

Package ‘pathMED’

April 21, 2026

Title Scoring Personalized Molecular Portraits

Version 1.3.0

Description PathMED is a collection of tools to facilitate precision medicine studies with omics data (e.g. transcriptomics). Among its functionalities, genesets scores for individual samples may be calculated with several methods. These scores may be used to train machine learning models and to predict clinical features on new data. For this, several machine learning methods are evaluated in order to select the best method based on internal validation and to tune the hyperparameters. Performance metrics and a ready-to-use model to predict the outcomes for new patients are returned.

Depends R (>= 4.5.0)

Suggests ada, AUCCell, Biobase, BiocGenerics, BiocStyle, fgsea (>= 1.15.4), gam, GSEABase, import, kernlab, klaR, knitr, mboost, MLeval, randomForest, ranger, rmarkdown, RUnit, SummarizedExperiment, utils, xgboost

Imports BiocParallel, caret, caretEnsemble, decoupleR, ggplot2, GSVA, factoextra, FactoMineR, magrittr, matrixStats, methods, metRica, pbapply, reshape2, singscore, stats, stringi, dplyr,

VignetteBuilder knitr

biocViews Pathways, Classification, FeatureExtraction, Transcriptomics

BugReports <https://github.com/jordimartorell/pathMED/issues>

URL <https://github.com/jordimartorell/pathMED>

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| | |
|----------|---|
| ann2term | <i>Annotate the pathways from a scores matrix</i> |
|----------|---|

Description

Annotate the pathways from a scores matrix

Usage

```
ann2term(scoresMatrix)
```

Arguments

scoresMatrix Matrix with pathways IDs as row names

Value

A data frame with the input IDs and their corresponding terms

Author(s)

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References

Toro-Domínguez, D. et al (2022). *Scoring personalized molecular portraits identify Systemic Lupus Erythematosus subtypes and predict individualized drug responses, symptomatology and disease progression* . Briefings in Bioinformatics. 23(5)

See Also

[getScores](#)

Examples

```
data(pathMEExampleData)
scoresExample <- getScores(pathMEExampleData, geneSets = "tmod",
                           method = "GSVA")
annotatedTerms <- ann2term(scoresExample)
```

| | |
|----------------|--|
| buildRefObject | <i>Create a reference data object for input to the pathMED functions</i> |
|----------------|--|

Description

Create a reference data object for input to the pathMED functions

Usage

```
buildRefObject(data, metadata = NULL, groupVar, controlGroup, use.assay = 1)
```

Arguments

| | |
|--------------|---|
| data | A list of matrices, data frames, ExpressionSets or SummarizedExperiments with samples in columns and features in rows. A single matrix, dataframe, ExpressionSet or SummarizedExperiment may be also used. |
| metadata | A list of data frames or a single data frame with information for each sample. Samples in rows and variables in columns. If a list of ExpressionSets or SummarizedExperiments are used as @data, it is not necessary to provide @metadata. |
| groupVar | Character or list of characters indicating the column name of @metadata classifying the samples in controls and cases. If several metadata objects are provided a @groupVar can be specified for each metadata. |
| controlGroup | Character or list of characters indicating which @groupVar level corresponds to the control group, usually healthy samples. All other samples will be considered as cases, usually disease samples. If several @groupVar are provided a @controlGroup can be specified for each @groupVar |
| use.assay | If SummarizedExperiments are used, the number of the assay to extract the data. |

Value

A refObject that serves as input for mScores_createReference and dissectDB functions.

