Package ‘gespeR’

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Description Estimates gene-specific phenotypes from off-target confounded RNAi screens. The phenotype of each siRNA is modeled based on on-targeted and off-targeted genes, using a regularized linear regression model.

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URL http://www.cbg.ethz.ch/software/gespeR

Collate ‘Phenotypes-class.R’ ‘TargetRelations-class.R’
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Package: Gene-Specific Phenotype EstimatoR

gespeR-package

Description

This package provides a model to deconvolute off-target confounded RNAi knockdown phenotypes, and methods to investigate concordance between ranked lists of (estimated) phenotypes. The regularized linear regression model can be fitted using two different strategies. (a) Cross-validation over regularization parameters optimising the mean-squared-error of the model and (b) stability selection of covariates (genes) based on a method by Nicolai Meinshausen et al.

Author(s)

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References

Fabian Schmich et. al, Deconvoluting Off-Target Confounded RNA Interference Screens (2014).

See Also

gespeR

Examples

```r
# Read phenotypes
phenos <- lapply(LETTERS[1:4], function(x) {
    sprintf("Phenotypes_screen_%s.txt", x)
})
phenos <- lapply(phenos, function(x) {
    Phenotypes(system.file("extdata", x, package="gespeR"),
                type = "SSP",
                col.id = 1,
                col.score = 2)
})
phenos
plot(phenos[[1]])

# Read target relations
tr <- lapply(LETTERS[1:4], function(x) {
    sprintf("TR_screen_%s.rds", x)
})
tr <- lapply(tr, function(x) {
    TargetRelations(system.file("extdata", x, package="gespeR"))
})
tr[[1]]
tempfile <- paste(tempfile(pattern = "file", tmpdir = tempdir()), ".rds", sep="")
tr[[1]] <- unloadValues(tr[[1]], writeValues = TRUE, path = tempfile)
tr[[1]]
tr[[1]] <- loadValues(tr[[1]])
tr[[1]]

# Fit gespeR models with cross validation
res.cv <- lapply(1:length(phenos), function(i) {
    gespeR(phenotypes = phenos[[i]],
           target.relations = tr[[i]],
           mode = "cv",
           alpha = 0.5,
           ncores = 1)
})
summary(res.cv[[1]])
res.cv[[1]]
plot(res.cv[[1]])

# Extract scores
ssp(res.cv[[1]])
gsp(res.cv[[1]])
head(scores(res.cv[[1]]))
```
# Fit gespeR models with stability selection
res.stab <- lapply(1:length(phenos), function(i) {
  gespeR(phenotypes = phenos[[i]],
         target.relations = tr[[i]],
         mode = "stability",
         nbootstrap = 100,
         fraction = 0.67,
         threshold = 0.75,
         EV = 1,
         weakness = 0.8,
         ncores = 1)
})
summary(res.stab[[1]])
res.stab[[1]]
plot(res.stab[[1]])

# Extract scores
ssp(res.stab[[1]])
gsp(res.stab[[1]])
head(scores(res.stab[[1]]))

# Compare concordance between stability selected GSPs and SSPs
conc.gsp <- concordance(lapply(res.stab, gsp))
conc.ssp <- concordance(lapply(res.stab, ssp))
pl.gsp <- plot(conc.gsp) + ggtitle("GSPs\n")
pl.ssp <- plot(conc.ssp) + ggtitle("SSPs\n")
if (require(grid)) {
  grid.newpage()
  pushViewport(viewport(layout = grid.layout(1, 2) ) )
  print(pl.gsp, vp = viewport(layout.pos.row = 1, layout.pos.col = 1))
  print(pl.ssp, vp = viewport(layout.pos.row = 1, layout.pos.col = 2))
} else {
  plot(pl.gsp)
  plot(pl.ssp)
}

---

**Description**

Query Biomart HGNC symbols for the entrez identifiers of estimated GSPs. Currently, only implemented for species "hsapiens".

