

Package ‘pareg’

September 16, 2024

Title Pathway enrichment using a regularized regression approach

Version 1.8.0

Description Compute pathway enrichment scores while accounting for term-term relations.

This package uses a regularized multiple linear regression to regress differential expression p-values obtained from multi-condition experiments on a pathway membership matrix.

By doing so, it is able to incorporate additional biological knowledge into the enrichment analysis and to estimate pathway enrichment scores more robustly.

URL <https://github.com/cbg-ethz/pareg>

BugReports <https://github.com/cbg-ethz/pareg/issues>

biocViews Software, StatisticalMethod, GraphAndNetwork, Regression, GeneExpression, DifferentialExpression, NetworkEnrichment, Network

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as.data.frame.pareg *as.data.frame for an object of class pareg.*

Description

Retrieve dataframe with enrichment information.

Usage

```
## S3 method for class 'pareg'
as.data.frame(x, row.names = NULL, optional = FALSE, ...)
```

Arguments

x	An object of class pareg.
row.names	Optional character vector of rownames.
optional	Allow optional arguments.
...	Additional arguments.

Value

Dataframe containing enrichment score and name for each pathway.

Examples

```
df_genes <- data.frame(
  gene = paste("g", 1:20, sep = ""),
  pvalue = c(
    rbeta(10, .1, 1),
    rbeta(10, 1, 1)
  )
)
df_terms <- rbind(
  data.frame(
    term = "foo",
    gene = paste("g", 1:10, sep = "")
  ),
  data.frame(
    term = "bar",
    gene = paste("g", 11:20, sep = "")
  )
)
fit <- pareg(df_genes, df_terms, max_iterations = 10)
as.data.frame(fit)
```

as_dense_sim

Convert matrices.

Description

Convert sparse similarity matrix from package data to a dense version with 1 on its diagonal. This matrix can then be used by pareg.

Usage

```
as_dense_sim(mat_sparse)
```

Arguments

mat_sparse	Sparse matrix.
------------	----------------

Value

Dense matrix

Examples

```
transform_y(c(0, 0.5, 1))
```

as_enrichplot_object *Convert object of class pareg to class enrichResult.*

Description

The resulting object can be passed to any method from the enrichplot package and thus allows for nice visualizations of the enrichment results. Note: term similarities are included if available.

Usage

```
as_enrichplot_object(x, pvalue_threshold = 0.05)
```

Arguments

x An object of class pareg.
pvalue_threshold Threshold to select genes for count statistics.

Value

Object of class enrichResult.

Examples

```
df_genes <- data.frame(  
  gene = paste("g", 1:20, sep = ""),  
  pvalue = c(  
    rbeta(10, .1, 1),  
    rbeta(10, 1, 1)  
  )  
)  
df_terms <- rbind(  
  data.frame(  
    term = "foo",  
    gene = paste("g", 1:10, sep = "")  
  ),  
  data.frame(  
    term = "bar",  
    gene = paste("g", 11:20, sep = "")  
  )  
)  
fit <- pareg(df_genes, df_terms, max_iterations = 10)  
as_enrichplot_object(fit)
```

`cluster_apply`*Parallelize function calls on LSF cluster.*

Description

Run function for each row of input dataframe in LSF job.

Usage

```
cluster_apply(  
  df_iter,  
  func,  
  .bsub_params = c("-n", "2", "-W", "24:00", "-R", "rusage[mem=10000]"),  
  .tempdir = ".",  
  .packages = c(),  
  ...  
)
```

Arguments

<code>df_iter</code>	Dataframe over whose rows to iterate.
<code>func</code>	Function to apply to each dataframe row. Its arguments must be all dataframe columns.
<code>.bsub_params</code>	Parameters to pass to 'bsub' during job submission.
<code>.tempdir</code>	Location to store auxiliary files in.
<code>.packages</code>	Packages to import in each job.
<code>...</code>	Extra arguments for function.

Value

Dataframe created by concatenating results of each function call.

