Package ‘CytoMDS’

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Title Low Dimensions projection of cytometry samples

Version 1.0.0

Description This package implements a low dimensional visualization of a set of cytometry samples, in order to visually assess the 'distances' between them. This, in turn, can greatly help the user to identify quality issues like batch effects or outlier samples, and/or check the presence of potential sample clusters that might align with the experimental design. The CytoMDS algorithm combines, on the one hand, the concept of Earth Mover's Distance (EMD), a.k.a. Wasserstein metric and, on the other hand, the Multi Dimensional Scaling (MDS) algorithm for the low dimensional projection. Also, the package provides some diagnostic tools for both checking the quality of the MDS projection, as well as tools to help with the interpretation of the axes of the projection.

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BugReports https://github.com/UCLouvain-CBIO/CytoMDS/issues

URL https://uclouvain-cbio.github.io/CytoMDS

biocViews FlowCytometry, QualityControl, DimensionReduction, MultidimensionalScaling, Software, Visualization

Collate 'CytoMDS-package.R' 'stats.R' 'ggplots.R' 'MDS-class.R'

Depends R (>= 4.3)

Imports methods, stats, rlang, pracma, withr, flowCore, reshape2, ggplot2, ggrepel, ggforce, patchwork, transport, smacof, BiocParallel, CytoPipeline

Suggests testthat (>= 3.0.0), vdiffr, diffviewer, knitr, rmarkdown, BiocStyle, HDCytoData

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CytoMDS-package

CytoMDS: Low Dimensions projection of cytometry samples

Description

This package implements a low dimensional visualization of a set of cytometry samples, in order to visually assess the 'distances' between them. This, in turn, can greatly help the user to identify quality issues like batch effects or outlier samples, and/or check the presence of potential sample clusters that might align with the experimental design. The CytoMDS algorithm combines, on the one hand, the concept of Earth Mover’s Distance (EMD), a.k.a. Wasserstein metric and, on the other hand, the Multi Dimensional Scaling (MDS) algorithm for the low dimensional projection. Also, the package provides some diagnostic tools for both checking the quality of the MDS projection, as well as tools to help with the interpretation of the axes of the projection.
channelSummaryStats

Summary statistics per channel computation

Description

Computation of summary statistic for selected channels, for all flowFrames of a flowSet. This method provides two different input modes:

- the user provides directly a flowSet loaded in memory (RAM).
- the user provides (1.) a number of samples nSamples; (2.) an ad-hoc function that takes as input an index between 1 and nSamples, and codes the method to load the corresponding flowFrame in memory; Optional row and column ranges can be provided to limit the calculation to a specific rectangle of the matrix. These i.e. can be specified as a way to split heavy calculations of large distance matrices on several computation nodes.

Usage

channelSummaryStats(
  x,
  loadFlowFrameFUN = NULL,
  loadFlowFrameFUNArgs = NULL,
  channels = NULL,
  statFUNs = stats::median,
  verbose = FALSE,
  BPPARAM = BiocParallel::SerialParam(),
  BPOPTIONS = BiocParallel::bpoptions(packages = c("flowCore"))
)

See Also

Useful links:

- https://uclouvain-cbio.github.io/CytoMDS
- Report bugs at https://github.com/UCLouvain-CBIO/CytoMDS/issues
Arguments

x

either a flowCore::flowSet, or the number of samples (integer >=1)

loadFlowFrameFUN

the function used to translate a flowFrame index into a flowFrame. In other words, the function should code how to load a specific flowFrame into memory. Important: the flowFrame index should be the first function argument and should be named ffIndex.

loadFlowFrameFUNArgs

(optional) a named list containing additional input parameters of loadFlowFrameFUN()

channels

which channels (integer index(ices) or character(s)):

• if it is a character vector, it can refer to either the channel names, or the marker names
• if it is a numeric vector, it refers to the indexes of channels in fs
• if NULL all scatter and fluorescent channels of fs will be selected

statFUNs

a list (possibly of length one) of functions to call to calculate the statistics, or a simple function This list can be named, in that case, these names will be transferred to the returned value.

verbose

if TRUE, output a message after each single distance calculation

BPPARAM

sets the BPPARAM back-end to be used for the computation. If not provided, will use BiocParallel::SerialParam() (no task parallelization)

BPOPTIONS

sets the BPOPTIONS to be passed to bplapply() function. Note that if you use a SnowParams back-end, you need to specify all the packages that need to be loaded for the different CytoProcessingStep to work properly (visibility of functions). As a minimum, the flowCore package needs to be loaded. (hence the default BPOPTIONS = bpoptions(packages = c("flowCore")))

Value

a list of named statistic matrices. In each stat matrix, the columns are the channel statistics for all flowFrames of the flowSet. Exception: if only one stat function (and not a list) is passed in statFUNs, the return value is simplified to the stat matrix itself.

