assignment for each observation. Cluster names are integer numbers from 1 to k , 0 indicates trimmed observations.

par A list, containing the parameters the algorithm has been called with (`x`, if not suppressed by `store.x = FALSE`, `k`, `alpha`, `restr.fact`, `nstart`, `KStep`, and `equal.weights`).

weights A numerical vector of length k , containing the weights of each cluster.

obj the value of the objective function of the best (returned) solution.

References

Fritz, H., Garcia-Escudero, L. A., & Mayo-Isacar, A. (2012). `tclust`: An R package for a trimming approach to cluster analysis. *Journal of Statistical Software*, 47(12), 1-26.

Examples

```
x <- rbind(matrix(rnorm(100), ncol = 2), matrix(rnorm(100) + 2, ncol = 2),
           matrix(rnorm(100) + 4, ncol = 2))
## robust cluster obtention from a sample x asking for 3 clusters,
## trimming level 0.05 and constrain level 12
k <- 3; alpha <- 0.05; restr.fact <- 12
output <- tclust_H(x = x, k = k, alpha = alpha, nstart = 50, iter.max = 20,
                  restr = "eigen", restr.fact = restr.fact, sol_ini_p = FALSE, sol_ini = NA,
                  equal.weights = FALSE, trace = 0, zero.tol = 1e-16)
## cluster assignment
output$cluster
plot(x, col = output$cluster)
```

trimmedKBarycenter	<i>trimmedKBarycenter</i>
--------------------	---------------------------

Description

Calculates a 2-Wasserstein k-barycenter of a list of multivariate normal distributions.

Usage

```
trimmedKBarycenter(k, alpha0, type.ini = "rnd", reps.list)
```

Arguments

<code>k</code>	Number k of elements in the k-barycenter.
<code>alpha0</code>	Level of trimming.
<code>type.ini</code>	of initialization in c('rnd', 'plus-plus'). 'rnd' makes the common random initialization while 'plus-plus' initializes in a similar fashion to k-means++.
<code>reps.list</code>	List of multivariate normals for which the trimmed k-barycenter should be performed.

Value

A list with values:

variacion_wasser A double giving the Wasserstein variation.

baricentro A list of k elements, each of which is a member of the k-barycenter. Each element is a normal distribution characterized by a mean and a covariance.

cluster The assignment of the original entries to each member of the k-barycenter.

Examples

```
normals <- list(list(mean = c(1, 1), cov = diag(2, 2)), list(mean = c(1, 1), cov = diag(1, 2)),
  list(mean = c(3, 3), cov = diag(1, 2)))
trimmedKBarycenter(2, 0, 'rnd', normals)
```

voteLabelTransfer	<i>voteLabelTransfer</i>
-------------------	--------------------------

Description

A wrapper for doing either labelTransfer or labelTransferEllipse.

Usage

```

voteLabelTransfer(
  type = "points",
  test.partition,
  test.cytometry,
  test.partition.ellipse,
  training.cytometries,
  training.cytometries.barycenter,
  test = 1,
  op.syst,
  cl.paral = 1,
  equal.weights = FALSE
)

```

Arguments

`type` 'points' indicates use of labelTransfer; 'ellipses' of labelTransferEllipse.

`test.partition` Only when type = 'points'. Labels of a partition of the test data.

`test.cytometry` Only when type = 'points'. Test data, a dataframe without labels.

`test.partition.ellipse`
Only when type = 'ellipses'. A test clustering viewed as a mixture of multivariate normal distributions.

`training.cytometries`
Only when type = 'points'. List of partitions, where each partition is a dataframe where the last column contains the labels of the partition.

`training.cytometries.barycenter`
Only when type = 'ellipses'. A training partition viewed as a mixture of multivariate normal distributions.

`test` Only when type = 'ellipses'. A dummy variable, should be any integral. Ment for use with lapply.

`op.syst` Type of system, takes values in c('unix', 'windows').

`cl.paral` Number of cores to be used in parallel procedures.

`equal.weights` If True, weights assigned to every cluster in a partition are uniform (1/number of clusters) when calculating the similarity distance. If False, weights assigned to clusters are the proportions of points in every cluster compared to the total amount of points in the partition.

Value

A list containing:

final.vote A list for the votes on each cell.

complete.vote A more complete list for the votes on each cell.

Examples

```

data.example <- data.frame(v1 = c(rnorm(50, 2, 1), rnorm(50, -2, 1)),
  v2 = c(rnorm(50, 2, 1), rnorm(50, -2, 1)), id = c(rep(0, 50), rep(1, 50)))
test.labels <- c(rep('a', 50), rep('b', 50))
voteLabelTransfer(test.partition = test.labels, test.cytometry = data.example[, 1:2],
  training.cytometries = list(data.example), op.syst = .Platform$OS.type)$final.vote[[1]]

```

`w2dist``w2dist`

Description

The 2-Wasserstein distance between two multivariate normal distributions

Usage

```
w2dist(P, Q)
```

Arguments

`P` A multivariate normal distribution given as a list with arguments mean and cov.
`Q` A multivariate normal distribution given as a list with arguments mean and cov.

Value

A double giving the 2-Wasserstein distance between the two distributions.

Examples

```
P <- list(mean = c(1, 1), cov = diag(1, 2))
Q <- list(mean = c(0, 0), cov = 1.1*diag(1, 2))
Q <- list(mean = c(0, 0), cov = 1.1*diag(1, 2))
w2dist(P, Q)
```

`wasserCostFunction``wasserCostFunction`

Description

Calculates the similarity distance between elements `j` and `i` of a list of partitions.

Usage

```
wasserCostFunction(j, i, cytometries, equal.weights = FALSE)
```

Arguments

`j` An entry of the list of partitions.
`i` An entry of the list of partitions.
`cytometries` The list of partitions.
`equal.weights` If True, weights assigned to every cluster in a partition are uniform (1/number of clusters) when calculating the similarity distance. If False, weights assigned to clusters are the proportions of points in every cluster compared to the total amount of points in the partition.

Value

A double giving the value of the similarity distance.

Examples

```
# # We construct a simple database selecting only some of the Cytometries and some cell types for simplicity and
database <- buildDatabase(
  dataset_names = paste0('Cytometry', c(2:5, 7:9, 12:17, 19, 21)),
  population_ids = c('Monocytes', 'CD4+CD8-', 'Mature SIg Kappa', 'TCRgd-'))

templates.optimalFlow <- optimalFlowTemplates(database = database, templates.number = 5,
  cl.paral = 1)
print(wasserCostFunction(1, 2, list(templates.optimalFlow$database.elliptical[[1]],
  templates.optimalFlow$database.elliptical[[2]])))
```

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