Package 'BioCor'

April 15, 2020

```
Description Calculates functional similarities based on the
      pathways described on KEGG and REACTOME or in gene sets. These
      similarities can be calculated for pathways or gene sets, genes, or
      clusters and combined with other similarities. They can be used to
      improve networks, gene selection, testing relationships...
License MIT + file LICENSE
URL https://llrs.github.io/BioCor/
BugReports https://github.com/llrs/BioCor/issues
Depends R (>= 3.4.0)
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```

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Description

Calculates a functional similarity measure between gene identifiers based on the pathways described on KEGG and REACTOME.

Important functions

```
pathSim Calculates the similarity between two pathways
geneSim Calculates the similarity (based on pathSim) between two genes
clusterSim Calculates the similarity between two clusters of genes by joining pathways of each gene.
clusterGeneSim Calculates the similarity between two clusters of genes by comparing the similarity between the genes of a cluster
similarities Allows to combine the value of matrices of similarities
conversions Two functions to convert similarity measures
weighted Functions provided to combine similarities
```

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addSimilarities

Additive integration of similarities

Description

Function that use the previously calculated similarities into a single similarity matrix.

Usage

```
addSimilarities(x, bio_mat, weights = c(0.5, 0.18, 0.1, 0.22))
```

Arguments

x A matrix with the similarity of expression
 bio_mat A list of matrices of the same dimension as x.
 weights A numeric vector of weight to multiply each similarity

Details

The total weight can't be higher than 1 to prevent values above 1 but can be below 1. It uses weighted.sum with abs = TRUE internally.

Value

A square matrix of the same dimensions as the input matrices.

Author(s)

Lluís Revilla

See Also

```
similarities, weighted.
```

```
set.seed(100)  a \leftarrow seq2mat(LETTERS[1:5], rnorm(10)) \\ b \leftarrow seq2mat(LETTERS[1:5], seq(from = 0.1, to = 1, by = 0.1)) \\ sim \leftarrow list(b) \\ addSimilarities(a, sim, c(0.5, 0.5))
```

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AintoB

Insert a matrix into another

Description

Insert values from a matrix into another matrix based on the rownames and colnames replacing the values.

Usage

```
AintoB(A, B)
```

Arguments

A matrix to be inserted.

B A matrix to insert in.

Details

If all the genes with pathway information are already calculated but you would like to use more genes when performing analysis. insert the once you have calculated on the matrix of genes.

Value

A matrix with the values of A in the matrix B.

Author(s)

Lluís Revilla

clusterGeneSim 5

Description

Looks for the similarity between genes of a group and then between each group's genes.

Usage

```
clusterGeneSim(cluster1, cluster2, info, method = c("max", "rcmax.avg"),
    ...)
## S4 method for signature 'character, character, GeneSetCollection'
clusterGeneSim(cluster1,
    cluster2, info, method = c("max", "rcmax.avg"), ...)
```

Arguments

cluster1	A vector with genes.
cluster2	A vector with genes.
info	A GeneSetCollection or a list of genes and the pathways they are involved.
method	A vector with two or one argument to be passed to combineScores the first one is used to summarize the similarities of genes, the second one for clusters.
	Other arguments passed to combineScores

Details

Differs with clusterSim that first each combination between genes is calculated, and with this values then the comparison between the two clusters is done. Thus applying combineScores twice, one at gene level and another one at cluster level.

Value

Returns a similarity score between the genes of the two clusters.

Methods (by class)

• cluster1 = character, cluster2 = character, info = GeneSetCollection: Calculates the gene similarities in a GeneSetCollection and combine them using combineScoresPar

Author(s)

Lluís Revilla

See Also

 ${\tt mclusterGeneSim,\,combineScores\,and\,clusterSim}$

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Examples

clusterSim

Similarity score between clusters of genes based on pathways similarity

Description

Looks for the similarity between genes in groups

Usage

```
clusterSim(cluster1, cluster2, info, method = "max", ...)
## S4 method for signature 'character, character, GeneSetCollection'
clusterSim(cluster1,
    cluster2, info, method = "max", ...)
```

Arguments

```
A vector with genes.

info A GeneSetCollection or a list of genes and the pathways they are involved.

method one of c("avg", "max", "rcmax", "rcmax.avg", "BMA", "reciprocal"), see Details.