Examples

```
## Not run:  
foo <- 42  
cluster_apply(  
  data.frame(i = seq_len(3), group = c("A", "B", "C")),  
  function(i, group) {  
    log_debug("hello")  
    data.frame(group = group, i = i, foo = foo, result = foo + 2 * i)  
  },  
  .packages = c(logger)  
)  
  
## End(Not run)
```

compute_term_similarities

Term similarity computation.

Description

Generate similarity matrix for input terms.

Usage

```
compute_term_similarities(  
  df_terms,  
  similarity_function = jaccard,  
  max_similarity = 1  
)
```

Arguments

df_terms Dataframe storing pathway database.
similarity_function Function to compute similarity between two sets.
max_similarity Value to fill diagonal with.

Value

Symmetric matrix of similarity scores.

Examples

```
df_terms <- data.frame(  
  term = c("A", "A", "B", "B", "C", "C", "C"),  
  gene = c("a", "b", "a", "b", "c", "a", "c", "d")  
)  
compute_term_similarities(df_terms)
```

create_model_df

Create design matrix.

Description

Store term membership for each gene.

Usage

```
create_model_df(df_genes, df_terms, pvalue_threshold = 0.05)
```

Arguments

df_genes Dataframe storing gene names and DE p-values.
df_terms Dataframe storing pathway database.
pvalue_threshold P-value threshold to create binary columns 'pvalue_sig' and 'pvalue_notsig'.

Value

Dataframe.

Examples

```
df_genes <- data.frame(
  gene = c("g1", "g2"),
  pvalue = c(0.1, 0.2)
)
df_terms <- data.frame(
  term = c("A", "A", "B", "B", "C"),
  gene = c("g1", "g2", "g1", "g2", "g2")
)
create_model_df(df_genes, df_terms)
```

cv_edgenet

Find the optimal shrinkage parameters for edgenet

Description

Finds the optimal regularization parameters using cross-validation for edgenet. We use the BOBYQA algorithm to find the optimal regularization parameters in a cross-validation framework.

Usage

```
cv_edgenet(
  X,
  Y,
  G.X = NULL,
  G.Y = NULL,
  lambda = NA_real_,
  psigx = NA_real_,
  psigy = NA_real_,
  thresh = 1e-05,
  maxit = 1e+05,
  learning.rate = 0.01,
  family = gaussian,
  optim.thresh = 0.01,
  optim.maxit = 100,
  lambda_range = seq(0, 2, length.out = 10),
```

```

    psigx_range = seq(0, 500, length.out = 10),
    psigy_range = seq(0, 500, length.out = 10),
    nfolds = 2,
    cv_method = c("grid_search", "grid_search_lsf", "optim"),
    tempdir = "."
)

```

```
## S4 method for signature 'matrix,numeric'
```

```

cv_edgenet(
  X,
  Y,
  G.X = NULL,
  G.Y = NULL,
  lambda = NA_real_,
  psigx = NA_real_,
  psigy = NA_real_,
  thresh = 1e-05,
  maxit = 1e+05,
  learning.rate = 0.01,
  family = gaussian,
  optim.thresh = 0.01,
  optim.maxit = 100,
  lambda_range = seq(0, 2, length.out = 10),
  psigx_range = seq(0, 500, length.out = 10),
  psigy_range = seq(0, 500, length.out = 10),
  nfolds = 2,
  cv_method = c("grid_search", "grid_search_lsf", "optim"),
  tempdir = "."
)

```

```
## S4 method for signature 'matrix,matrix'
```

```

cv_edgenet(
  X,
  Y,
  G.X = NULL,
  G.Y = NULL,
  lambda = NA_real_,
  psigx = NA_real_,
  psigy = NA_real_,
  thresh = 1e-05,
  maxit = 1e+05,
  learning.rate = 0.01,
  family = gaussian,
  optim.thresh = 0.01,
  optim.maxit = 100,
  lambda_range = seq(0, 2, length.out = 10),
  psigx_range = seq(0, 500, length.out = 10),
  psigy_range = seq(0, 500, length.out = 10),

```



```

    nfolds = 2,
    cv_method = c("grid_search", "grid_search_lsf", "optim"),
    tempdir = "."
)