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References

Toro-Domínguez, D. et al (2022). *Scoring personalized molecular portraits identify Systemic Lupus Erythematosus subtypes and predict individualized drug responses, symptomatology and disease progression* . Briefings in Bioinformatics. 23(5)

See Also

[mScores_createReference](#), [dissectDB](#)

Examples

```
data(refData)

refObject <- buildRefObject(
  data = list(
    refData$dataset1, refData$dataset2,
    refData$dataset3, refData$dataset4
  ),
  metadata = list(
    refData$metadata1, refData$metadata2,
    refData$metadata3, refData$metadata4
  ),
  groupVar = "group",
  controlGroup = "Healthy_sample"
)

## Also works with a metadata for all datasets
metadata <- rbind(
  refData$metadata1, refData$metadata2,
  refData$metadata3, refData$metadata4
)
refObject <- buildRefObject(
  data = list(
    refData$dataset1, refData$dataset2,
    refData$dataset3, refData$dataset4
  ),
  metadata = metadata,
  groupVar = "group",
  controlGroup = "Healthy_sample"
)
```

dissectDB

*Split pathways into coexpressed subpathways***Description**

Split pathways into coexpressed subpathways

Usage

```
dissectDB(
  refObject,
  geneSets,
  minPathSize = 10,
  minSplitSize = 3,
  maxSplits = NULL,
  explainedVariance = 60,
  percSharedGenes = 90,
  use.assay = 1
)
```

Arguments

| | |
|-------------------|--|
| refObject | A refObject object structure: a list of lists, each one with a cases omic matrix and controls omic matrix (named as Disease and Healthy). It can be constructed with the buildRefObject function. A list with one or more expression matrices, ExpressionSets or SummarizedExperiments without controls, can also be used. Data should be normalized and log2-transformed. Feature names must match the gene sets nomenclature. To use preloaded databases, they must be gene symbols. |
| geneSets | A named list with each gene set, or the name of one preloaded database (go_bp, go_cc, go_mf, kegg, reactome, pharmgkb, lincs, ctd, disgenet, hpo, wikipathways, tmod) or a GeneSetCollection. |
| minPathSize | numeric, minimum number of genes in a pathway to consider splitting it. |
| minSplitSize | numeric, minimum number of genes in a subpathway. Smaller splits will be merged with the closest coexpressed subpathway. |
| maxSplits | numeric, maximum number of subpathways for a pathway. If NULL (default), there is not limit. |
| explainedVariance | numeric, percentage of cumulative variance explained within a pathway. This parameter is used to select the number of subdivisions of a pathway that manage to explain at least the percentage of variance defined by explainedVariance. |
| percSharedGenes | numeric, minimum percentage of common genes across datasets to merge them before clustering. If NULL or this percentage is not reached, clustering is performed for each dataset independently and consensus subpathways are obtained from co-occurrence across datasets. |
| use.assay | If SummarizedExperiments are used, the number of the assay to extract the data. |

Value

A list with the subpathways.

Author(s)

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References

Toro-Domínguez, D. et al (2022). *Scoring personalized molecular portraits identify Systemic Lupus Erythematosus subtypes and predict individualized drug responses, symptomatology and disease progression*. Briefings in Bioinformatics. 23(5)

See Also

[buildRefObject](#), [mScores_createReference](#), [getScores](#)

Examples

```
data(refData)

refObject <- buildRefObject(
  data = list(
    refData$dataset1, refData$dataset2,
    refData$dataset3, refData$dataset4
  ),
  metadata = list(
    refData$metadata1, refData$metadata2,
    refData$metadata3, refData$metadata4
  ),
  groupVar = "group",
  controlGroup = "Healthy_sample"
)

set.seed(123)
custom.tmod <- dissectDB(refObject, geneSets = "tmod")
```

genesetsData

Preloaded gene sets

Description

genesetsData was constructed from the GeneCodis database (<https://genecodis.genyo.es/>)

Usage

```
data(genesetsData)
```

Format

An object of class "list" with one list per database. Each database consists on a list of gene sets, containing the gene symbols associated to it.

getScores

Calculate pathways scores for a dataset

Description

Calculate pathways scores for a dataset

Usage

```
getScores(
  inputData,
  geneSets,
  method = "GSVA",
  labels = NULL,
  cores = 1,
  use.assay = 1,
  ...
)
```