Other arguments passed to combineScores
```

Details

Once the pathways for each cluster are found they are combined using combineScores.

Value

clusterSim returns a similarity score of the two clusters

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Methods (by class)

• cluster1 = character, cluster2 = character, info = GeneSetCollection: Calculates all the similarities of the GeneSetCollection and combine them using combineScoresPar

Author(s)

Lluís Revilla

See Also

For a different approach see clusterGeneSim, combineScores and conversions

Examples

```
if (require("org.Hs.eg.db")) {
    #Extract the paths of all genes of org.Hs.eg.db from KEGG (last update in
    # data of June 31st 2011)
    genes.kegg <- as.list(org.Hs.egPATH)
    clusterSim(c("9", "15", "10"), c("33", "19", "20"), genes.kegg)
    clusterSim(c("9", "15", "10"), c("33", "19", "20"), genes.kegg, NULL)
    clusterSim(c("9", "15", "10"), c("33", "19", "20"), genes.kegg, "avg")
} else {
    warning('You need org.Hs.eg.db package for this example')
}</pre>
```

combinadic

i-th combination of n elements taken from r

Description

Function similar to combn but for larger vectors. To avoid allocating a big vector with all the combinations each one can be computed with this function.

Usage

```
combinadic(n, r, i)
```

Arguments

n Elements to extract the combination fromr Number of elements per combination

i ith combination

Value

The combination ith of the elements

Author(s)

Joshua Ulrich

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References

StackOverflow answer 4494469/2886003

See Also

combn

Examples

```
#Output of all combinations
combn(LETTERS[1:5], 2)
# Otuput of the second combination
combinadic(LETTERS[1:5], 2, 2)
```

combineScores

Combining values

Description

Combine several similarities into one using several methods.

Usage

```
combineScores(scores, method = c("max", "avg", "rcmax", "rcmax.avg",
   "BMA", "reciprocal"), round = FALSE, t = 0)

combineScoresPar(scores, method, subSets = NULL, BPPARAM = NULL, ...)
```

Arguments

scores method	Matrix of scores to be combined one of c("avg", "max", "rcmax", "rcmax.avg", "BMA", "reciprocal"), see Details.
round	Should the resulting value be rounded to the third digit?
t	Numeric value to filter scores below this value. Only used in the reciprocal method.
subSets	List of combinations as info in other functions.
BPPARAM	BiocParallel back-end parameters. By default (NULL) a for loop is used.
	Other arguments passed to combineScores

Details

The input matrix can be a base matrix or a matrix from package Matrix. The methods return:

avg The average or mean value

max The max value

rcmax The max of the column means or row means

rcmax.avg The sum of the max values by rows and columns divided by the number of columns and rows

BMA The same as rcmax.avg

reciprocal The double of the sum of the reciprocal maximal similarities (above a threshold) divided by the number of elements. See equation 3 of the Tao *et al* 2007 article

combineSources 9

Value

A numeric value as described in details.

Note

combineScores is a version of the function of the same name in package GOSemSim (combineScores) with optional rounding and some internal differences.

Author(s)

Lluís Revilla based on Guangchuang Yu

References

Ying Tao, Lee Sam, Jianrong Li, Carol Friedman, Yves A. Lussier; Information theory applied to the sparse gene ontology annotation network to predict novel gene function. Bioinformatics 2007; 23 (13): i529-i538. doi: 10.1093/bioinformatics/btm195

See Also

register in BiocParallel about the arguments accepted by BPPARAM

Examples

combineSources

Combine different sources of pathways

Description

Given several sources of pathways with the same for the same id of the genes it merge them.

Usage