```

Arguments

X	input matrix, of dimension (n x p) where n is the number of observations and p is the number of covariables. Each row is an observation vector.
Y	output matrix, of dimension (n x q) where n is the number of observations and q is the number of response variables. Each row is an observation vector.
G.X	non-negativ affinity matrix for X, of dimensions (p x p) where p is the number of covariables. Providing a graph G.X will optimize the regularization parameter <code>psi.gx</code> . If this is not desired just set G.X to NULL.
G.Y	non-negativ affinity matrix for Y, of dimensions (q x q) where q is the number of responses Y. Providing a graph G.Y will optimize the regularization parameter <code>psi.gy</code> . If this is not desired just set G.Y to NULL.
lambda	numerical shrinkage parameter for LASSO. Per default this parameter is set to <code>NA_real_</code> which means that lambda is going to be estimated using cross-validation. If any numerical value for lambda is set, estimation of the optimal parameter will <i>not</i> be conducted.
psigx	numerical shrinkage parameter for graph-regularization of G.X. Per default this parameter is set to <code>NA_real_</code> which means that psigx is going to be estimated in the cross-validation. If any numerical value for psigx is set, estimation of the optimal parameter will <i>not</i> be conducted.
psigy	numerical shrinkage parameter for graph-regularization of G.Y. Per default this parameter is set to <code>NA_real_</code> which means that psigy is going to be estimated in the cross-validation. If any numerical value for psigy is set, estimation of the optimal parameter will <i>not</i> be conducted.
thresh	numerical threshold for the optimizer
maxit	maximum number of iterations for the optimizer (integer)
learning.rate	step size for Adam optimizer (numerical)
family	family of response, e.g. <i>gaussian</i> or <i>binomial</i>
optim.thresh	numerical threshold criterion for the optimization to stop. Usually 1e-3 is a good choice.
optim.maxit	the maximum number of iterations for the optimization (integer). Usually 1e4 is a good choice.
lambda_range	range of lambda to use in CV grid.
psigx_range	range of psigx to use in CV grid.
psigy_range	range of psigy to use in CV grid.
nfolds	the number of folds to be used - default is 10.
cv_method	which cross-validation method to use.
tempdir	where to store auxiliary files.

Value

An object of class `cv_edgenet`

<code>parameters</code>	the estimated, optimal regularization parameters
<code>lambda</code>	optimal estimated value for regularization parameter <code>lambda</code> (or, if provided as argument, the value of the parameter)
<code>psigx</code>	optimal estimated value for regularization parameter <code>psigx</code> (or, if provided as argument, the value of the parameter)
<code>psigy</code>	optimal estimated value for regularization parameter <code>psigy</code> (or, if provided as argument, the value of the parameter)
<code>estimated.parameters</code>	names of parameters that were estimated
<code>family</code>	family used for estimated
<code>fit</code>	an <code>edgenet</code> object fitted with the optimal, estimated parameters
<code>call</code>	the call that produced the object

Examples

```
X <- matrix(rnorm(100 * 10), 100, 10)
b <- matrix(rnorm(100), 10)
G.X <- abs(rWishart(1, 10, diag(10))[, , 1])
G.Y <- abs(rWishart(1, 10, diag(10))[, , 1])
diag(G.X) <- diag(G.Y) <- 0

# estimate the parameters of a Gaussian model
Y <- X %*% b + matrix(rnorm(100 * 10), 100)

## dont use affinity matrices and estimate lambda
fit <- cv_edgenet(
  X = X,
  Y = Y,
  family = gaussian,
  maxit = 1,
  lambda_range = c(0, 1)
)
## only provide one matrix and estimate lambda
fit <- cv_edgenet(
  X = X,
  Y = Y,
  G.X = G.X,
  psigx = 1,
  family = gaussian,
  maxit = 1,
  lambda_range = c(0, 1)
)
## estimate only lambda with two matrices
fit <- cv_edgenet(
  X = X,
  Y = Y,
```

```

    G.X = G.X,
    G.Y,
    psigx = 1,
    psigy = 1,
    family = gaussian,
    maxit = 1,
    lambda_range = c(0, 1)
)
## estimate only psigx
fit <- cv_edgenet(
  X = X,
  Y = Y,
  G.X = G.X,
  G.Y,
  lambda = 1,
  psigy = 1,
  family = gaussian,
  maxit = 1,
  psigx_range = c(0, 1)
)
## estimate all parameters
fit <- cv_edgenet(
  X = X,
  Y = Y,
  G.X = G.X,
  G.Y,
  family = gaussian,
  maxit = 1,
  lambda_range = c(0, 1),
  psigx_range = c(0, 1),
  psigy_range = c(0, 1)
)
## if Y is vectorial, we cannot use an affinity matrix for Y
fit <- cv_edgenet(
  X = X,
  Y = Y[, 1],
  G.X = G.X,
  family = gaussian,
  maxit = 1,
  lambda_range = c(0, 1),
  psigx_range = c(0, 1),
)