Examples

library(CytoPipeline)

data(OMIP021Samples)

# estimate scale transformations
# and transform the whole OMIP021Samples

transList <- estimateScaleTransforms(
  ff = OMIP021Samples[[1]],
  fluoMethod = "estimateLogicle",
  scatterMethod = "linearQuantile",
  scatterRefMarker = "BV785 - CD3")
computeMetricMDS <- CytoPipeline::applyScaleTransforms(
  OMIP021Samples,
  transList)

channelsOrMarkers <- c("FSC-A", "SSC-A", "BV785 - CD3")

# calculate mean for each 4 selected channels, for each 2 samples
channelMeans <- channelSummaryStats(
  OMIP021Trans,
  channels = channelsOrMarkers,
  statFUNs = mean)

# calculate median AND std deviation
# for each 4 selected channels, for each 2 samples
channelMedians <- channelSummaryStats(
  OMIP021Trans,
  channels = channelsOrMarkers,
  statFUNs = list("median" = stats::median,
                  "std.dev" = stats::sd))

computeMetricMDS  metric MDS projection of sample

Description
Multi-dimensional scaling projection of samples, using a distance matrix as an input. The MDS algorithm is not the classical MDS (cmdscale alike, aka Torgerson’s algorithm), but is the SMA-COF algorithm for metric distances that are not necessarily euclidean. After having obtained the projections on the \( n_{\text{Dim}} \) dimensions, we always apply svd decomposition to visualize as first axes the ones that contain the most variance of the projected dataset in \( n_{\text{Dim}} \) dimensions. Instead of being provided directly by the user, the \( n_{\text{Dim}} \) parameter can otherwise be found iteratively by finding the minimum \( n_{\text{Dim}} \) parameter that allows the projection to reach a target pseudo RSquare. If this is the case, the maxDim parameter is used to avoid looking for too big projection spaces.

Usage
computeMetricMDS(
  pwDist,
  nDim = NULL,
  seed = NULL,
  targetPseudoRSq = 0.95,
  maxDim = 128,
  ...
)
Arguments

`pwDist` (nSamples rows, nSamples columns), previously calculated pairwise distances between samples, must be provided as a full symmetric square matrix, with 0. diagonal

`nDim` number of dimensions of projection, as input to SMACOF algorithm if not provided, will be found iteratively using `targetPseudoRSq`

`seed` seed to be set when launching SMACOF algorithm (e.g. when `init` is set to "random" but not only)

`targetPseudoRSq` target pseudo RSquare to be reached (only used when `nDim` is set to NULL)

`maxDim` in case `nDim` is found iteratively, maximum number of dimensions the search procedure is allowed to explore

... additional parameters passed to SMACOF algorithm

Value

a list with six elements:

• `pwDist` the initial pair-wise distance (same as input)
• `$proj` the final configuration, i.e. the projected data matrix (nSamples rows, nDim columns) in nDim dimensions
• `$projDist` the distance matrix of projected data
• `stress` the global stress loss function final value obtained from the SMACOF algorithm
• `spp` the stress per point obtained from the SMACOF algorithm, i.e. the contribution of each point to the stress loss function
• `$RSq` R squares, for each d, from 1 to nDim: the (pseudo) R square when taking all dims from 1 to d.
• `$GoF` Goodness of fit, for each d, from 1 to nDim: the goodness of fit indicator (b/w 0 and 1) when taking all dims from 1 to d. Note pseudo R square and goodness of fit indicators are essentially the same indicator, only the definition of total sum of squares differ:
  • for pseudo RSq: TSS is calculated using the mean pairwise distance as minimum
  • for goodness of fit: TSS is calculated using 0 as minimum

Examples

```r
library(CytoPipeline)
data(OMIP021Samples)

# estimate scale transformations
# and transform the whole OMIP021Samples
transList <- estimateScaleTransforms(
  ff = OMIP021Samples[[1]],
  fluoMethod = "estimateLogicle",
  scatterMethod = "linearQuantile",
  scatterRefMarker = "BV785 - CD3")
```
OMIP021Trans <- CytoPipeline::applyScaleTransforms(
    OMIP021Samples,
    transList)