```
combineSources(...)
```

Arguments

.. Lists of genes and their pathways.

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Details

It assumes that the identifier of the genes are the same for both sources but if many aren't equal it issues a warning. Only unique pathways identifiers are returned.

Value

A single list with the pathways of each source on the same gene.

Examples

conversions

Convert the similarities formats

Description

Functions to convert the similarity coefficients between Jaccard and Dice. D2J is the opposite of J2D.

Usage

D2J(D)

J2D(J)

Arguments

D Dice coefficient, as returned by diceSim, geneSim, clusterSim and clusterGeneSim

J Jaccard coefficient

Value

A numeric value.

Author(s)

Lluís Revilla

```
D2J(0.5)
J2D(0.5)
D2J(J2D(0.5))
```

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diceSim

Compare pathways

Description

Function to estimate how much two list of genes overlap by looking how much of the nodes are shared. Calculates the Dice similarity

Usage

```
diceSim(g1, g2)
```

Arguments

g1, g2

A character list with the names of the proteins in each pathway.

Details

It requires a vector of characters otherwise will return an NA.

Value

A score between 0 and 1 calculated as the double of the proteins shared by g1 and g2 divided by the number of genes in both groups.

Author(s)

Lluís Revilla

See Also

Used for geneSim, see conversions help page to transform Dice score to Jaccard score.

```
genes.id2 <- c("52", "11342", "80895", "57654", "548953", "11586", "45985") genes.id1 <- c("52", "11342", "80895", "57654", "58493", "1164", "1163", "4150", "2130", "159") diceSim(genes.id1, genes.id2) diceSim(genes.id2, genes.id2)
```

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duplicateIndices

Finds the indices of the duplicated events of a vector

Description

Finds the indices of duplicated elements in the vector given.

Usage

```
duplicateIndices(vec)
```

Arguments

vec

Vector of identifiers presumably duplicated

Details

For each duplication it can return a list or if all the duplication events are of the same length it returns a matrix, where each column is duplicated.

Value

The format is determined by the simplify2array

Author(s)

Lluís Revilla

See Also

removeDup

Examples

geneSim

Similarity score genes based on pathways similarity

Description

Given two genes, calculates the Dice similarity between each pathway which is combined to obtain a similarity between the genes.

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Usage

```
geneSim(gene1, gene2, info, method = "max", ...)
## S4 method for signature 'character, character, GeneSetCollection'
geneSim(gene1, gene2,
  info, method = "max", ...)
```

Arguments

gene1, gene2 Ids of the genes to calculate the similarity, to be found in genes.

A GeneSetCollection or a list of genes and the pathways they are involved.

method one of c("avg", "max", "rcmax", "rcmax.avg", "BMA", "reciprocal"), see Details.

Other arguments passed to combineScores

Details

Given the information about the genes and their pathways, uses the ids of the genes to find the Dice similarity score for each pathway comparison between the genes. Later this similarities are combined using combineScoresPar.

Value

The highest Dice score of all the combinations of pathways between the two ids compared if a method to combine scores is provided or NA if there isn't information for one gene. If an NA is returned this means that there isn't information available for any pathways for one of the genes. Otherwise a number between 0 and 1 (both included) is returned. Note that there isn't a negative value of similarity.

Methods (by class)

• gene1 = character, gene2 = character, info = GeneSetCollection: Calculates all the similarities of the GeneSetCollection and combine them using combineScoresPar

Author(s)

Lluís Revilla

See Also

mgeneSim, conversions help page to transform Dice score to Jaccard score. For the method to combine the scores see combineScoresPar.

```
if (require("org.Hs.eg.db") & require("reactome.db")) {
    # Extract the paths of all genes of org.Hs.eg.db from KEGG
    # (last update in data of June 31st 2011)
    genes.kegg <- as.list(org.Hs.egPATH)
    # Extracts the paths of all genes of org.Hs.eg.db from reactome
    genes.react <- as.list(reactomeEXTID2PATHID)
    geneSim("81", "18", genes.react)
    geneSim("81", "18", genes.kegg)</pre>
```

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```
geneSim("81", "18", genes.react, NULL)
geneSim("81", "18", genes.kegg, NULL)
} else {
  warning('You need reactome.db and org.Hs.eg.db package for this example')
}
```

inverseList

Invert a list

Description

Calculate the pathways per gene of list

Usage

```
inverseList(x)
```

Arguments

Χ

A list with genes as names and names of pathways as values of the list

Value

The number of pathways each gene has.

