Package 'statTarget'

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Type Package

Title Statistical Analysis of Molecular Profiles

Version 2.0

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Imports randomForest,plyr,pdist,ROC,utils,grDevices,graphics,rrcov,stats, pls,impute

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Description A streamlined tool provides a graphical user interface for quality control based signal drift correction, integration of data from multi-batch MS-based experiments, and the comprehensive statistical analysis in metabolomics and targeted proteomics.

License LGPL (>= 3)

URL https://stattarget.github.io

biocViews Metabolomics, Proteomics, Machine Learning, MassSpectrometry, QualityControl, Normalization, DifferentialExpression, BatchEffect, Visualization, MultipleComparison,Preprocessing, GUI, Software

RoxygenNote 6.0.1

LazyData true

NeedsCompilation no

BuildVignettes true

R topics documented:

`statTarget-package` *Statistical Analysis of Molecular Profiles*

Description

An streamlined tool provides graphical user interface for quality control based signal correction, integration of MS-based data from multiple batches, and the comprehensive statistical analysis for omics studies.

Usage

```
statTarget()
```

Details

Package: statTarget

Type: package

License: LGPL (>= 3)

Value

A description of statTarget. See the details at https://stattarget.github.io

Author(s)

Hemi Luan

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`mdsPlot` *MDSplot in statTarget*

Description

Multi-dimensional scaling plot of proximity matrix from randomForest.

Usage

```
mdsPlot(rForest,pimpModel,Labels = TRUE,slink = FALSE,
slinkDat, ...)
```

Arguments

rForest	An object of class randomForest that contains the proximity component from statTarget_rForest function.
pimpModel	An object of permutation-based variable Gini importance measures (PIMP-algorithm) from statTarget_rForest function.
Labels	Labels is TRUE for visible the sample name in the figure else with the index for class.
slink	Logical indicating if slinkDat is active for extenal classID.
slinkDat	A data frame for the extenal classID.
...	A generic MDSplot function in randomForest package

Value

The output of cmdscale on 1 - rf$proximity is returned invisibly.

Author(s)

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See Also

MDSplot

Examples

```
datpath <- system.file('extdata',package = 'statTarget')
statFile <- paste(datpath,'data_example.csv', sep='/')
getFile <- read.csv(statFile,header=TRUE)
rFtest <- rForest(getFile,ntree = 10,times = 5)
mdsPlot(rFtest$randomForest,rFtest$pimpTest)
```

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predict_RF *preidict function for random forest objects in statTarget*

Description

Prediction of test data using random forest in statTarget.

Usage

```
predict_RF(object, newdata, type='response',...)
```

Arguments

object	An object created by the function statTarget_rForest.
newdata	A data frame or matrix containing new data. (Note: If not given, the out-of-bag prediction in object is returned. see randomForest package.
type	One of response, prob. or votes, indicating the type of output: predicted values, matrix of class probabilities, or matrix of vote counts. class is allowed, but automatically converted to 'response', for backward compatibility.
...	A generic predict function from randomForest package.

Value

A class of predicted values is returned. Object type is classification, for detail see randomForest package.

Author(s)

Hemi Luan, hemi.luan@gmail.com

See Also

randomForest

Examples

```
datpath <- system.file('extdata',package = 'statTarget')
statFile <- paste(datpath,'data_example.csv', sep='/')
getFile <- read.csv(statFile,header=TRUE)
rFtest <- rForest(getFile,ntree = 10,times = 5)
predictOutput <- predict_RF(rFtest, getFile[1:19,3:8])
```

---

pvimPlot *Gini importance and permutation-based variable importance measures plots*

Description

Create plots for Gini importance and permutation-based variable Gini importance measures.

Usage

```
pvimPlot(rForest,pimpModel,nvarRF = 6,border= NA,
space = 0.3,...)
```

Arguments

rForest	an object of class randomForest that contains the proximity component from statTarget rForest function.
pimpModel	an object of permutation-based variable Gini importance measures (PIMP-algorithm) from statTarget rForest function.
nvarRF	The number of variables in importance plot of randomForest.
border	The color to be used for the border of the bars. Use border = NA to omit borders. see also barplot.
space	The amount of space (as a fraction of the average bar width) left before each bar. May be given as a single number or one number per bar. see also barplot
...	A generic barplot function from graphics package.

Value

The output of the name of selected variable importance.