**Usage**

```r
## S4 method for signature 'Phenotypes'
```
annotate.gsp(object, organism = "hsapiens")

## S4 method for signature 'gespeR'
annotate.gsp(object, organism = "hsapiens")

Arguments

object A gespeR or Phenotypes object
organism String indicating the biomaRt organism

Value
data.frame containing gene identifier, gene symbol and phenotypic score

Author(s)

Fabian Schmich

See Also
gsp
ssp
scores

Examples
data(stabilityfits)
gspA <- gsp(stabilityfits$A)
## Not run:
annotate.gsp(gspA)
## End(Not run)

as.data.frame,Phenotypes-method

Convert Phenotypes object to a data.frame

Description

Convert Phenotypes object to a data.frame

Usage

## S4 method for signature 'Phenotypes'
as.data.frame(x)
Arguments

x A Phenotypes object

Value

A data.frame

Author(s)

Fabian Schmich

Examples

phenos <- Phenotypes(system.file("extdata", "Phenotypes_screen_A.txt", package = "gespeR"),
type = "SSP",
col.id = 1,
col.score = 2)
as.data.frame(phenos)

as.data.frame.concordance

Coerce method

Description

Coerce method

Usage

## S3 method for class 'concordance'
as.data.frame(x, ...)

Arguments

x concordance object

... additional arguments

Value

data.frame

Author(s)

Fabian Schmich
Description
Concatenate Phenotypes objects

Usage
## S4 method for signature 'Phenotypes'
c(x, ..., recursive = FALSE)

Arguments
x
A Phenotypes object

... additional Phenotypes objects

recursive
recursive

Value
A concatenated Phenotypes object

Author(s)
Fabian Schmich

Examples
phenos.a <- Phenotypes(system.file("extdata","Phenotypes_screen_A.txt", package = "gespeR"),
type = "SSP",
col.id = 1,
col.score = 2)
phenos.b <- Phenotypes(system.file("extdata","Phenotypes_screen_B.txt", package = "gespeR"),
type = "SSP",
col.id = 1,
col.score = 2)
c(phenos.a, phenos.b)
concordance

Evaluate the concordance between Phenotype objects

Description

Measures include the correlation (rho) between pairs of phenotypes for the same gene, the rank biased overlap (rbo) of the top and bottom of ranked lists, and the Jaccard index (J) of selected genes.

Usage

concordance(..., min.overlap = 10, cor.method = "spearman", rbo.p = 0.98, rbo.k = NULL, rbo.mid = 0, uneven.lengths = TRUE)

Arguments

... The phenotypes to be evaluated for concordance
min.overlap The minimum number of overlapping genes required
cor.method A character string indicating which correlation coefficient is to be computed
rbo.p The weighting parameter for rank biased overlap (rbo) in [0, 1]. High p implies strong emphasis on top ranked elements
rbo.k The evaluation depth for rank biased overlap extrapolation
rbo.mid The mid point to split a ranked list, e.g. in order to split positive and negative scores choose mid=0
uneven.lengths Indicator if lists have uneven lengths

Value

A concordance object with the following elements:

pair.test Indicator of compared phenotypes
cor The correlation between pairs of phenotypes for the same gene
rbo.top The rank biased overlap of genes evaluated at the top of the ranked list
rbo.bottom The rank biased overlap of genes evaluated at the bottom of the ranked list
jaccard The Jaccard index of selected genes

Author(s)

Fabian Schmich

See Also

Phenotypes
plot.concordance
rbo
Examples

```r
data(stabilityfits)
conc <- concordance(gsp(stabilityfits$A), gsp(stabilityfits$B),
gsp(stabilityfits$C), gsp(stabilityfits$D))
plot(conc)
```

---

**Description**

Dimension of a `Phenotypes` object

**Usage**

```r
## S4 method for signature 'Phenotypes'
dim(x)
```

**Arguments**

- `x` `Phenotypes` object

**Value**

Dimension of the `Phenotypes` object

**Author(s)**

Fabian Schmich

---

**gespeR-class**

**gespeR**

**Description**

Class that represents a gespeR model. It contains a SSP `Phenotypes` and `TargetRelations` representing a siRNA knockdown experiment. When the model is fitted, it additionally contains estimated GSP `Phenotypes`. 
Usage

gespeR(phenotypes, target.relations, ...)

## S4 method for signature 'Phenotypes,TargetRelations'
gespeR(phenotypes, target.relations,
    mode = c("cv", "stability"), alpha = 0.5, nbootstrap = 100,
    fraction = 0.67, threshold = 0.9, EV = 1, weakness = 0.8,
    ncores = 1, ...)