Author(s)

Lluís Revilla

mclusterGeneSim

Similarity score between clusters of genes based on genes similarity

Description

Looks for the similarity between genes of a group and then between each group's genes.

Usage

```
mclusterGeneSim(clusters, info, method = c("max", "rcmax.avg"), ...)
## S4 method for signature 'list,GeneSetCollection'
mclusterGeneSim(clusters, info,
    method = c("max", "rcmax.avg"), ...)
```

Arguments

clusters A list of clusters of genes to be found in id.

A GeneSetCollection or a list of genes and the pathways they are involved.

A vector with two or one argument to be passed to combineScores the first one is used to summarize the similarities of genes, the second one for clusters.

... Other arguments passed to combineScores

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Value

Returns a matrix with the similarity scores for each cluster comparison.

Methods (by class)

• clusters = list, info = GeneSetCollection: Calculates all the similarities of the Gene-SetCollection and combine them using combineScoresPar

Author(s)

Lluís Revilla

See Also

clusterGeneSim, clusterSim and combineScores

Examples

mclusterSim

Similarity score between clusters of genes based on pathways similarity

Description

Looks for the similarity between genes in groups. Once the pathways for each cluster are found they are combined using codecombineScores.

Usage

```
mclusterSim(clusters, info, method = "max", ...)
## S4 method for signature 'list,GeneSetCollection'
mclusterSim(clusters, info,
    method = "max", ...)
```

Arguments

```
clusters A list of clusters of genes to be found in id.

A GeneSetCollection or a list of genes and the pathways they are involved.

method one of c("avg", "max", "rcmax", "rcmax.avg", "BMA", "reciprocal"), see Details.

Other arguments passed to combineScores
```

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Value

mclusterSim returns a matrix with the similarity scores for each cluster comparison.

Methods (by class)

• clusters = list,info = GeneSetCollection: Calculates all the similarities of the Gene-SetCollection and combine them using combineScoresPar

Author(s)

Lluís Revilla

See Also

For a different approach see clusterGeneSim, combineScores and conversions

Examples

mgeneSim

Similarity score genes based on pathways similarity

Description

Given two genes, calculates the Dice similarity between each pathway which is combined to obtain a similarity between the genes.

Usage

```
mgeneSim(genes, info, method = "max", ...)
## S4 method for signature 'character,GeneSetCollection'
mgeneSim(genes, info,
  method = "max", ...)
## S4 method for signature 'missing,GeneSetCollection'
mgeneSim(genes, info,
  method = "max", ...)
```

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Arguments

genes	A vector of genes.
info	A GeneSetCollection or a list of genes and the pathways they are involved.
method	one of c("avg","max","rcmax","rcmax.avg","BMA","reciprocal"), see Details.
	Other arguments passed to combineScores

Details

Given the information about the genes and their pathways, uses the ids of the genes to find the Dice similarity score for each pathway comparison between the genes. Later this similarities are combined using combineScoresPar.

Value

mgeneSim returns the matrix of similarities between the genes in the vector

Methods (by class)

- genes = character, info = GeneSetCollection: Calculates all the similarities of the list and combine them using combineScoresPar
- genes = missing, info = GeneSetCollection: Calculates all the similarities of the list and combine them using combineScoresPar

Note

genes accept named characters and the output will use the names of the genes.

See Also

geneSim, conversions help page to transform Dice score to Jaccard score. For the method to combine the scores see combineScoresPar.

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mpathSim

Calculates the Dice similarity between pathways

Description

Calculates the similarity between several pathways using dice similarity score. If one needs the matrix of similarities between pathways set the argument methods to NULL.