Author(s)

Hemi Luan, hemi.luan@gmail.com

Examples

```
datpath <- system.file('extdata',package = 'statTarget')
statFile <- paste(datpath,'data_example.csv', sep='/')
getFile <- read.csv(statFile,header=TRUE)
rFtest <- rForest(getFile,ntree = 10,times = 5)
pvimPlot(rFtest$randomForest,rFtest$pimpTest)
```

---

rForest *Random Forest classfication in statTarget*

Description

rForest provides the Breiman's random forest algorithm for classification and permutation-based variable importance measures (PIMP-algorithm).

Usage

```
rForest(file,ntree = 100,times = 100, gDist = TRUE,
seed = 123,...)
```

Arguments

file	An data frame or 'Stat File' from statTarget software.
ntree	Number of trees to grow. This should not be set to too small a number, to ensure that every input row gets predicted at least a few times.
times	The number of permutations for permutation-based variable importance measures.
gDist	If gDist is TRUE the null importance distributions are approximated with Gaussian distributions else with empirical cumulative distributions.
seed	For the same set of random variables and reproducible results.
...	A generic function in randomForest package

Value

Objects Two objects from statTarget_rForest (1. randomForest,rfModel; 2. PIMPresult, pimpModel)

VarImp The original Gini importance

PerVarImp A matrix, where the permuted VarImp measures for the predictor variable.

p-value The probability of observing the original VarImp or a larger value, given the fitted null importance distribution.

p.ks.test The p-values of the Kolmogorov-Smirnov Tests for each row PerVarImp.

Author(s)

Hemi Luan, hemi.luan@gmail.com

References

Altmann A.,Tolosi L.,Sander O. and Lengauer T. (2010) Permutation importance: a corrected feature importance measure, Bioinformatics 26 (10), 1340-1347.

Ender Celik. (2015) vita: Variable Importance Testing Approaches. R package version 1.0.0 https://CRAN.R-project.org/package=vita

Examples

```
datpath <- system.file('extdata',package = 'statTarget')
statFile <- paste(datpath,'data_example.csv', sep='/')
getFile <- read.csv(statFile,header=TRUE)
rFtest <- rForest(getFile,ntree = 10,times = 5)
```

`shiftCor` *shiftCor for GUI*

Description

shiftCor provides the QC based signal correction for large scale metabolomics and targeted proteomics.

Usage

```
shiftCor(samPeno, samFile, Frule = 0.8, MLmethod = "QCRFSC", ntree = 500,
  QCspan = 0, degree = 2, imputeM = "KNN")
```

Arguments

`samPeno`	The file with the meta information including the sample name, batches, class and order.
`samFile`	The file with the expression information.
`Frule`	Modified n precent rule function. A variable will be kept if it has a non-zero value for at least n precent of samples in any one group. (Default: 0.8)
`MLmethod`	The machine learning method for QC based signal correction. i.e. QC based random forest signal correction (QC-RFSC) and QC based LOESS signal correction (QC-RLSC).
`ntree`	Number of trees to grow in random forest model.
`QCspan`	The smoothing parameter for QC-RLSC which controls the bias-variance trade-off in QC-RLSC method if the QCspan is set at '0', the generalised cross-validation will be performed to avoid overfitting the observed data.
`degree`	Lets you specify local constant regression (i.e., the Nadaraya-Watson estimator, degree=0), local linear regression (degree=1), or local polynomial fits (degree=2, the default) for QC-RLSC.
`imputeM`	The parameter for imputation method i.e., nearest neighbor averaging, 'KNN'; minimum values, 'min'; Half of minimum values, 'minHalf'; median values, 'median'.

Value

the shiftCor files.

Examples

```
datpath <- system.file('extdata',package = 'statTarget')
samPeno <- paste(datpath,'MTBLS79_sampleList.csv', sep='/')
samFile <- paste(datpath,'MTBLS79.csv', sep='/')
shiftCor(samPeno,samFile, Frule = 0.8, MLmethod = 'QCRFSC', QCspan = 0,imputeM = 'KNN')
```

`statAnalysis` *statAnalysis for statistical analysis for omics data or others.*

Description

statAnalysis provides the statistical analysis for metabolomics data or others.