Arguments

| | |
|-----------|---|
| inputData | Matrix, data frame, ExpressionSet or SummarizedExperiment with omics data. Feature names must match the gene sets nomenclature. To use preloaded databases, they must be gene symbols. |
| geneSets | A named list with each gene set, or the name of one preloaded database (go_bp, go_cc, go_mf, kegg, reactome, pharmgkb, lincs, ctd, disgenet, hpo, wikipathways, tmod) or a GeneSetCollection. For using network methods, a data frame including columns: "source", "target", "weight" and "mor" (optional). |
| method | Scoring method: M-Scores, GSVA, ssGSEA, singscore, Plage, Z-score, AUCell, MDT, MLM, ORA, UDT, ULM, FGSEA, norm_FGSEA, WMEAN, norm_WMEAN, corr_WMEAN, WSUM, norm_WSUM or corr_WSUM. |
| labels | (Only for M-Scores) Vector with the samples class labels (0 or "Healthy" for control samples). Optional. |
| cores | Number of cores to be used. |
| use.assay | If SummarizedExperiments are used, the number of the assay to extract the data. |
| ... | Additional parameters for the scoring functions. |

Value

A list with the results of each of the analyzed regions. For each region type, a data frame with the results and a list with the probes associated to each region are generated. In addition, this list also contains the input methData, pheno and platform objects

Author(s)

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References

Toro-Domínguez, D. et al (2022). *Scoring personalized molecular portraits identify Systemic Lupus Erythematosus subtypes and predict individualized drug responses, symptomatology and disease progression* . Briefings in Bioinformatics. 23(5)

See Also

[trainModel](#)

Examples

```
data(pathMEExampleData)
scoresExample <- getScores(pathMEExampleData, geneSets = "tmod",
                           method = "GSVA")
```

methodsML

Prepare the models parameter for the trainModel function

Description

Prepare the models parameter for the trainModel function

Usage

```
methodsML(algorithms = c("rf", "knn", "nb"), outcomeClass, tuneLength = 20)
```

Arguments

| | |
|--------------|--|
| algorithms | Vector with one or more of these methods: 'glm', 'lm', 'lda', 'xgbTree', 'rf', 'knn', 'svmLinear', 'nnet', 'svmRadial', 'nb', 'lars', 'rpart', 'gamboost', 'ada', 'brnn', 'enet', or 'all' to use all algorithms |
| outcomeClass | Predicted variable type ('character' or 'numeric') |
| tuneLength | maximum number of tuning parameter combinations |

Value

A list with the selected models ready to use as the 'models' parameter in the trainModel function

Author(s)

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References

Toro-Domínguez, D. et al (2022). *Scoring personalized molecular portraits identify Systemic Lupus Erythematosus subtypes and predict individualized drug responses, symptomatology and disease progression* . Briefings in Bioinformatics. 23(5)

See Also

[trainModel](#)

Examples

```
models <- methodsML(c("rf", "knn"), tuneLength = 20,  
                   outcomeClass = "character")
```

mScores_createReference

Create a reference dataset based on M-scores

Description

Create a reference dataset based on M-scores

Usage

```
mScores_createReference(refObject, geneSets, cores = 1)
```

Arguments

| | |
|-----------|---|
| refObject | A refObject object structure: a list of lists, each one with a cases omic matrix and controls omic matrix (named as Disease and Healthy). It can be constructed with the buildRefObject function. Feature names must match the gene sets nomenclature. To use preloaded databases, they must be gene symbols. |
| geneSets | A named list with each gene set, or the name of one preloaded database (go_bp, go_cc, go_mf, kegg, reactome, pharmgkb, lincs, ctd, disgenet, hpo, wikipathways, tmod) or a GeneSetCollection. |
| cores | Number of cores to be used. |

Value

A list with three elements. The first one is a list with the M-scores for each dataset. The second one is the geneSet used for the analysis and the third one is the input data.