# As there are only 2 samples in OMIP021Samples dataset,
# we create artificial samples that are random combinations of both samples

ffList <- c(  
    flowCore::flowSet_to_list(OMIP021Trans),
    lapply(3:5,
        FUN = function(i) {
            aggregateAndSample(  
                OMIP021Trans,
                seed = 10*i,
                nTotalEvents = 5000)
        }[1:22]
    )
)

fsNames <- c("Donor1", "Donor2", paste0("Agg",1:3))
names(ffList) <- fsNames

fsAll <- as(ffList,"flowSet")

flowCore::pData(fsAll)$type <- factor(c("real", "real", rep("synthetic", 3)))
flowCore::pData(fsAll)$grpId <- factor(c("D1", "D2", rep("Agg", 3)))

# calculate all pairwise distances

pwDist <- pairwiseEMDDist(fsAll,
    channels = c("FSC-A","SSC-A"),
    verbose = FALSE)

# compute Metric MDS object with explicit number of dimensions

mdsObj <- computeMetricMDS(pwDist, nDim = 4, seed = 0)

dim <- nDim(mdsObj) # should be 4

#' # compute Metric MDS object by reaching a target pseudo RSquare

mdsObj2 <- computeMetricMDS(pwDist, seed = 0, targetPseudoRSq = 0.999)

---

**EMDDist**

*Calculate Earth Mover’s distance between two flowFrames*

**EMDDist**

**Description**

Calculate Earth Mover’s distance between two flowFrames
EMDDist

Usage

EMDDist(
  ff1,
  ff2,
  channels = NULL,
  checkChannels = TRUE,
  binSize = 0.05,
  minRange = -10,
  maxRange = 10,
  returnAll = FALSE
)

Arguments

  ff1 a flowCore::flowFrame
  ff2 a flowCore::flowFrame
  channels
    which channels (integer index(ices) or character(s)):
    • if it is a character vector, it can refer to either the channel names, or the
      marker names
    • if it is a numeric vector, it refers to the indexes of channels in ff1
    • if NULL all scatter and fluorescent channels of ff1 will be selected
  checkChannels if TRUE, will explicitly check that all provided channels are present in both
    flowFrames
  binSize size of equal bins to approximate the marginal distributions.
  minRange minimum value taken when approximating the marginal distributions
  maxRange maximum value taken when approximating the marginal distributions
  returnAll If TRUE, distributions and marginal distribution distances are returned as well.
    Default = FALSE.

Value

the Earth Mover’s distance between ff1 and ff2, which is calculated by summing up all EMD
approximates for the marginal distributions of each channel

Examples

library(CytoPipeline)

data(OMIP021Samples)

# estimate scale transformations
# and transform the whole OMIP021Samples

transList <- estimateScaleTransforms(
  ff = OMIP021Samples[[1]],
  fluoMethod = "estimateLogicle",
  scatterMethod = "linearQuantile",
)
scatterRefMarker = "BV785 - CD3"

OMIP021Trans <- CytoPipeline::applyScaleTransforms(
  OMIP021Samples,
  transList)

# distance with itself (all channels at once)
# => should return 0
dist0 <- EMDDist(
  ff1 = OMIP021Trans[[1]],
  ff2 = OMIP021Trans[[1]])

# returning only distance, 2 channels
dist1 <- EMDDist(
  ff1 = OMIP021Trans[[1]],
  ff2 = OMIP021Trans[[2]],
  channels = c("FSC-A", "SSC-A"))

# using only one channel, passed by marker name
dist2 <- EMDDist(ff1 = OMIP021Trans[[1]],
  ff2 = OMIP021Trans[[2]],
  channels = c("BV785 - CD3"))

# using only one channel, passed by index
dist3 <- EMDDist(ff1 = OMIP021Trans[[1]],
  ff2 = OMIP021Trans[[2]],
  channels = 10)

dist2 == dist3

---

### ggplotMarginalDensities

*Plot of channel intensity marginal densities*

**Description**

`ggplotMarginalDensities` uses `ggplot2` to draw plots of marginal densities of selected channels of a `flowSet`. If the `flowSet` contains several `flowFrames`, all events are concatenated together. By default, a pseudo Rsquare projection quality indicator, and the number of dimensions of the MDS projection are provided in sub-title.

