

Package ‘fspls2’

September 12, 2026

Type Package

Title A Package to Find Minimal Transcriptional Signatures

Version 0.1.0

Date 2026-09-02

Author Lachlan Coin [aut, cre]

Imports R6, jsonlite, Matrix, glmnet, tidyr, MASS, ggplot2, pROC,
binom, confintr, DBI, RSQLite, methods, tibble, ggrepel,
RColorBrewer, data.table

Depends R (>= 4.1.0)

Maintainer Lachlan Coin <l.coin@imb.uq.edu.au>

Description Identifies minimal biomarker signatures for predicting phenotypes from multiomic data.
Integrates multiple omics layers, supports internal cross-
validation. Supports missing values in predictors and outcomes.
Enables model based imputation of uncertain values.
Supports continuous, binary, multi-class and ordinal outcomes.

License GPL-2

LazyLoad yes

NeedsCompilation no

Repository CRAN

Date/Publication 2026-09-12 12:30:02 UTC

Config/roxygen2/version 8.0.0

Encoding UTF-8

Suggests knitr, rmarkdown, testthat

VignetteBuilder knitr

Contents

analysisBase	2
analysisEnv	3
dataH	5

fspls.iterative	11
fspls.select	11
getFamily	12
getFolds	13
getTransform	13
plotEval	14

Index	16
--------------	-----------

analysisBase	<i>Analysis Base Class</i>
--------------	----------------------------

Description

A class that encapsulates a dataset holder and/or analysis of datasets

Details

Available methods:

- `new()` - Create a new instance
- `name()` - Get dataset name
- `clone()` - Clone the object

Methods

Public methods:

- `analysisBase$new()`
- `analysisBase$name()`
- `analysisBase$integrate()`
- `analysisBase$clone()`

`analysisBase$new()`: Create a new instance of base class

Usage:

```
analysisBase$new(nme, dims = NULL, flags = list(), dbDir = tempdir())
```

Arguments:

`nme` name

`dims` dims

`flags` a list object specifying options

`dbDir` location for database to be written, default to tempdir

`analysisBase$name()`: get dataset name;

Usage:

```
analysisBase$name()
```

Returns: assigned name of dataset

analysisBase\$integrate(): integrates variables from different CV runs

Usage:

analysisBase\$integrate(variables)

Arguments:

variables a variables object

analysisBase\$clone(): The objects of this class are cloneable with this method.

Usage:

analysisBase\$clone(deep = FALSE)

Arguments:

deep Whether to make a deep clone.

analysisEnv

Analysis Class

Description

A class that encapsulates analysis of one or more datasets. Only expert users will need access to this

Details

Available methods:

- new() - Create a new instance
- name() - Get dataset name
- clone() - Clone the object

@export

Super class

[analysisBase](#) -> analysisEnv

Methods

Public methods:

- [analysisEnv\\$new\(\)](#)
- [analysisEnv\\$plot_trajectory\(\)](#)
- [analysisEnv\\$select_k\(\)](#)
- [analysisEnv\\$getTodo\(\)](#)
- [analysisEnv\\$clear_db\(\)](#)
- [analysisEnv\\$savePvalsAndNextVars\(\)](#)
- [analysisEnv\\$select\(\)](#)

- `analysisEnv$clone()`

`analysisEnv$new()`: Create a new instance

Usage:

```
analysisEnv$new(flags = list(), dbDir = tempdir())
```

Arguments:

`flags` a list object specifying options

`dbDir` location for database to be written. If NULL then no DB gets the trajectory

`analysisEnv$plot_trajectory()`:

Usage:

```
analysisEnv$plot_trajectory(datasH)
```

Arguments:

`datasH` a list of dataH objects after variable selection selection for a single fold

`analysisEnv$select_k()`:

Usage:

```
analysisEnv$select_k(datasH, k1, vars_l_todo)
```

Arguments:

`datasH` a list of dataH objects

`k1` the fold

`vars_l_todo` an object representing what is left to do

Returns: `vars_l_todo` object Get todo

`analysisEnv$getTodo()`:

Usage:

```
analysisEnv$getTodo(flags, phens)
```

Arguments:

`flags` list of options

`phens` phenotypes

Returns: object outlining what is left to do for next iteration Clear the databases. Only necessary if using a database and re-running analyses

`analysisEnv$clear_db()`:

Usage:

```
analysisEnv$clear_db(drop = FALSE, exclude = "vars", datasH = NULL)
```

Arguments:

`drop` completely drop tables and start from scratch

`exclude` tables to exclude from clearing

`datasH` list of dataH objects to clear Get the next vars in iteration. Internal function

`analysisEnv$savePvalsAndNextVars()`:

Usage:

```
analysisEnv$savePvalsAndNextVars(vars_l_todo, comb2_new, data_nme, k1)
```

Arguments:

vars_l_todo vars_l_todo
 comb2_new results
 data_nme name of dataset
 k1 which repetition

Returns: object outlining what is left to do main function for variable selection

```
analysisEnv$select():
```

Usage:

```
analysisEnv$select(  
  datasH,  
  phens,  
  transform_x,  
  data_types = datasH[[1]]$data_types()  
)
```

Arguments:

datasH a list of dataH objects
 phens list of phenotypes
 transform_x transformation object
 data_types data_types object

analysisEnv\$clone(): The objects of this class are cloneable with this method.

Usage:

```
analysisEnv$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

dataH

Data holder class

Description

A class that encapsulates a dataset holder

Details

Available methods:

- new() - Create a new instance
- name() - Get dataset name
- clone() - Clone the object

Super class

analysisBase -> dataH

Methods**Public methods:**

- dataH\$new()
- dataH\$multiAnglesAndPv()
- dataH\$clear_db()
- dataH\$get_trajectory()
- dataH\$data_types()
- dataH\$split()
- dataH\$pheno()
- dataH\$dims()
- dataH\$nreps()
- dataH\$update()
- dataH\$select()
- dataH\$y()
- dataH\$plotPredictions()
- dataH\$extractPredictions()
- dataH\$plotData()
- dataH\$updateWeights()
- dataH\$getYNew()
- dataH\$getProjectedData()
- dataH\$getVariance()
- dataH\$makeAllModels()
- dataH\$evaluateAllModels()
- dataH\$clone()

dataH\$new(): Create a new instance

Usage:

```
dataH$new(  
  data,  
  y,  
  certainty = rep(1, nrow(y)),  
  nme,  
  flags,  
  family = getFamily(y),  
  dbDir = NULL  
)
```

Arguments:

data a list of matrices (of different modalities), with columns as variables and rows as samples

y phenotype matrix, with columns as outcomes and rows as samples

certainty the certainty of each observation, expressed as a probability of being correct. Default is to treat each observation as certain

nme The name of the data object.

flags list of options, described in the vignette

family the statistical family of phenotype y, can be calculated by getFamily

dbDir dir for database to store results to speed up re-runs. Can be NULL

transform_x a transformation object from the function getTransformation

`dataH$multiAnglesAndPv()`: Calculate the angles and pv across multiple phenotypes. This is an internal function and should not need to be called by user

Usage:

```
dataH$multiAnglesAndPv(comb20, k1, expt_id, vars_l_todo)
```

Arguments:

comb20 values from previous iteration

k1 k1 is the current fold

expt_id and ID for the experiment (can be 0)

vars_l_todo the variables under consideration clear database. This is only used if you want to clear the database. Internal function

phens1 phenotypes being used

flags list of options

`dataH$clear_db()`:

Usage:

```
dataH$clear_db(drop = FALSE, exclude = "vars")
```

Arguments:

drop drop the tables instead of clear

exclude which tables not to clear

`dataH$get_trajectory()`: returns data on trajectory

Usage:

```
dataH$get_trajectory()
```

Returns: a dataframe with information to plot trajectory get the data types

`dataH$data_types()`:

Usage:

```
dataH$data_types(
  data_nmes = list(all = names(private$data$data)),
  inds = lapply(data_nmes, function(x) list(pos_inds = c(), neg_inds = c(), max = 1000)),
  direction = lapply(inds, private$data$getDirection),
  incl = c(),
  excl = c()
)
```

Arguments:

data_nmes a list of names of the data names to include, optional
 inds a list of positive and negative inds, optional
 direction a direction object
 incl a list of variables to include
 excl a list of variables to exclude

Returns: an object which is used to specify both directionallity and data types

dataH\$split(): split dataset into smaller datasets

Usage:

```
dataH$split(proportions = c(0.5, 0.5))
```

Arguments:

proportions what proportions to split into

Returns: a list of dataH objects with data partiioned according to proportions

dataH\$pheno(): get the phenotypyps

Usage:

```
dataH$pheno()
```

Returns: phenotypes

dataH\$dims(): get the dimensions

Usage:

```
dataH$dims()
```

Returns: dimensions get the nreps

dataH\$nreps():

Usage:

```
dataH$nreps()
```

Returns: nreps

dataH\$update(): update the phenotypes without remaking the entire object. You can provide many phenotypes in the initialisation stage, but only consider a subset in model fitting stage in this way. Must run this before select

Usage:

```
dataH$update(
  phens = self$pheno()$all,
  flags = private$flags,
  transform_x = fromJSON(flags$transform_x),
  data_types = self$data_types()
)
```

Arguments:

phens phenotypes

flags list of options

transform_x transformation object

data_types a data_type object

dataH\$select(): main function for variable selection

Usage:

```
dataH$select(analysis = analysisEnv$new(flags = private$flags, dbDir = NULL))
```

Arguments:

analysis an analysisEnv object

dataH\$y(): provides access to internal storage of phenotype data

Usage:

```
dataH$y(phens = self$pheno()[[1]])
```

Arguments:

phens list of phenotypes

Returns: list of matrices

dataH\$plotPredictions(): ggplot to visualise predictions

Usage:

```
dataH$plotPredictions(all_modelsh, update = FALSE, liab = TRUE)
```

Arguments:

all_modelsh fitted models from makeAllModels

update whether to update

liab return liability score, or probability (for binomial, ordinal multinomial)

Returns: a ggplot

dataH\$extractPredictions(): extract the predictions for the fitted models

Usage:

```
dataH$extractPredictions(all_modelsh, liab = TRUE)
```

Arguments:

all_modelsh fitted models from makeAllModels

liab return liability score, or probability (for binomial, ordinal multinomial)

Returns: a table with results

dataH\$plotData(): plot all data for selected variables

Usage:

```
dataH$plotData(  
  variables,  
  all_types = FALSE,  
  violin = FALSE,  
  assoc = FALSE,  
  update = FALSE  
)
```

Arguments:

variables object returned by fspls.select
all_types use all types?
violin violin plots
assoc use association
update whether to use attributes from bariables to update this object, default is FALSE
Returns: a table with results

dataH\$updateWeights(): update the weights based on predictions from the model

Usage:

dataH\$updateWeights(all_models)

Arguments:

all_models the output of dataH function getAllModels

Returns: list of auc beta and updated sumdiff of weights used as stopping criteria

dataH\$getYNew(): return updated y after iterative imputation

Usage:

dataH\$getYNew()

Returns: updated y, updated certainty and indices which were updated

dataH\$getProjectedData(): get data after projection

Usage:

dataH\$getProjectedData(varnames)

Arguments:

varnames varnames

Returns: projected data after projecting out varnames

dataH\$getVariance(): get variance of data

Usage:

dataH\$getVariance(varnames)

Arguments:

varnames varnames

Returns: variance

dataH\$makeAllModels(): fit models based on variables

Usage:

dataH\$makeAllModels(variables, update = FALSE)

Arguments:

variables list of variables selected by select method

update whether to automatically update phens, transform_x and flags , default TRUE

Returns: fitted models

dataH\$evaluateAllModels(): evaluate the fit of models

Usage:

```
dataH$evaluateAllModels(all_modelsh, update = TRUE)
```

Arguments:

all_modelsh models fitted from makeAllModels

update whether to automatically update phens, transform_x and flags , default TRUE

Returns: evaluation of models

dataH\$clone(): The objects of this class are cloneable with this method.

Usage:

```
dataH$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

fspls.iterative	<i>main function for variable selection with unknown values</i>
-----------------	---

Description

main function for variable selection with unknown values

Usage

```
fspls.iterative(dataset, flags, transform_x)
```

Arguments

dataset a list with y and data value

flags list of options

transform_x transformation object

fspls.select	<i>main function for variable selection</i>
--------------	---

Description

main function for variable selection

Usage

```
fspls.select(
  datasH,
  flags,
  transform_x,
  phens = datasH[[1]]$pheno()$all,
  data_types = datasH[[1]]$data_types(),
  dbDir = NULL
)
```

Arguments

datasH	a list of dataH objects
flags	list of options
transform_x	transformation object
phens	list of phenotypes
data_types	a data type object
dbDir	database dir, can be NULL

getFamily

Infer the statistical families of the phenotypes

Description

Infer the statistical families of the phenotypes

Usage

```
getFamily(y_mat, max_ordinal = getOption("max_ordinal", 10))
```

Arguments

y_mat	a matrix of phenotypes, with columns as variables and rows as samples
max_ordinal	maximum number of values before we consider an ordinal value as a continuous value

Value

a list with the statistical families detected

getFolds	<i>extracts the full model variables from a cross validation run</i>
----------	--

Description

extracts the full model variables from a cross validation run

Usage

```
getFolds(leng, nrep = NA, batch = NA, randomize = TRUE)
```

Arguments

leng	length of dataset
nrep	number of reps
batch	batch size (one of batch or nrep is non NA)
randomize	whether to randomize

getTransform	<i>Get object for transforming the x variables</i>
--------------	--

Description

Get object for transforming the x variables

Usage

```
getTransform(  
  pows = c(1),  
  offset = 0,  
  n_random = 1,  
  perm = FALSE,  
  norm = 1,  
  CHECK = FALSE  
)
```

Arguments

pows	power to raise to
offset	offset to subtract
n_random	how many random variables
perm	whether random is permutation
norm	rescaling factor
CHECK	check whether inverse function works

Value

transformation object

plotEval

Plot the results from evaluateAll

Description

Plot the results from evaluateAll

Usage

```
plotEval(
  eval3,
  shape_color = c("pheno", "subpheno"),
  shape = shape_color,
  text = "variable",
  dotsize = "nsamps",
  color = shape_color,
  linetype = shape,
  showranges = TRUE,
  txtsize = 1,
  logy = FALSE,
  legend = FALSE,
  sep_by = "",
  scales = "free",
  point = TRUE,
  line = TRUE,
  labelsize = 2,
  grid0 = c("cohort", "measure"),
  grid1 = "cv_full",
  title = "",
  title1 = ""
)
```

Arguments

eval3	a tibble or data frame from evaluateAll method from dataH
shape_color	a list of column names to encode as both shape and color
shape	defaults to shape_color but can be specified separately
text	a list of column names to include as text labels
dotsize	a numerical column to encode dotsize, or a number for constant sizes
color	defaults to shape_color but can be specified separately
linetype	column controlling the type of line

<code>showranges</code>	whether to show 95% CI as ribbon
<code>txtsize</code>	size of text
<code>logy</code>	whether to log y axis
<code>legend</code>	whether to show a legend
<code>sep_by</code>	list of column names to separate into diff plots
<code>scales</code>	used in faceting can be free or fixed
<code>point</code>	whether to show dots
<code>line</code>	whether to include line
<code>labelsize</code>	the size of the text labels
<code>grid0</code>	how to facet on y
<code>grid1</code>	how to facet on x
<code>title</code>	the title
<code>title1</code>	columns to include in the title

Value

ggplot2 plot

Index

analysisBase, [2](#), [3](#), [6](#)

analysisEnv, [3](#)

dataH, [5](#)

fspls.iterative, [11](#)

fspls.select, [11](#)

getFamily, [12](#)

getFolds, [13](#)

getTransform, [13](#)

plotEval, [14](#)