Usage

```
mpathSim(pathways, info, method = NULL, ...)
## S4 method for signature 'character, GeneSetCollection, ANY'
mpathSim(pathways, info,
  method = NULL, ...)
## S4 method for signature 'missing, GeneSetCollection, ANY'
mpathSim(pathways, info,
  method = NULL, ...)
## S4 method for signature 'missing, list, ANY'
mpathSim(pathways, info, method = NULL, ...)
## S4 method for signature 'missing, list, missing'
mpathSim(pathways, info, method = NULL, ...)
```

Arguments

pathways	Pathways to calculate the similarity for
info	A list of genes and the pathways they are involved or a GeneSetCollection object
method	To combine the scores of each pathway, one of $c("avg", "max", "rcmax", "rcmax.avg", "BMA")$, if NULL returns the matrix of similarities.
	Other arguments passed to combineScoresPar

Value

The similarity between those pathways or all the similarities between each comparison.

Methods (by class)

- pathways = character, info = GeneSetCollection, method = ANY: Calculates the similarity between the provided pathways of the GeneSetCollection using combineScoresPar
- pathways = missing, info = GeneSetCollection, method = ANY: Calculates all the similarities of the GeneSetCollection and combine them using combineScoresPar
- pathways = missing,info = list,method = ANY: Calculates all the similarities of the list and combine them using combineScoresPar
- pathways = missing, info = list, method = missing: Calculates all the similarities of the list

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Note

pathways accept named characters, and then the output will have the names

See Also

pathSim For single pairwise comparison. conversions To convert the Dice similarity to Jaccard similarity

Examples

pathSim

Calculates the Dice similarity between pathways

Description

Calculates the similarity between pathways using dice similarity score. diceSim is used to calculate similarities between the two pathways.

Usage

```
pathSim(pathway1, pathway2, info)
## S4 method for signature 'character, character, GeneSetCollection'
pathSim(pathway1,
    pathway2, info)
```

Arguments

```
pathway1, pathway2

A single pathway to calculate the similarity

info

A GeneSetCollection or a list of genes and the pathways they are involved.
```

Value

The similarity between those pathways or all the similarities between each comparison.

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Methods (by class)

• pathway1 = character, pathway2 = character, info = GeneSetCollection: Calculates all the similarities of a GeneSetCollection and combine them using combineScoresPar

Author(s)

Lluís Revilla

See Also

conversions help page to transform Dice score to Jaccard score. mpathSim for multiple pairwise comparison of pathways.

Examples

```
if (require("reactome.db")){
    # Extracts the paths of all genes of org.Hs.eg.db from reactome
    genes.react <- as.list(reactomeEXTID2PATHID)
    (paths <- sample(unique(unlist(genes.react)), 2))
    pathSim(paths[1], paths[2], genes.react)
} else {
    warning('You need reactome.db package for this example')
}</pre>
```

removeDup

Remove duplicated rows and columns

Description

Given the indices of the duplicated entries remove the columns and rows until just one is left, it keeps the duplicated with the highest absolute mean value.

Usage

```
removeDup(cor_mat, dupli)
```

Arguments

cor_mat List of matrices

dupli List of indices with duplicated entries

Value

A matrix with only one of the columns and rows duplicated

Author(s)

Lluís Revilla

See Also

duplicateIndices to obtain the list of indices with duplicated entries.

seq2mat 21

Examples

```
a <- seq2mat(c("52", "52", "53", "55"), runif(choose(4, 2)))
b <- seq2mat(c("52", "52", "53", "55"), runif(choose(4, 2)))
mat <- list("kegg" = a, "react" = b)
mat
dupli <- duplicateIndices(rownames(a))
remat <- removeDup(mat, dupli)
remat</pre>
```

seq2mat

Transforms a vector to a symmetric matrix

Description

Fills a matrix of ncol = length(x) and nrow = length(x) with the values in dat and setting the diagonal to 1.

Usage

```
seq2mat(x, dat)
```

Arguments

x names of columns and rows, used to define the size of the matrix

dat Data to fill with the matrix with except the diagonal.