**Usage**

```r
ggplotMarginalDensities(
  x,
  sampleSubset,
  channels,
  pDataForColour,
```
Arguments

x
sampleSubset
channels
pDataForColour
pDataForGroup
nEventInSubsample
seed
transList

Value

a ggplot object

Examples

library(CytoPipeline)

data(OMIP021Samples)

# estimate scale transformations
# and transform the whole OMIP021Samples

transList <- estimateScaleTransforms(
  ff = OMIP021Samples[[1]],
  fluoMethod = "estimateLogicle",
  scatterMethod = "linearQuantile",
  scatterRefMarker = "BV785 - CD3")

OMIP021Trans <- CytoPipeline::applyScaleTransforms(
  OMIP021Samples,
  transList)

# As there are only 2 samples in OMIP021Samples dataset,
# we create artificial samples that are random combinations of both samples
ffList <- c(
    flowCore::flowSet_to_list(OMIP021Trans),
    lapply(3:5,
        FUN = function(i) {
            aggregateAndSample(
                OMIP021Trans,
                seed = 10*i,
                nTotalEvents = 5000)
        }[1:22])
)

fsNames <- c("Donor1", "Donor2", paste0("Agg", 1:3))
names(ffList) <- fsNames

fsAll <- as(ffList, "flowSet")

flowCore::pData(fsAll)$grpId <- factor(c("D1", "D2", rep("Agg", 3)))
flowCore::pData(fsAll)$lbl <- paste0("S", 1:5)

# plot densities, all samples together
p <- ggplotMarginalDensities(fsAll)

# plot densities, per sample
p <- ggplotMarginalDensities(fsAll, pDataForGroup = "lbl")

# plot densities, per sample and coloured by group
p <- ggplotMarginalDensities(fsAll, pDataForGroup = "lbl",
                              pDataForColour = "grpId")

---

ggplotSampleMDS  
Plot of Metric MDS object

---

Description

`ggplotSampleMDS` uses `ggplot2` to provide plots of Metric MDS results. By default, a pseudo R-square projection quality indicator, and the number of dimensions of the MDS projection are provided in sub-title.

Usage

```r
ggplotSampleMDS(
    mdsObj,  
    pData,  
    sampleSubset,  
    projectionAxes = c(1, 2),  
    biplot = FALSE,  
    biplotType = c("correlation", "regression"),
```
ggplotSampleMDS

extVariables,
pDataForColour,
pDataForShape,
pDataForLabel,
pDataForAdditionalLabelling,
sizeReflectingStress = FALSE,
title = "Multi Dimensional Scaling",
displayPointLabels = TRUE,
pointLabelSize = 3.88,
repelPointLabels = TRUE,
displayArrowLabels = TRUE,
arrowLabelSize = 3.88,
repelArrowLabels = FALSE,
arrowThreshold = 0.8,
flipXAxis = FALSE,
flipYAxis = FALSE,
displayPseudoRSq = TRUE,
...

Arguments

mdsObj a MDS object, output of the computeMetricMDS() method.
pData (optional) a data.frame providing user input sample data. These can be design of experiment variables, phenotype data per sample,... and will be used to highlight sample categories in the plot and/or for subsetting.
sampleSubset (optional) a logical vector, of size nrow(pData), which is by construction the nb of samples, indicating which samples to keep in the plot. Typically it is obtained through the evaluation of a logical condition on pData rows.
projectionAxes which two axes should be plotted (should be a numeric vector of length 2)
biplot if TRUE, adds projection of external variables
biplotType type of biplot used:
  • if "correlation", projection of external variables will be according to Pearson correlations w.r.t. projection axes (arrow x & y coordinates)
  • if "regression", a linear regression of external variables using the 2 projection axes as explanatory variables is performed, and the projection of external variables will be according to regression coefficients (arrow direction) and R square of regression (arrow size)
extVariables are used to generate a biplot these are the external variables that will be used in the biplot. They should be provided as a matrix with named columns corresponding to the variables. The number of rows should be the same as the number of samples. The matrix might contain some NA's, in that case only complete rows will be used to calculate biplot arrows.
pDataForColour (optional) which pData variable will be used as colour aesthetic. Should be a character.
pDataForShape (optional) which pData variable will be used as shape aesthetic. Should be a character.

pDataForLabel (optional) which pData variable will be used as point labels in the plot. Should be a character. If missing, point labels will be set equal to point names defined in MDS object (if not NULL, otherwise no labels will be set).

pDataForAdditionalLabelling (optional) which pData variable(s) will be add to the ggplot mapping, as to make them available for plotly tooltipping. Should be an array of character of maximum length 3. Note this works only if biplot=FALSE, as biplots contain circle and arrows that are currently not supported under ggplotly.