```

edgenet

Fit a graph-regularized linear regression model using edge-based regularization. Adapted from <https://github.com/dirmeier/netReg>.

Description

Fit a graph-regularized linear regression model using edge-penalization. The coefficients are computed using graph-prior knowledge in the form of one/two affinity matrices. Graph-regularization

is an extension to previously introduced regularization techniques, such as the LASSO. See the vignette for details on the objective function of the model: `vignette("edgenet", package="netReg")`

Usage

```
edgenet(  
  X,  
  Y,  
  G.X = NULL,  
  G.Y = NULL,  
  lambda = 0,  
  psigx = 0,  
  psigy = 0,  
  thresh = 1e-05,  
  maxit = 1e+05,  
  learning.rate = 0.01,  
  family = gaussian  
)  
  
## S4 method for signature 'matrix,numeric'  
edgenet(  
  X,  
  Y,  
  G.X = NULL,  
  G.Y = NULL,  
  lambda = 0,  
  psigx = 0,  
  psigy = 0,  
  thresh = 1e-05,  
  maxit = 1e+05,  
  learning.rate = 0.01,  
  family = gaussian  
)  
  
## S4 method for signature 'matrix,matrix'  
edgenet(  
  X,  
  Y,  
  G.X = NULL,  
  G.Y = NULL,  
  lambda = 0,  
  psigx = 0,  
  psigy = 0,  
  thresh = 1e-05,  
  maxit = 1e+05,  
  learning.rate = 0.01,  
  family = gaussian  
)
```

Arguments

X	input matrix, of dimension (n x p) where n is the number of observations and p is the number of covariables. Each row is an observation vector.
Y	output matrix, of dimension (n x q) where n is the number of observations and q is the number of response variables. Each row is an observation vector.
G.X	non-negativ affinity matrix for X, of dimensions (p x p) where p is the number of covariables
G.Y	non-negativ affinity matrix for Y, of dimensions (q x q) where q is the number of responses
lambda	numerical shrinkage parameter for LASSO.
psigx	numerical shrinkage parameter for graph-regularization of G.X
psigy	numerical shrinkage parameter for graph-regularization of G.Y
thresh	numerical threshold for optimizer
maxit	maximum number of iterations for optimizer (integer)
learning.rate	step size for Adam optimizer (numerical)
family	family of response, e.g. <i>gaussian</i> or <i>binomial</i>

Value

An object of class edgenet

beta	the estimated (p x q)-dimensional coefficient matrix B.hat
alpha	the estimated (q x 1)-dimensional vector of intercepts
parameters	regularization parameters
lambda	regularization parameter lambda
psigx	regularization parameter psigx
psigy	regularization parameter psigy
family	a description of the error distribution and link function to be used. Can be a pareg::family function or a character string naming a family function, e.g. <i>gaussian</i> or "gaussian".
call	the call that produced the object

References

Cheng, Wei and Zhang, Xiang and Guo, Zhishan and Shi, Yu and Wang, Wei (2014), Graph-regularized dual Lasso for robust eQTL mapping.
Bioinformatics