Details

dat should be at least choose(length(x), 2) of length. It assumes that the data provided comes from using the row and column id to obtain it.

Value

A square matrix with the diagonal set to 1 and dat on the upper and lower triangle with the columns ids and row ids from x.

Author(s)

Lluís Revilla

See Also

```
upper.tri and lower.tri
```

```
seq2mat(LETTERS[1:5], 1:10)

seq2mat(LETTERS[1:5], seq(from = 0.1, to = 1, by = 0.1))
```

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Apply a function to a list of similarities

Description

Function to join list of similarities by a function provided by the user.

Usage

```
similarities(sim, func, ...)
```

Arguments

sim	list of similarities to be joined. All similarities must have the same dimensions. The genes are assumed to be in the same order for all the matrices.
func	function to perform on those similarities: prod, sum It should accept as many arguments as similarities matrices are provided, and should use numbers.
	Other arguments passed to the function func. Usually na.rm or similar.

Value

A matrix of the size of the similarities

Note

It doesn't check that the columns and rows of the matrices are in the same order or are the same.

Author(s)

Lluís Revilla

See Also

weighted for functions that can be used, and addSimilarities for a wrapper to one of them

```
set.seed(100)
a <- seq2mat(LETTERS[1:5], rnorm(10))
b <- seq2mat(LETTERS[1:5], seq(from = 0.1, to = 1, by = 0.1))
sim <- list(b, a)
similarities(sim, weighted.prod, c(0.5, 0.5))
# Note the differences in the sign of some values
similarities(sim, weighted.sum, c(0.5, 0.5))</pre>
```

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WAIG	ghted
***	JIICCA

Weighted operations

Description

Calculates the weighted sum or product of x. Each values should have its weight, otherwise it will throw an error.

Usage

```
weighted.sum(x, w, abs = TRUE)
weighted.prod(x, w)
```

Arguments

X	an object containing the values whose weighted operations is to be computed
W	a numerical vector of weights the same length as \boldsymbol{x} giving the weights to use for elements of \boldsymbol{x} .
abs	If any x is negative you want the result negative too?

Details

This functions are thought to be used with similarities. As some similarities might be positive and others negative the argument abs is provided for weighted.sum, assuming that only one similarity will be negative (usually the one coming from expression correlation).

Value

weighted.sum returns the sum of the product of x*weights removing all NA values. See parameter abs if there are any negative values.

weighted.prod returns the product of product of x*weights removing all NA values.

Author(s)

Lluís Revilla

See Also

weighted.mean, similarities and addSimilarities

```
\begin{split} & \exp r <- c(-0.2,\ 0.3,\ 0.5,\ 0.8,\ 0.1) \\ & \text{weighted.sum}(\exp r,\ c(0.5,\ 0.2,\ 0.1,\ 0.1,\ 0.1)) \\ & \text{weighted.sum}(\exp r,\ c(0.5,\ 0.2,\ 0.1,\ 0.2,\ 0.1),\ FALSE) \\ & \text{weighted.sum}(\exp r,\ c(0.4,\ 0.2,\ 0.1,\ 0.2,\ 0.1)) \\ & \text{weighted.sum}(\exp r,\ c(0.4,\ 0.2,\ 0.1,\ 0.2,\ 0.1),\ FALSE) \\ & \text{weighted.sum}(\exp r,\ c(0.4,\ 0.2,\ 0,\ 0.2,\ 0.1)) \\ & \text{weighted.sum}(\exp r,\ c(0.5,\ 0.2,\ 0,\ 0.2,\ 0.1)) \\ & \text{\# Compared to weighted.prod:} \\ & \text{weighted.prod}(\exp r,\ c(0.5,\ 0.2,\ 0.1,\ 0.1,\ 0.1)) \end{split}
```

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```
weighted.prod(expr, c(0.4, 0.2, 0.1, 0.2, 0.1)) weighted.prod(expr, c(0.4, 0.2, 0, 0.2, 0.1)) weighted.prod(expr, c(0.5, 0.2, 0, 0.2, 0.1))
```

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