sizeReflectingStress if TRUE, size of points will appear proportional to stress by point, i.e. the bigger the sample point appears, the less accurate its representation is (in terms of distances w.r.t. other points)

title title to give to the plot
displayPointLabels if TRUE, displays labels attached to points (see pDataForLabels for the setting of the label values)

pointLabelSize size of point labels (default: 3.88 as in geom_text())

repelPointLabels if TRUE, uses ggrepel::geom_text_repel() instead of ggplot2::geom_text() (try to split the labels such that they do not overlap) for the points
displayArrowLabels if TRUE, displays arrows labels (only with biplot)

arrowLabelSize size of arrow labels (default: 3.88 as in geom_text())

repelArrowLabels if TRUE, uses ggrepel::geom_text_repel() instead of ggplot2::geom_text() for the arrows (only with biplot)

arrowThreshold (only with biplot), arrows will be made barely visible if their length is (in absolute value) less than this threshold.

flipXAxis if TRUE, take the opposite of x values (provided as it might ease low dimensional projection comparisons)

flipYAxis if TRUE, take the opposite of y values (provided as it might ease low dimensional projection comparisons)
displayPseudoRSq if TRUE, display pseudo RSquare in subtitle, on top of nb of dimensions

... additional parameters passed to ggrepel::geom_text_repel() (if used)

Value

a ggplot object

See Also

ggplotSampleMDSWrapBiplots, ggplotSampleMDSShepard, computeMetricMDS
Examples

library(CytoPipeline)

data(OMIP021Samples)

# estimate scale transformations
# and transform the whole OMIP021Samples

transList <- estimateScaleTransforms(
  ff = OMIP021Samples[[1]],
  fluoMethod = "estimateLogicle",
  scatterMethod = "linearQuantile",
  scatterRefMarker = "BV785 - CD3")

OMIP021Trans <- CytoPipeline::applyScaleTransforms(
  OMIP021Samples,
  transList)

# As there are only 2 samples in OMIP021Samples dataset,
# we create artificial samples that are random combinations of both samples

ffList <- c(
  flowCore::flowSet_to_list(OMIP021Trans),
  lapply(3:5,
    FUN = function(i) {
      aggregateAndSample(
        OMIP021Trans,
        seed = 10*i,
        nTotalEvents = 5000)
    [1:22]
  } ))

fsNames <- c("Donor1", "Donor2", paste0("Agg", 1:3))
names(ffList) <- fsNames

fsAll <- as(ffList, "flowSet")

flowCore::pData(fsAll)$type <- factor(c("real", "real", rep("synthetic", 3)))
flowCore::pData(fsAll)$grpId <- factor(c("D1", "D2", rep("Agg", 3)))

# calculate all pairwise distances

pwDist <- pairwiseEMDDist(fsAll,
  channels = c("FSC-A", "SSC-A"),
  verbose = FALSE)

# compute Metric MDS object with explicit number of dimensions
mdsObj <- computeMetricMDS(pwDist, nDim = 4, seed = 0)

dim <- nDim(mdsObj) # should be 4

# compute Metric MDS object by reaching a target pseudo RSquare
mdsObj2 <- computeMetricMDS(pwDist, seed = 0, targetPseudoRSq = 0.999)
# plot mds projection on axes 1 and 2, # use 'grpId' for colour, 'type' for shape, and no label

```r
p_12 <- ggplotSampleMDS(
  mdsObj = mdsObj,
  pData = flowCore::pData(fsAll),
  projectionAxes = c(1,2),
  pDataForColour = "grpId",
  pDataForShape = "type"
)
```

# plot mds projection on axes 3 and 4, # use 'grpId' for colour, and 'name' as point label

```r
p_34 <- ggplotSampleMDS(
  mdsObj = mdsObj,
  pData = flowCore::pData(fsAll),
  projectionAxes = c(3,4),
  pDataForColour = "grpId",
  pDataForLabel = "name"
)
```

# plot mds projection on axes 1 and 2, # use 'group' for colour, 'type' for shape, and 'name' as point label # have sample point size reflecting 'stress' # i.e. quality of projection w.r.t. distances to other points

```r
p12_Stress <- ggplotSampleMDS(
  mdsObj = mdsObj,
  pData = flowCore::pData(fsAll),
  projectionAxes = c(1,2),
  pDataForColour = "grpId",
  pDataForLabel = "name",
  pDataForShape = "type",
  sizeReflectingStress = TRUE
)
```