Examples

```

X <- matrix(rnorm(100 * 10), 100, 10)
b <- matrix(rnorm(100), 10)
G.X <- abs(rWishart(1, 10, diag(10))[, , 1])
G.Y <- abs(rWishart(1, 10, diag(10))[, , 1])
diag(G.X) <- diag(G.Y) <- 0

# estimate the parameters of a Gaussian model
Y <- X %*% b + matrix(rnorm(100 * 10), 100)
## dont use affinity matrices
fit <- edgenet(X = X, Y = Y, family = gaussian, maxit = 10)
## only provide one matrix
fit <- edgenet(
  X = X,
  Y = Y,
  G.X = G.X,
  psigx = 1,
  family = gaussian,
  maxit = 10
)
## use two matrices
fit <- edgenet(X = X, Y = Y, G.X = G.X, G.Y, family = gaussian, maxit = 10)
## if Y is vectorial, we cannot use an affinity matrix for Y
fit <- edgenet(X = X, Y = Y[, 1], G.X = G.X, family = gaussian, maxit = 10)

```

family

Family objects for models

Description

Family objects provide a convenient way to specify the details of the models used by `pareg`. See also `stats::family` for more details.

Usage

```

family(object, ...)

gaussian(link = c("identity"))

bernoulli(link = c("logit", "probit", "log"))

beta(link = c("logit", "probit", "log"))

beta_phi_lm(link = c("logit", "probit", "log"))

beta_phi_var(link = c("logit", "probit", "log"))

```

Arguments

object	a object for which the family should be returned (e.g. edgenet)
...	further arguments passed to methods
link	name of a link function

Value

An object of class <code>pareg.family</code>	
family	name of the family
link	name of the link function
linkinv	inverse link function
loss	loss function

Examples

```
gaussian()  
bernoulli("probit")$link  
beta()$loss
```

```
generate_similarity_matrix  
      Similarity matrix generation.
```

Description

Generate block-structured similarity matrices corresponding to cluster structures.

Usage

```
generate_similarity_matrix(cluster_sizes)
```

Arguments

`cluster_sizes` List of cluster sizes.

Value

Similarity matrix with samples as row-/colnames.

Examples

```
generate_similarity_matrix(c(1, 2, 3))
```

jaccard	<i>Jaccard similarity.</i>
---------	----------------------------

Description

Compute Jaccard similarity between two sets.

Usage

```
jaccard(x, y)
```

Arguments

x	First set.
y	Second set.

Value

Jaccard similarity between set x and y.

See Also

Other pathway similarity methods: [overlap_coefficient\(\)](#)

Examples

```
jaccard(c(1, 2, 3), c(2, 3, 4))
```

overlap_coefficient	<i>Overlap coefficient.</i>
---------------------	-----------------------------

Description

Compute overlap coefficient between two sets.

Usage

```
overlap_coefficient(x, y)
```

Arguments

x	First set.
y	Second set.

Value

Overlap coefficient between set x and y.

See Also

Other pathway similarity methods: [jaccard\(\)](#)

Examples

```
overlap_coefficient(c(1, 2, 3), c(2, 3, 4))
```

pareg

Pathway enrichment using a regularized regression approach.

Description

Run model to compute pathway enrichments. Can model inter-pathway relations, cross-validation and much more.

Usage

```
pareg(  
  df_genes,  
  df_terms,  
  lasso_param = NA_real_,  
  network_param = NA_real_,  
  term_network = NULL,  
  cv = FALSE,  
  cv_cores = NULL,  
  family = beta,  
  response_column_name = "pvalue",  
  max_iterations = 1e+05,  
  lasso_param_range = seq(0, 2, length.out = 10),  
  network_param_range = seq(0, 500, length.out = 10),  
  log_level = NULL,  
  ...  
)
```

Arguments

df_genes	Dataframe storing gene names and DE p-values.
df_terms	Dataframe storing pathway database.
lasso_param	Lasso regularization parameter.
network_param	Network regularization parameter.
term_network	Term similarity network as adjacency matrix.
cv	Estimate best regularization parameters using cross-validation.