## S4 method for signature 'numeric,Matrix'
gespeR(phenotypes, target.relations, ...)

Arguments

phenotypes The siRNA-specific phenotypes. Single object for univariate phenotypes and list of Phenotypes objects for multivariate phenotypes.
target.relations The siRNA-to-gene target relations
...
mode The mode of covariate selection ("cv" or "stability")
alpha The glmnet mixing parameter
nbootstrap The number of bootstrap samples
fraction The fraction for each bootstrap sample
threshold The selection threshold
EV The expected value of wrongly selected elements
weakness The weakness parameter for randomised lasso
ncores The number of cores for parallel computation

Value

A gespeR object

Slots

SSP The observed siRNA-specific phenotypes
GSP The deconvoluted gene-specific phenotypes
target.relations The siRNA-to-gene target relations, e.g. predicted by TargetScan
is.fitted An indicator whether the gespeR model was fitted
model The fitted regularized linear regression model

Author(s)

Fabian Schmich
gsp

See Also
gespeR-package
plot.gespeR
gsp
ssp
scores
stability
target.relations

Examples
phenos <- Phenotypes(system.file("extdata", "Phenotypes_screen_A.txt", package = "gespeR"),
type = "SSP",
col.id = 1,
col.score = 2)
trels <- TargetRelations(readRDS(system.file("extdata", "TR_screen_A.rds", package = "gespeR")))
res <- gespeR(phenotypes = phenos,
    target.relations = trels,
    mode = "stability",
    nbootstrap = 100,
    fraction = 0.67,
    threshold = 0.75,
    EV = 1,
    weakness = 0.8,
    ncores = 1)
gsp(res)

Description
Retrieve GSPs and SSPs from gespeR objects

Usage
gsp(object)

## S4 method for signature 'gespeR'
gsp(object)

ssp(object)

## S4 method for signature 'gespeR'
ssp(object)
Arguments

    object A gespeR object

Value

    A Phenotypes object of GSPs and SSPs, respectively

Author(s)

    Fabian Schmich

See Also

    annotate.gsp
      scores

Examples

    data(stabilityfits)
    gsp(stabilityfits$A)
    ssp(stabilityfits$B)

Description

    Join a TargetRelations object and a Phenotype object

Usage

    join(targets, phenotypes)

      ## S4 method for signature 'TargetRelations,Phenotypes'
      join(targets, phenotypes)

Arguments

    targets A TargetRelations object.
    phenotypes A Phenotypes object.

Value

    List containing the matched targets and phenotypes

Author(s)

    Fabian Schmich
```
lasso.rand <- Phenotypes(system.file("extdata", "Phenotypes_screen_A.txt", package = "gespeR"),
type = "SSP",
col.id = 1,
col.score = 2)
trels <- TargetRelations(readRDS(system.file("extdata", "TR_screen_A.rds", package = "gespeR")))
phenos <- phenos[1:17]
stripped_down <- join(targets = trels, phenotypes = phenos)
```

---

**lasso.rand**  
*Randomized Lasso*

**Description**

Based on Meinshausen and Buehlmann (2009)

**Usage**

```
lasso.rand(x, y, weakness = 1, subsample = 1:nrow(x), dfmax = (ncol(x) + 1), lambda = NULL, standardize = FALSE, intercept = FALSE, ...)
```

**Arguments**

- `x`: The design matrix
- `y`: The response vector
- `weakness`: The weakness parameter
- `subsample`: The data subsample (default: none)
- `dfmax`: The maximum number of degrees of freedom
- `lambda`: The regularisation parameter
- `standardize`: Indicator, whether to standardize the design matrix
- `intercept`: Indicator, whether to fit an intercept
- `...`: Additional arguments to `glmnet`

**Value**

A `glmnet` object

**Author(s)**

Fabian Schmich

**Examples**

```
y <- rnorm(50)
x <- matrix(runif(50 * 20), ncol = 20)
lasso.rand(x = x, y = y)
```
Methods for values of `TargetRelations` objects

Description
Load, unload or write to file the values of a `TargetRelations` object