# try to associate axes with median of each channel # => use bi-plot

```r
extVars <- channelSummaryStats(
  fsAll,
  channels = c("FSC-A", "SSC-A"),
  statFUNs = stats::median)
```

```r
bp_12 <- ggplotSampleMDS(
  mdsObj = mdsObj,
  pData = flowCore::pData(fsAll),
  projectionAxes = c(1,2),
  biplot = TRUE,
  extVariables = extVars,
  pDataForColour = "grpId",
  sizeReflectingStress = TRUE
)
```
ggplotSampleMDSShepard

Plot of Metric MDS object - Shepard diagram

Description

ggplotSampleMDSShepard uses ggplot2 to provide plot of Metric MDS results. Shepard diagram provides a scatter plot of:

- on the x axis, the high dimensional pairwise distances between each sample pairs
- on the y axis, the corresponding pairwise distances in the obtained low dimensional projection

Usage

ggplotSampleMDSShepard(
  mdsObj,
  nDim,
  title = "Multi Dimensional Scaling - Shepard's diagram",
  pointSize = 0.5,
  lineWidth = 0.5,
  displayPseudoRSq = TRUE
)

Arguments

- `mdsObj` a MDS object, output of the `computeMetricMDS()` method.
- `nDim` (optional) number of dimensions to use when calculating Shepard’s diagram and pseudoRSquare. If missing, it will be set equal to the number of projection dimensions as calculated in `mdsObj`
- `title` title to give to the plot
- `pointSize` point size in plot
- `lineWidth` line width in plot
- `displayPseudoRSq` if TRUE, display pseudo RSquare in subtitle, on top of nb of dimensions
**Value**

a ggplot object

**See Also**

`ggplotSampleMDS`, `computeMetricMDS`

**Examples**

```r
library(CytoPipeline)

data(OMIP021Samples)

# estimate scale transformations
# and transform the whole OMIP021Samples

transList <- estimateScaleTransforms(
  ff = OMIP021Samples[[1]],
  fluoMethod = "estimateLogicle",
  scatterMethod = "linearQuantile",
  scatterRefMarker = "BV785 - CD3")

OMIP021Trans <- CytoPipeline::applyScaleTransforms(
  OMIP021Samples,
  transList)

ffList <- c(
  flowCore::flowSet_to_list(OMIP021Trans),
  lapply(3:5,
    FUN = function(i) {
      aggregateAndSample(
        OMIP021Trans,
        seed = 10*i,
        nTotalEvents = 5000)[,1:22]
    })))

fsNames <- c("Donor1", "Donor2", paste0("Agg",1:3))
names(ffList) <- fsNames

fsAll <- as(ffList,"flowSet")

flowCore::pData(fsAll)$type <- factor(c("real", "real", rep("synthetic", 3)))
flowCore::pData(fsAll)$grpId <- factor(c("D1", "D2", rep("Agg", 3)))

# calculate all pairwise distances

pwDist <- pairwiseEMDDist(fsAll,
    channels = c("FSC-A", "SSC-A"),
    verbose = FALSE)

# compute Metric MDS object with explicit number of dimensions
```
mdsObj <- computeMetricMDS(pwDist, nDim = 4, seed = 0)

dim <- nDim(mdsObj) # should be 4

#' # compute Metric MDS object by reaching a target pseudo RSquare
mdsObj2 <- computeMetricMDS(pwDist, seed = 0, targetPseudoRSq = 0.999)

# Shepard diagrams
p2D <- ggplotSampleMDSShepard(
    mdsObj, 
    nDim = 2, 
    pointSize = 1, 
    title = "Shepard with 2 dimensions")

p3D <- ggplotSampleMDSShepard(
    mdsObj, 
    nDim = 3, 
    title = "Shepard with 3 dimensions")

#' pDefD <- ggplotSampleMDSShepard(
    mdsObj, 
    title = "Shepard with default nb of dimensions")

---

ggplotSampleMDSWrapBiplots

SampleMDS biplot wrapping

Description

ggplotSampleMDSWrapBiplots calls ggplotSampleMDS repeatedly to generate biplots with different sets of external variables and align them in a grid using the patchwork package, in a similar fashion as ggplot2::facet_wrap() does.