Author(s)

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References

Toro-Domínguez, D. et al (2022). *Scoring personalized molecular portraits identify Systemic Lupus Erythematosus subtypes and predict individualized drug responses, symptomatology and disease progression*. Briefings in Bioinformatics. 23(5)

See Also

[mScores_imputeFromReference](#), [dissectDB](#), [mScores_filterPaths](#), [trainModel](#)

Examples

```

data(refData)

refObject <- buildRefObject(
  data = list(
    refData$dataset1, refData$dataset2,
    refData$dataset3, refData$dataset4
  ),
  metadata = list(
    refData$metadata1, refData$metadata2,
    refData$metadata3, refData$metadata4
  ),
  groupVar = "group",
  controlGroup = "Healthy_sample"
)

refMscore <- mScores_createReference(refObject, geneSets = "tmod")

```

mScores_filterPaths *Filter pathways from the reference M-scores dataset*

Description

Filter pathways from the reference M-scores dataset

Usage

```

mScores_filterPaths(
  MRef,
  min_datasets = round(length(MRef[[1]]) * 0.34),
  perc_samples = 10,
  Pcutoff = 0.05,
  plotMetrics = TRUE
)

```

Arguments

| | |
|--------------|---|
| MRef | output from the mScores_createReference function |
| min_datasets | number of datasets that each pathway must meet the perc_samples threshold |
| perc_samples | minimum percentage of samples in a dataset in which a pathway must be significant |
| Pcutoff | P-value cutoff for significance |
| plotMetrics | Plot number of significant pathways selected based on the different combination of perc_samples and min_datasets parameters |

Value

A list with the selected pathways

Author(s)

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References

Toro-Domínguez, D. et al (2022). *Scoring personalized molecular portraits identify Systemic Lupus Erythematosus subtypes and predict individualized drug responses, symptomatology and disease progression*. Briefings in Bioinformatics. 23(5)

See Also

[mScores_createReference](#)

Examples

```
data(refData)

refObject <- buildRefObject(
  data = list(
    refData$dataset1, refData$dataset2,
    refData$dataset3, refData$dataset4
  ),
  metadata = list(
    refData$metadata1, refData$metadata2,
    refData$metadata3, refData$metadata4
  ),
  groupVar = "group",
  controlGroup = "Healthy_sample"
)

exampleRefMScore <- mScores_createReference(refObject, geneSets = "tmod")
relevantPaths <- mScores_filterPaths(exampleRefMScore, min_datasets = 3)
```

mScores_imputeFromReference

Estimate M-scores for a dataset without healthy controls

Description

Estimate M-scores for a dataset without healthy controls

Usage

```
mScores_imputeFromReference(
  inputData,
  geneSets,
  externalReference,
  nk = 5,
  distance.threshold = 30,
  cores = 1,
  use.assay = 1
)
```

Arguments

| | |
|--------------------|---|
| inputData | Data matrix, data frame ExpressionSet or SummarizedExperiment. Feature names must match the gene sets nomenclature. To use preloaded databases, they must be gene symbols. |
| geneSets | A named list with each gene set, or the name of one preloaded database (go_bp, go_cc, go_mf, kegg, reactome, pharmgkb, lincs, ctd, disgenet, hpo, wikipathways, tmod) or a GeneSetCollection. |
| externalReference | External reference created with the mScores_createReference function. |
| nk | Number of most similar samples from the external reference to impute M-scores. |
| distance.threshold | Only samples that do not surpass the mean Euclidean distance of distance.threshold (by default = 30) with the external reference are imputed. If NULL, impute all samples. |
| cores | Number of cores to be used. |
| use.assay | If SummarizedExperiments are used, the number of the assay to extract the data. |

Value

A list with the results of each of the analyzed regions. For each region type, a data frame with the results and a list with the probes associated to each region are generated. In addition, this list also contains the input methData, pheno and platform objects

Author(s)

Jordi Martorell-Marugán, <jordi.martorell@genyo.es>

Daniel Toro-Dominguez, <danieltorodominguez@gmail.com>

References

Toro-Domínguez, D. et al (2022). *Scoring personalized molecular portraits identify Systemic Lupus Erythematosus subtypes and predict individualized drug responses, symptomatology and disease progression*. Briefings in Bioinformatics. 23(5)