Usage

```r
loadValues(object)

## S4 method for signature 'TargetRelations'
loadValues(object)

## S4 method for signature 'gespeR'
loadValues(object)

unloadValues(object, ...)

## S4 method for signature 'TargetRelations'
unloadValues(object, writeValues = TRUE, overwrite = FALSE, path = NULL)

## S4 method for signature 'gespeR'
unloadValues(object, writeValues = TRUE, overwrite = FALSE, path = NULL)

writeValues(object, ...)

## S4 method for signature 'TargetRelations'
writeValues(object, overwrite = FALSE)
```

Arguments

- `object`: A `TargetRelations` object or `gespeR` object
- `...`: Additional arguments
- `writeValues`: Indicator, whether to write values
- `overwrite`: Indicator, whether to overwrite values if file exists at path
- `path`: The path to write out values

Value

A `TargetRelations` object or `gespeR` object

Author(s)

Fabian Schmich
Examples

data(stabilityfits)
## Not run:
loadValues(stabilityfits$A)

## End(Not run)

na.rem

Remove NA/Inf values from phenotype vectors

Description

Remove NA/Inf values from phenotype vectors

Usage

na.rem(object)

## S4 method for signature 'Phenotypes'
na.rem(object)

Arguments

object A Phenotypes object

Value

A Phenotypes object without NA scores values

Author(s)

Fabian Schmich

Examples

phenos <- Phenotypes(system.file("extdata", "Phenotypes_screen_A.txt", package = "gespeR"),
type = "SSP",
col.id = 1,
col.score = 2)
na.rem(phenos)
Description
Set the path of a TargetRelations object object

Usage
path(object) <- value

## S4 replacement method for signature 'TargetRelations,character'
path(object) <- value

Arguments
object A TargetRelations object
value A string defining the path

Value
A TargetRelations object with set path

Author(s)
Fabian Schmich

Examples
trels <- TargetRelations(readRDS(system.file("extdata","TR_screen_A.rds", package = "gespeR")))
path(trels) <- "/dev/null"

Phenotypes-class Phenotypes

Description
Class used to represent various types of phenotypes, e.g. from siRNA-specific (SSP) or estimated gene-specific phenotypes (GSP).
Usage

Phenotypes(phenotypes, ...)

## S4 method for signature 'character'
Phenotypes(phenotypes, type = c("SSP", "GSP"),
    sep = "\t", col.id = 1, col.score = 2)

## S4 method for signature 'cellHTS'
Phenotypes(phenotypes, channel, sample)

## S4 method for signature 'Matrix'
Phenotypes(phenotypes, ids = NULL, pnames = NULL,
    type = c("SSP", "GSP"))

Arguments

- **phenotypes**: The phenotypes as numeric vector, path to a .txt file with two columns (1: identifiers, 2: values), or a cellHTS object
- ... Additional arguments
- **type**: The type of phenotype (GSP, SSP)
- **sep**: The separator string
- **col.id**: Column number for the siRNA identifiers
- **col.score**: Column number(s) for the phenotype score
- **channel**: The cellHTS channel identifier
- **sample**: The cellHTS sample index
- **ids**: The siRNA/gene identifiers
- **pnames**: The phenotype identifiers

Value

A Phenotypes object

Slots

- **type**: The type of represented phenotypes (i.e., "SSP" or "GSP")
- **ids**: The entity identifiers (i.e., siRNA or gene ids)
- **pnames**: The phenotype identifiers
- **values**: The phenotypic values

Author(s)

Fabian Schmich
See Also

plot.Phenotypes
join
gsp
ssp
scores
concordance

Examples

phenos <- Phenotypes(system.file("extdata", "Phenotypes_screen_A.txt", package = "gespeR"),
  type = "SSP",
  col.id = 1,
  col.score = 2)

plot.concordance  Plot concordance

Description

Plots boxplots of concordance evaluated between multiple Phenotype objects. Measures include the correlation (rho) between pairs of phenotypes for the same gene, the rank biased overlap (rbo) of the top and bottom of ranked lists, and the Jaccard index (J) of selected genes.