Usage

ggplotSampleMDSWrapBiplots(
    mdsObj, 
    extVariableList, 
    ncol = NULL, 
    nrow = NULL, 
    byrow = NULL, 
    displayLegend = TRUE, 
    ... 
)
Arguments

- mdsObj: a MDS object, output of the `computeMetricMDS()` method
- extVariableList: should be a named list of external variable matrices. Each element of the list should be a matrix with named columns corresponding to the variables. The number of rows should be the same as the number of samples.
- ncol: passed to `patchwork::wrap_plots()`
- nrow: passed to `patchwork::wrap_plots()`
- byrow: passed to `patchwork::wrap_plots()`
- displayLegend: if FALSE, will de-active the legend display
- ...: additional parameters passed to `ggplotSampleMDS()` (if used)

Value

- a ggplot object

See Also

- `ggplotSampleMDS`, `ggplotSampleMDSShepard`, `computeMetricMDS`

Examples

```r
library(CytoPipeline)
data(OMIP021Samples)

# estimate scale transformations
# and transform the whole OMIP021Samples

transList <- estimateScaleTransforms(
  ff = OMIP021Samples[[1]],
  fluoMethod = "estimateLogicle",
  scatterMethod = "linearQuantile",
  scatterRefMarker = "BV785 - CD3")

OMIP021Trans <- CytoPipeline::applyScaleTransforms(
  OMIP021Samples,
  transList)

# As there are only 2 samples in OMIP021Samples dataset,
# we create artificial samples that are random combinations of both samples

ffList <- c(
  flowCore::flowSet_to_list(OMIP021Trans),
  lapply(3:5, FUN = function(i) {
    aggregateAndSample(
      OMIP021Trans,
```
seed = 10*i,
        nTotalEvents = 5000[,1:22]
    )

fsNames <- c("Donor1", "Donor2", paste0("Agg",1:3))
names(ffList) <- fsNames

fsAll <- as(ffList,"flowSet")
flowCore::pData(fsAll)$type <- factor(c("real", "real", rep("synthetic", 3)))
flowCore::pData(fsAll)$grpId <- factor(c("D1", "D2", rep("Agg", 3)))

# calculate all pairwise distances
pwDist <- pairwiseEMDDist(fsAll,
                           channels = c("FSC-A", "SSC-A"),
                           verbose = FALSE)

# compute Metric MDS object with explicit number of dimensions
mdsObj <- computeMetricMDS(pwDist, nDim = 4, seed = 0)
dim <- nDim(mdsObj) # should be 4

#' # compute Metric MDS object by reaching a target pseudo RSquare
mdsObj2 <- computeMetricMDS(pwDist, seed = 0, targetPseudoRSq = 0.999)

# plot mds projection on axes 1 and 2,
# use 'group' for colour, 'type' for shape, and no label
p_12 <- ggplotSampleMDS(
            mdsObj = mdsObj,
            pData = flowCore::pData(fsAll),
            projectionAxes = c(1,2),
            pDataForColour = "grpId",
            pDataForShape = "type")

# try to associate axes with median or std deviation of each channel
# => use bi-plots
extVarList <- channelSummaryStats(
            fsAll,
            channels = c("FSC-A", "SSC-A"),
            statFUNs = c("median" = stats::median,
                         "std.dev" = stats::sd))

bpFull <- ggplotSampleMDSWrapBiplots(
            mdsObj = mdsObj,
            extVariableList = extVarList,
            pData = flowCore::pData(fsAll),
            projectionAxes = c(1,2),
            pDataForColour = "group",
            pDataForShape = "type",
            seed = 0)
MDS-class

Description

Class representing Multi Dimensional Scaling (MDS) projection.
returns the value of the stress criterion, minimized by the SMACOF algorithm.
returns a vector of nPoints dimension, containing the stress indicator per point. The stress mini-
mization criterion can indeed be allocated per represented point. The more the stress of a particular
point, the less accurate its distances w.r.t. the other points.

Usage

## S4 method for signature 'MDS'
show(object)

nDim(x)
nPoints(x)
pwDist(x)
projections(x)
projDist(x)
stress(x)
spp(x)
eigenVals(x)
pctvar(x)
RSq(x)
RSqVec(x)
GoF(x)
smacofRes(x)

Arguments

object a MDS object
x a MDS object
Value

nothing

Slots

nDim numeric, nb of dimensions of the projection

pwDist An object of class dist storing the triangular relevant part of the symmetric, zero diagonal pairwise distance matrix (nPoints * nPoints), BEFORE projection.

proj The projection matrix, resulting from MDS

projDist An object of class dist storing the triangular relevant part of the symmetric, zero diagonal pairwise distance matrix (nPoints * nPoints), AFTER projection.

eigen numeric, vector of nDim length, containing the eigen values of the PCA that is applied after the Smacof algorithm.

pctvar numeric, vector of nDim length, containing the percentage of explained variance per axis.