See Also

[mScores_filterPaths](#), [trainModel](#)

Examples

```
data(refData, pathMEExampleData)

refObject <- buildRefObject(
  data = list(
    refData$dataset1, refData$dataset2,
    refData$dataset3, refData$dataset4
  ),
  metadata = list(
    refData$metadata1, refData$metadata2,
    refData$metadata3, refData$metadata4
  ),
  groupVar = "group",
```

```
    controlGroup = "Healthy_sample"
  )

  refMScores <- mScores_createReference(refObject,
    geneSets = "tmod", cores = 1
  )

  exampleMScores <- mScores_imputeFromReference(pathMEDEExampleData,
    geneSets = "tmod",
    externalReference = refMScores,
    distance.threshold = 50
  )
```

pathMEDEExampleData *Example of test gene expression data*

Description

pathMEDEExampleData was obtained from a dataset downloaded from NCBI GEO (GSE224705), that contains lupus patients treated with Micophenolate mofetil. The same preprocessing was done as for the datasets used to create refData. 40 patients were randomly selected, 20 samples from responding patients and 20 from non-responders.

Usage

```
data(pathMEDEExampleData)
```

Format

An object of class "data.frame" with genes in rows and samples in columns.

pathMEDEExampleMetadata *Metadata of test gene expression data*

Description

Metadata from the dataset GSE224705. Response column contains the information about the response and non-response to the drug for each sample.

Usage

```
data(pathMEDEExampleMetadata)
```

Format

An object of class "data.frame" with samples in rows and variables in columns.

predictExternal *Predict conditions in external datasets*

Description

Predict conditions in external datasets

Usage

```
predictExternal(  
  testData,  
  model,  
  realValues = NULL,  
  positiveClass = NULL,  
  use.assay = 1  
)
```

Arguments

| | |
|---------------|--|
| testData | Numerical matrix or data frame with the same features used for the model construction in rows, and the samples (new observations) in columns. An ExpressionSet may or SummarizedExperiment may also be used. |
| model | trainModel output or a caret-like model object |
| realValues | Optional, named vector (for numerical variables) or named factor (for categorical variables) with real values for each sample |
| positiveClass | Optional, positive class to get confusion matrix. Only needed when realValues = TRUE and for categorical variables |
| use.assay | If SummarizedExperiments are used, the number of the assay to extract the data. |

Value

A dataframe with predictions (if realValues is not provided) or a list with the dataframe with predictions and a dataframe with the performance metrics (if realValues is provided)

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References

Toro-Domínguez, D. et al (2022). *Scoring personalized molecular portraits identify Systemic Lupus Erythematosus subtypes and predict individualized drug responses, symptomatology and disease progression*. Briefings in Bioinformatics. 23(5)

Examples

```
data(refData)

commonGenes <- intersect(rownames(refData$dataset1),
                        rownames(refData$dataset2))
dataset1 <- refData$dataset1[commonGenes, ]
dataset2 <- refData$dataset2[commonGenes, ]

scoresExample <- getScores(dataset1, geneSets = "tmod", method = "Z-score")

set.seed(123)
trainedModel <- trainModel(
  inputData = scoresExample,
  metadata = refData$metadata1,
  var2predict = "group",
  models = methodsML("svmLinear",
                    outcomeClass = "character"
  ),
  Koutter = 2,
  Kinner = 2,
  repeatsCV = 1
)

externalScores <- getScores(dataset2, geneSets = "tmod", method = "Z-score")
realValues <- refData$metadata2$group
names(realValues) <- rownames(refData$metadata2)
predictions <- predictExternal(externalScores, trainedModel,
                              realValues = realValues
)

print(predictions)
```

refData

Example of reference gene expression datasets

Description

refData contains processed gene expression data from four datasets, including Systemic Lupus Erythematosus patients and healthy controls. Raw data for each dataset were downloaded from NCBI GEO (GSE65391, GSE45291, GSE61635, and GSE72509, respectively). Platform-dependent pre-processing was performed following established guidelines (Martorell-Marugán et al., 2021). Gene expression data were log₂-transformed, and probe sets were annotated to gene symbols. To reduce computational cost in examples, 20 patient and 10 control samples were randomly selected from each dataset.