Usage

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

Arguments

x  The data of class concordance
...
Additional parameters for plot

Value

Boxplots of concordance measures

Author(s)

Fabian Schmich
Description

Plot method for gespeR objects

Usage

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

Arguments

x
A gespeR object

... Additional parameters for plot

Value

Histogram of SSPs or GSPs

Author(s)

Fabian Schmich

---

Description

Plot method for Phenotype objects

Usage

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

Arguments

x
A Phenotypes object

... Additional arguments for plot

Value

Histogram of scores phenos <- Phenotypes(system.file("extdata", "Phenotypes_screen_A.txt", package = "gespeR"), type = "SSP", col.id = 1, col.score = 2) plot(phenos)
Author(s)

Fabian Schmich

---

rbo  
*Rank biased overlap (Webber et al., 2010)*

Description

Evaluates the rank biased overlap (rbo) of two ranked lists based on formula based on (32) from "A Similarity Measure for Indefinite Rankings" (Webber et al.). Two ranked lists with high rbo are very similar, whereas low rbo indicates dissimilar lists. rbo ranges between 0 and 1. In this method the extrapolated version of rbo is implemented.

Usage

```
rbo(s, t, p, k = floor(max(length(s), length(t))/2), side = c("top", "bottom"), mid = NULL, uneven.lengths = TRUE)
```

Arguments

- **s**: List 1
- **t**: List 2
- **p**: Weighting parameter in \([0, 1]\). High p implies strong emphasis on top ranked elements
- **k**: Evaluation depth for extrapolation
- **side**: Evaluate similarity between the top or the bottom of the ranked lists
- **mid**: Set the mid point to for example only consider positive or negative scores
- **uneven.lengths**: Indicator if lists have uneven lengths

Value

rank biased overlap (rbo)

Author(s)

Fabian Schmich

See Also

- concordance

Examples

```
a <- rnorm(26)
b <- rnorm(26)
names(a) <- names(b) <- LETTERS
rbo(a, b, p = 0.95)
```
Description

Return a named vector of phenotype scores

Usage

```r
## S4 method for signature 'Phenotypes'
scores(object)
```

```r
## S4 method for signature 'gespeR'
scores(object, type = c("GSP", "SSP"))
```

Arguments

- `object`: A `gespeR` or `Phenotypes` object
- `type`: The type of phenotype scores (GSP, SSP)

Value

A named vector of scores for each phenotype identifier

Author(s)

Fabian Schmich

See Also

`gespeR`

`Phenotypes`

Examples

```r
data(stabilityfits)
scores(stabilityfits$A)
```
Example data: Simulated phenotypes and target relations for 4 screens (A, B, C, D)

Description

The data set contains simulated data for four screens. Each screen consists of a phenotype vector and target relations between siRNAs and genes, i.e. which siRNA binds which genes (on- and off-targets). The size of each simulated screen is $N = 1000$ siRNAs x $p = 1500$ genes. SSPs are generated by first defining GSPs and multiplying the true GSPs with the sampled target relation matrices. For sampling the GSPs, we set the number of effect genes to 5 from Normal$(0, 3)$. Target relation matrices are simulated by sampling the number of off-targets per siRNA from Normal$(3e-2 \times N, 3e-3 \times N)$ and the strength of off-targets is sampled from Beta$(2, 5)$. On-target components are set to 0.75.

Details

The code used to simulate the data can be found in `system.file("example", "data_simulation.R", package="gespeR")`

Examples

```r
pheno.a <- Phenotypes(system.file("extdata", "Phenotypes_screen_A.txt", package="gespeR"), type = "SSP", col.id = 1, col.score = 2)
targets.a <- TargetRelations(system.file("extdata", "TR_screen_A.rds", package="gespeR"))
```

Description

Retrieve a Phenotypes object with stability values from a gespeR object.