`cv_cores` How many cores to use for CV parallelization.
`family` Distribution family of response.
`response_column_name`
 Which column of model dataframe to use as response.
`max_iterations` How many iterations to maximally run optimizer for.
`lasso_param_range`
 LASSO regularization parameter search space in grid search of CV.
`network_param_range`
 Network regularization parameter search space in grid search of CV.
`log_level` Control verbosity (logger::INFO, logger::DEBUG, ...).
`...` Further arguments to pass to '(cv.)edgenet'.

Value

An object of class `pareg`.

Examples

```

df_genes <- data.frame(
  gene = paste("g", 1:20, sep = ""),
  pvalue = c(
    rbeta(10, .1, 1),
    rbeta(10, 1, 1)
  )
)
df_terms <- rbind(
  data.frame(
    term = "foo",
    gene = paste("g", 1:10, sep = "")
  ),
  data.frame(
    term = "bar",
    gene = paste("g", 11:20, sep = "")
  )
)
pareg(df_genes, df_terms, max_iterations = 10)

```

`pareg_env`

Conda environment definition.

Description

Declare Python packages needed to run this R package.

Usage

`pareg_env`

Format

An object of class BasiliskEnvironment of length 1.

pathway_similarities *Collection of pathway similarity matrices.*

Description

Contains matrices for various pathway databases and similarity measures. Note that the matrices are sparse, upper triangular and subsampled to a maximum size of \$1000x1000\$ if necessary. They can be transformed to a dense representation using `pareg::as_dense_sim`.

Usage

```
pathway_similarities
```

Format

A list of lists of matrices. * Pathway database 1 * Similarity measure 1 * Similarity measure 2 * ...
* Pathway database 2 * ...

plot.pareg *Plot pareg object.*

Description

Check `pareg::plot_pareg_with_args` for details. Needed because of WARNING in "checking S3 generic/method consistency"

Usage

```
## S3 method for class 'pareg'
plot(x, ...)
```

Arguments

x An object of class pareg.
... Parameters passed to `pareg::plot_pareg_with_args`

Value

ggplot object.

plot_pareg_with_args *Plot result of enrichment computation.*

Description

Visualize pathway enrichments as network.

Usage

```
plot_pareg_with_args(  
  x,  
  show_term_names = TRUE,  
  min_similarity = 0,  
  term_subset = NULL  
)
```

Arguments

x An object of class pareg.
show_term_names Whether to plot node labels.
min_similarity Don't plot edges for similarities below this value.
term_subset Subset of terms to show.

Value

ggplot object.

Examples

```
df_genes <- data.frame(  
  gene = paste("g", 1:20, sep = ""),  
  pvalue = c(  
    rbeta(10, .1, 1),  
    rbeta(10, 1, 1)  
  )  
)  
df_terms <- rbind(  
  data.frame(  
    term = "foo",  
    gene = paste("g", 1:10, sep = "")  
  ),  
  data.frame(  
    term = "bar",  
    gene = paste("g", 11:20, sep = "")  
  )  
)  
fit <- pareg(df_genes, df_terms, max_iterations = 10)  
plot(fit)
```

similarity_sample	<i>Sample elements based on similarity structure.</i>
-------------------	---

Description

Choose similar object more often, depending on 'similarity_factor'.

Usage

```
similarity_sample(sim_mat, size, similarity_factor = 1)
```

Arguments

sim_mat	Similarity matrix with samples as row/col names.
size	How many samples to draw.
similarity_factor	Uniform sampling for 0. Weights mixture of uniform and similarity vector for each draw.

Value

Vector of samples.

Examples

```
similarity_sample(matrix(runif(100), nrow = 10, ncol = 10), 3)
```

transform_y	<i>Transform vector from [0, 1] to (0, 1).</i>
-------------	--

Description

Make (response) vector conform to Beta assumptions as described in section 2 of the betareg vignette <https://cran.r-project.org/web/packages/betareg/vignettes/betareg.pdf>.

Usage

```
transform_y(y)
```

Arguments

y	Numeric vector in $[0, 1]^N$
---	------------------------------

Value

Numeric vector in $(0, 1)^N$

Examples

```
transform_y(c(0, 0.5, 1))
```

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