Usage

```
data(refData)
```

Format

An object of class "list" containing eight objects (dataset1-4 and metadata1-4). Each dataset is a matrix of normalized gene expression values (genes in rows, samples in columns). Each metadata is a dataframe with two columns: samples and group.

trainModel

Train ML models and perform internal validation

Description

Train ML models and perform internal validation

Usage

```
trainModel(
  inputData,
  metadata = NULL,
  models = methodsML(outcomeClass = "character"),
  var2predict,
  positiveClass = NULL,
  pairingColumn = NULL,
  Koutter = 5,
  Kinner = 4,
  repeatsCV = 5,
  filterFeatures = NULL,
  filterSizes = seq(2, 100, by = 2),
  rerank = FALSE,
  continue_on_fail = TRUE,
  saveLogFile = NULL,
  use.assay = 1
)
```

Arguments

| | |
|---------------|---|
| inputData | Numerical matrix or data frame with samples in columns and features in rows. An ExpressionSet or SummarizedExperiment may also be used. |
| metadata | Data frame with information for each sample. Samples in rows and variables in columns. If @inputData is an ExpressionSet or SummarizedExperiment, the metadata will be extracted from it. |
| models | Named list with the ML models generated with caret::caretModelSpec function. methodsML function may be used to prepare this list. |
| var2predict | Character with the column name of the @metadata to predict |
| positiveClass | Value that must be considered as positive class (only for categoric variables). If NULL, the last class by alphabetical order is considered as the positive class. |
| pairingColumn | Optional. Character with the column name of the @metadata with pairing information (e.g. technical replicates). Paired samples will always be assigned to the same set (training/test) to avoid data leakage. |

| | |
|------------------|---|
| Koutter | Number of outer cross-validation folds. A list of integer with elements for each resampling iteration is admitted. Each list element is a vector of integers corresponding to the rows used for training on that iteration. |
| Kinner | Number of inner cross-validation folds (for parameter tuning). |
| repeatsCV | Number of repetitions of the parameter tuning process. |
| filterFeatures | "rfe" (Recursive Feature Elimination), "sbf" (Selection By Filtering) or NULL (no feature selection). |
| filterSizes | Only for filterFeatures = "rfe". A numeric vector of integers corresponding to the number of features that should be retained. |
| rerank | Only for filterFeatures = "rfe". A boolean indicating if the variable importance must be re-calculated each time features are removed. |
| continue_on_fail | Whether or not to continue training the models if any of them fail. |
| saveLogFile | Path to a .txt file in which to save error and warning messages. |
| use.assay | If SummarizedExperiments are used, the number of the assay to extract the data. |

Value

A list with four elements. The first one is the model. The second one is a table with different metrics obtained. The third one is a list with the best parameters selected in tuning process. The last element contains data for AUC plots

Author(s)

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References

Toro-Domínguez, D. et al (2022). *Scoring personalized molecular portraits identify Systemic Lupus Erythematosus subtypes and predict individualized drug responses, symptomatology and disease progression*. Briefings in Bioinformatics. 23(5)

Examples

```
data(pathMEExampleData, pathMEExampleMetadata)

scoresExample <- getScores(pathMEExampleData, geneSets = "tmod",
                           method = "GSVA")

modelsList <- methodsML("svmLinear", outcomeClass = "character")

set.seed(123)
trainedModel <- trainModel(
  inputData = scoresExample,
  metadata = pathMEExampleMetadata,
  var2predict = "Response",
  models = modelsList,
  Koutter = 2,
  Kinner = 2,
  repeatsCV = 1
)
```

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