Usage

```
statAnalysis(file, Frule = 0.8, normM = "NONE", imputeM = "KNN",
  glog = TRUE, FDR = TRUE, ntree = 500, nvarRF = 5,
  scaling = "Pareto", silt = 20, pcax = 1, pcay = 2, Labels = TRUE,
  upper.lim = 2, lower.lim = 0.5, sig.lim = 0.05)
```

Arguments

`file`	The file with the expression information.
`Frule`	Modified n precent rule function. A variable will be kept if it has a non-zero value for at least n precent of samples in any one group. (Default: 0.8)
`normM`	The parameter for normalization method (i.e median quotient normalization, 'PQN'; integral normalization , 'SUM', and 'NONE').
`imputeM`	The parameter for imputation method i.e., nearest neighbor averaging, 'KNN'; minimum values, 'min'; Half of minimum values, 'minHalf'; median values, 'median'.
`glog`	Generalised logarithm (glog) transformation, with the default value TRUE. The glog is a better behaved log transformation when some data values are zero or just near zero.
`FDR`	The false discovery rate for conceptualizing the rate of type I errors in null hypothesis testing when conducting multiple comparisons.
`ntree`	Number of trees to grow for randomForest model. This should not be set to too small a number, to ensure that every input row gets predicted at least a few times.
`nvarRF`	The number of the variables with top importance in randomforest model
`scaling`	Scaling method before statistic analysis (PCA or PLS-DA). 'pareto', 'Pareto', 'p' or 'P' can be used for specifying the Pareto scaling. 'auto', 'Auto', 'auto', 'a' or 'A' can be used for specifying the Auto scaling (or unit variance scaling). 'vast', 'Vast', 'v' or 'V' can be used for specifying the vast scaling. 'range', 'Range', 'r' or 'R' can be used for specifying the Range scaling.
`silt`	The number of permutation for PLS-DA model and variable importance of randomForest.
`pcax`	Principal components in PCA model for the x-axis.
`pcay`	Principal components in PCA model for the y-axis.

Labels	Name labels for score plot of multiple statistical analysis
upper.lim	The up-regulated metabolites using Fold Changes cut off values in the Volcano plot. Fold change values will be calculated before normalization step.
lower.lim	The down-regulated metabolites using Fold Changes cut off values in the Volcano plot. Fold change values will be calculated before normalization step.
sig.lim	The significance level for metabolites in the Pvalues file in the Volcano plot.
DataPretreatment	shows pretreatmented data that is processed with normalization or glog transformation procedure.
dataSummary	produces the results summaries of various statistics .
scaleData	shows the results of scaling procedure.
PCA_Data_xx	shows the results of PCA analysis.
PLS_DA_xx	shows the results of PLS(-DA) analysis.
randomForest	shows results of randomForest analysis and permutation based variable importance.
Univariate	shows fold changes, P value, ROC, odd ratio, volcano plot between any two groups, and box plot for all groups.

Value

The statAnalsis output files. See the details at https://stattarget.github.io

Author(s)

Hemi Luan, hemi.luan@gmail.com

Examples

```
datpath <- system.file('extdata',package = 'statTarget')
file <- paste(datpath,'data_example.csv', sep='/')
statAnalysis(file,Frule = 0.8, normM = 'NONE', imputeM = 'KNN', glog = TRUE,scaling = 'Pareto')
```

---

statTargetGUI *statTargetGUI for statTarget software*

Description

The statTarget GUI session. The Signal Correction and Statistical Analysis session are included in statTarget 2.0 software. See the details at https://stattarget.github.io

Usage

```
statTargetGUI()
```

Value

The output of GUI

Author(s)

Hemi Luan hemi.luan@gmail.com

References

Dunn WB., et al. Nat Protoc. 2011, 6, pp1060. Luan H., et al. GigaScience 2015, 4, pp16. Luan H., et al. J. Proteome Res., 2015, 14, pp467.

Examples

```
if (interactive()) {statTargetGUI()}
```

---

transX *transX for statTarget inputs*

Description

transX is to generate statTarget input file formats from Mass Spectrometry Data softwares, such as XCMS, SIEVE and SKYLINE

Usage

```
transX(data, type)
```

Arguments

data	A transX objects. The output file from Mass Spectrometry Data softwares.
type	The output file formats from Mass Spectrometry Data software, including 'XCMS' or 'xcms','SIEVE' or 'sieve' and 'skyline' or 'SKYLINE';

Value

An output directory named 'statTargetDirectory'

Author(s)

Hemi Luan, hemi.luan@gmail.com

Examples

```
datpath <- system.file('extdata',package = 'statTarget')
dataXcms <- paste(datpath,'xcmsOutput.tsv', sep='/')
dataSkyline <- paste(datpath,'skylineDemo.csv', sep='/')
transX(dataXcms,'xcms')
```

Index