Usage

```r
stability(object)
```

## S4 method for signature 'gespeR'
```r
stability(object)
```

Arguments

- `object` A gespeR object

Value

A Phenotypes object of SSPs
stability.selection

Author(s)
Fabian Schmich

Examples

```r
phenos <- Phenotypes(system.file("extdata", "Phenotypes_screen_A.txt", package = "gespeR"),
  type = "SSP",
  col.id = 1,
  col.score = 2)
trels <- TargetRelations(readRDS(system.file("extdata", "TR_screen_A.rds", package = "gespeR")))
res <- gespeR(phenotypes = phenos,
  target.relations = trels,
  mode = "stability",
  nbootstrap = 100,
  fraction = 0.67,
  threshold = 0.75,
  EV = 1,
  weakness = 0.8,
  ncores = 1)
stab <- stability(res)
ans <- merge(as.data.frame(gsp(res)), as.data.frame(stability(res)), by = "ID")
colnames(ans)[2:3] <- c("Phenotype", "Stability")
ans[order(ans$Stability, decreasing = TRUE),]
```

---

**stability.selection**  
**Stability Selection**

Description

Based on Meinshausen and Buehlmann (2009)

Usage

```r
stability.selection(x, y, fraction = 0.5, threshold = 0.75, EV = 1,
  nbootstrap = 100, weakness = 1, intercept = FALSE, ncores = 1, ...)
```

Arguments

- **x**  
The design matrix
- **y**  
The response vector
- **fraction**  
The fraction for each bootstrap sample
- **threshold**  
The selection threshold
- **EV**  
The expected value of wrongly selected elements
- **nbootstrap**  
The number of bootstrap samples
- **weakness**  
The weakness parameter for randomised lasso
- **intercept**  
Indicator, whether to fit an intercept
- **ncores**  
The number of cores for parallel computation
- **...**  
Additional arguments to `lasso.rand`
Value

A list containing selected covariates with frequencies, and the fitted model

Author(s)

Fabian Schmich

data(stabilityfits)
target.relations

Description

The data set contains four fitted gespeR models using stability selection from the four simulated screens.

Examples

Usage

target.relations(object)

Arguments

object A gespeR object

Value

A TargetRelations object

Author(s)

Fabian Schmich
Examples

```r
data(stabilityfits)
target.relations(stabilityfits$A)
```

Description

Class used to represent siRNA-to-gene on- and off-target relations for a knockdown library and a set of genes.

Usage

```r
TargetRelations(targets)
```

Arguments

targets Path to a .rds target relations matrix file or `Matrix` object

Value

A `TargetRelations` object

Slots

- siRNAs The siRNA identifiers
- genes The gene identifiers (Entrez)
- path The path to and .rds `TargetRelations` file
- is.loaded An indicator if target relations values are loaded
- values The quantitative target relation values between siRNAs and genes

Author(s)

Fabian Schmich
See Also

join
loadValues
unloadValues
writeValues
values
path<-

Examples

trels <- TargetRelations(readRDS(system.file("extdata", "TR_screen_A.rds", package = "gespeR")))

\begin{verbatim}
values values
\end{verbatim}

Description

Retrieve the numeric values from a TargetRelations or Phenotypes object

Usage

values(object)

\# S4 method for signature 'TargetRelations'
values(object)

\# S4 method for signature 'Phenotypes'
values(object)

Arguments

object A TargetRelations or Phenotypes object

Value

A Matrix object

Author(s)

Fabian Schmich
Examples

trels <- TargetRelations(readRDS(system.file("extdata", "TR_screen_A.rds", package = "gespeR")))
values(trels)[1:5, 1:5]

phenos <- Phenotypes(system.file("extdata", "Phenotypes_screen_A.txt", package = "gespeR"),
type = "SSP",
col.id = 1,
col.score = 2)
values(phenos)

Description

Subsetting for Phenotype objects.

Usage

```r
## S4 method for signature 'Phenotypes,ANY,ANY,ANY'
x[i, j, ..., drop = TRUE]
```

Arguments

- `x`: A `Phenotypes` object
- `i`: The subsetting indices for siRNAs
- `j`: Subsetting indices for multivariate phenotypes
- `...`: Additional parameters
- `drop`: Drop Redundant Extent Information

Value

A `Phenotypes` object

Author(s)

Fabian Schmich
Description

Subsetting for TargetRelations objects.

Usage

```r
## S4 method for signature 'TargetRelations,ANY,ANY,ANY'
x[i, j, ..., drop = TRUE]
```

Arguments

- `x` A `TargetRelations` object
- `i` The row subsetting indices (siRNAs)
- `j` The column subsetting indeces (genes)
- `...` Additional parameters
- `drop` Drop Redundant Extent Information

Value

A `TargetRelations` object

Author(s)

Fabian Schmich
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