# Package 'optimalFlow'

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**Author** Hristo Inouzhe <hristo.inouzhe@gmail.com>

**Maintainer** Hristo Inouzhe <hristo.inouzhe@gmail.com>

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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 clusetering 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

| | |
|---|---|
| `cytometry.as.mixture` | 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. |

| | |
|---|---|
| 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. |

## 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

| | |
|---|---|
| cytometry.as.mixture | 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 three 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. |

## 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), z
```

---

cytoPlotDatabase *cytoPlotDatabase*

---

## 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

| | |
|---|---|
| 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. |
| 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. |
| colour | If TRUE plots elements of a mixture distribution in different colours. If FALSE 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)], dimen
```

---

## 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)], di
```

`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` *estimCovCellGeneral*

## Description

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

## Usage

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

### Arguments

| | |
|---|---|
| cell | Labell of the clsuter 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 *f1Score*

---

### Description

Calculates the F1 score fore 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` *f1ScoreVoting*

---

## 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 for
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.opti
 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), ],
```

---

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 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 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 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 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 initilized by templates. Unsupevized usese 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.

`restr.factor.tclust`
Fixes the restr.fact parameter in tclust. Only when initial.method = supervized.

`classif.method` Indicates what type of supervised learning we want to do. Takes values on c("matching", "qda", "random forest").

`qda.bar` Only if classif.method = "qda". If True then the appropriate consensus clustering (template, prototype) is used for learning. If False, the closest partition in the appropriate group is used.

`cost.function` Only if classif.method = "matching". Indicates the cost function, distance between clusters, to be used for label matching.

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

`equal.weights.voting`
only when classif.method = "qda" and qda.bar =F, or when classif.method = "random forest". Indicates the weights structure when looking for the most similar partition in a group.

`equal.weights.template`
If True, weights assigned to every cluster in a partion 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.

## Value

A list formed by:

**cluster** Labels assigned to the input data.

**clusterings** A list that contains the initial unsupervized or semi-supervized clusterings of the cytometry of interest. Can have as much entries as the number of templates in the semi-supervized case (initial.method = "supervized), or only one entry in the case of initial.method = "unsupervized". 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 ares used for classification there is a secon 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 for
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 clu
# templates.optimalFlow <- optimalFlowTemplates(database = database)
templates.optimalFlow <- optimalFlowTemplates(database = database, templates.number = 5,
                                              cl.paral = 1)
classification.optimalFlow <- optimalFlowClassification(Cytometry1[
 which(match(Cytometry1$`Population ID (name)`,c("Monocytes", "CD4+CD8-", "Mature SIg Kappa",
                                  "TCRgd-"), nomatch = 0) > 0), 1:10], database, templates.optimalFlow, cl.paral =
scoreF1.optimalFlow <- optimalFlow::f1Score(classification.optimalFlow$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 partion 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. |
| hclust.method | Indicates what kind of hierarchical clustering to do with the similarity distances matrix of the partitions. Takes values in c('complete', 'single', 'average', 'hdbscan', 'dbscan'). |
| trimm.template | Logical value. Indicates if it is allowed to not take into account some of the entries of database. Default is False. |
| templates.number | Only if hclust.method in c('complete', 'single', 'average'). Indicates the number of clusters to use with cutree. If set to NA (default), plots the hierarchical tree and asks the user to introduce an appropriate number of clusters. |
| minPts | Only if hclust.method in c('hdbscan', 'dbscan'). Indicates the value of argument minPts in dbscan::dbscan and dbscan::hdbscan. |
| eps | Only if hclust.method = 'dbscan'. Indicates the value of eps in dbscan::dbscan. |
| consensus.method | Sets the way of doing consensus clustering when clusters are viewed as Multivariate Distributions. Can take values in c('pooling', 'k-barycenter', 'hierarchical'). See details. |
| barycenters.number | Only if consensus.method = 'k-barycenter'. Sets the number, k, of barycenters when using k-barycenters. |
| bar.repetitions | Only if consensus.method = 'k-barycenter'. How many times to repeat the k-barycenters procedure. Equivalent to nstart in kmeans. |
| alpha.bar | Only if consensus.method = 'k-barycenter'. The level of trimming allowed during the k-barycenters procedure. |
| bar.ini.method | Only if consensus.method = 'k-barycenter'. Takes values in c('rnd', 'plus-plus'). See details. |
| consensus.minPts | Only if consensus.method = 'hierarchical'. The value of argument minPts for dbscan::hdbscan. |
| cl.paral | Number of cores to be used in parallel procedures. |

## Value

A list containting:

**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, containig 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 containig 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, containig 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 for
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 clu
# 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 anc cluster assignations or can be a list spesifying a multivariate mixture of gaussians. |
| `cytometry` | A matrix or data.frame of dimension n x 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** he 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 assigment
output2 <- tclustWithInitialization(data.frame(x, output$cluster), x, 'points', 0.05, 10)
```

---

tclust_H *tclust_H*

---

## Description

A wrapper for the internal fucntion 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

| | |
|---|---|
| x | A matrix or data.frame of dimension n x p, containing the observations (row-wise). |
| k | The number of clusters initially searched for. |
| alpha | The proportion of observations to be trimmed. |
| nstart | The number of random initializations to be performed. Only when sol_ini_p = FALSE. |
| iter.max | The maximum number of concentration steps to be performed. The concentration steps are stopped, whenever two consecutive steps lead to the same data partition. |
| restr | The type of restriction to be applied on the cluster scatter matrices. Valid values are "eigen" (default). |
| 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. |
| sol_ini_p | Initial solution for parameters provided by the user TRUE/FALSE, if TRUE is stored in sol_ini. |
| sol_ini | Initial solution for parameters provided by the user. |
| equal.weights | A logical value, specifying whether equal cluster weights (TRUE) or not (FALSE) shall be considered in the concentration and assignment steps. |
| trace | 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. |
| zero.tol | 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 then 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 x k containing the centers (column-wise) of each cluster.

**cov** An array of size p x p x 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** he value of the objective function of the best (returned) solution.

## References

Fritz, H., Garcia-Escudero, L. A., & Mayo-Iscar, 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 assigment
output$cluster
plot(x, col = output$cluster)
```

---

`trimmedKBarycenter` *trimmedKBarycenter*

---

## Description

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

## Usage

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

## Arguments

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

## Value

A list with values:

**variacion_wasser** A double giving the Waserstein variation.

**baricentro** A list of k elements, each of which is a member of the k-barycenter. Each eement 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` *voteLabelTransfer*

---

## 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 wher 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 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 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 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 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 for
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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