RSq numeric, vector of pseudo R square indicators, as a function of number of dimensions. RSq[nDim] is the global pseudo R square, as displayed on plots.

GoF numeric, vector of goodness of fit indicators, as a function of number of dimensions. GoF[nDim] is the global goodness of fit.

smacofRes an object of class 'smacofB' containing the algorithmic optimization results, for example stress and stress per point, as returned by smacof::smacofSym() method.

Examples

nHD <- 10
nLD <- 2
nPoints <- 20

# generate uniformly distributed points in 10 dimensions
points <- matrix(
  data = runif(n = nPoints * nHD),
  nrow = nPoints)

# calculate euclidian distances
pwDist <- dist(points)

# compute Metric MDS object by reaching a target pseudo RSquare
mdsObj <- computeMetricMDS(pwDist, targetPseudoRSq = 0.95)

show(mdsObj)
pairwiseEMDDist

Pairwise Earth Mover’s Distance calculation

Description

Computation of all EMD between pairs of flowFrames belonging to a flowSet. This method provides two different input modes:

- the user provides directly a flowSet loaded in memory (RAM).
- the user provides (1.) a number of samples nSamples; (2.) an ad-hoc function that takes as input an index between 1 and nSamples, and codes the method to load the corresponding flowFrame in memory; Optional row and column ranges can be provided to limit the calculation to a specific rectangle of the matrix. These i.e. can be specified as a way to split heavy calculations of large distance matrices on several computation nodes.

Usage

```r
pairwiseEMDDist(
  x,
  rowRange = c(1, nSamples),
  colRange = c(min(rowRange), nSamples),
  loadFlowFrameFUN = NULL,
  loadFlowFrameFUNArgs = NULL,
  channels = NULL,
  verbose = FALSE,
  BPPARAM = BiocParallel::SerialParam(),
  BPOPTIONS = BiocParallel::bpoptions(packages = c("flowCore")),
  binSize = 0.05,
  minRange = -10,
  maxRange = 10
)
```

Arguments

- `x` either a flowCore::flowSet, or the number of samples (integer >=1)
- `rowRange` the range of rows of the distance matrix to be calculated
- `colRange` the range of columns of the distance matrix to be calculated
- `loadFlowFrameFUN` the function used to translate a flowFrame index into a flowFrame. In other words, the function should code how to load a specific flowFrame into memory. Important: the flowFrame index should be the first function argument and should be named ffIndex.
- `loadFlowFrameFUNArgs` (optional) a named list containing additional input parameters of `loadFlowFrameFUN()`
- `channels` which channels (integer index(ices) or character(s)):
pairwiseEMDDist

- if it is a character vector, it can refer to either the channel names, or the marker names
- if it is a numeric vector, it refers to the indexes of channels in fs
- if NULL all scatter and fluorescent channels of fs will be selected

verbose

if TRUE, output a message after each single distance calculation

BPPARAM

sets the BPPARAM back-end to be used for the computation. If not provided, will use BiocParallel::SerialParam() (no task parallelization)

BPOPTIONS

sets the BPOPTIONS to be passed to bplapply() function. Note that if you use a SnowParams back-end, you need to specify all the packages that need to be loaded for the different CytoProcessingStep to work properly (visibility of functions). As a minimum, the flowCore package needs to be loaded. (hence the default BPOPTIONS = bpoptions(packages = c("flowCore")))

binSize

size of equal bins to approximate the marginal distributions.

minRange

minimum value taken when approximating the marginal distributions

maxRange

maximum value taken when approximating the marginal distributions

Value

a distance matrix of pairwise distances (full symmetric with 0. diagonal)

Examples

library(CytoPipeline)

data(OMIP021Samples)

# estimate scale transformations
# and transform the whole OMIP021Samples

transList <- estimateScaleTransforms(
  ff = OMIP021Samples[[1]],
  fluoMethod = "estimateLogicle",
  scatterMethod = "linearQuantile",
  scatterRefMarker = "BV785 - CD3")

OMIP021Trans <- CytoPipeline::applyScaleTransforms(
  OMIP021Samples,
  transList)

# calculate pairwise distances using only FSC-A & SSC-A channels
pwDist <- pairwiseEMDDist(
  x = OMIP021Trans,
  channels = c("FSC-A", "SSC-A"))
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