

Package ‘WebGestaltR’

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Type Package

Title The R Version of WebGestalt

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Description The web version WebGestalt <<http://www.webgestalt.org>> supports 12 organisms, 354 gene identifiers and 321,251 function categories. Users can upload the data and functional categories with their own gene identifiers. In addition to the Over-Representation Analysis, WebGestalt also supports Gene Set Enrichment Analysis and Network Topology Analysis. The user-friendly output report allows interactive and efficient exploration of enrichment results. The WebGestaltR package not only supports all above functions but also can be integrated into other pipeline or simultaneously analyze multiple gene lists.

License LGPL

URL <https://github.com/bzhanglab/WebGestaltR>

LazyLoad yes

Depends R (>= 3.3)

Imports methods, dplyr, doRNG, readr, parallel (>= 3.3.2), doParallel (>= 1.0.10), foreach (>= 1.4.0), rjson (>= 0.2.15), httr, rlang, igraph, whisker, apcluster, Rcpp

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affinityPropagation *Affinity Propagation*

Description

Use affinity propagation to cluster similar gene sets to reduce redundancy in report.

Usage

```
affinityPropagation(idsInSet, score)
```

Arguments

idsInSet A list of set names and their member IDs.
score A vector of addible scores with the same length used to assign input preference; higher score has larger weight, i.e. $-\log P$.

Value

A list of clusters and representatives for each cluster.

clusters A list of character vectors of set IDs in each cluster.

representatives A character vector of representatives for each cluster.

Author(s)

Zhiao Shi, Yuxing Liao

formatCheck	<i>Check Format and Read Data</i>
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Description

Check Format and Read Data

Usage

```
formatCheck(dataType = "list", inputGeneFile = NULL,
            inputGene = NULL)
```

Arguments

dataType	Type of data, either list, rnk or gmt. Could be list, rnk or matrix for idToSymbol.
inputGeneFile	The data file to be mapped.
inputGene	Or the input could be given as an R object. GMT file should be read with readGmt.

Value

A list of data frame

goSlimSummary	<i>GO Slim Summary</i>
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Description

Outputs a brief summary of input genes based on GO Slim data.

Usage

```
goSlimSummary(organism = "hsapiens", geneList, outputFile,
              outputType = "pdf", isOutput = TRUE,
              hostName = "http://www.webgestalt.org")
```

Arguments

organism	Currently, WebGestaltR supports 12 organisms. Users can use the function listOrganism to check available organisms. Users can also input others to perform the enrichment analysis for other organisms not supported by WebGestaltR. For other organisms, users need to provide the functional categories, interesting list and reference list (for ORA method). Because WebGestaltR does not perform the ID mapping for the other organisms, the above data should have the same ID type.
----------	--

geneList	A list of input genes.
outputFile	Output file name.
outputType	File format of the plot: pdf, bmp or png.
isOutput	Boolean if a plot is save to outputFile.
hostName	The server URL for accessing data. Mostly for development purposes.

Value

A list of the summary result.

idMapping	<i>ID Mapping</i>
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Description

ID mapping utility with WebGestalt server.

Usage

```
idMapping(organism = "hsapiens", dataType = "list",
  inputGeneFile = NULL, inputGene = NULL, sourceIdType,
  targetIdType = NULL, collapseMethod = "mean",
  mappingOutput = FALSE, outputFileName = "",
  hostName = "http://www.webgestalt.org/")
```

```
idToSymbol(organism = "hsapiens", dataType = "list",
  inputGeneFile = NULL, inputGene = NULL,
  sourceIdType = "ensembl_gene_id", collapseMethod = "mean",
  mappingOutput = FALSE, outputFileName = NULL,
  hostName = "http://www.webgestalt.org/")
```

Arguments

organism	Currently, WebGestaltR supports 12 organisms. Users can use the function <code>listOrganism</code> to check available organisms. Users can also input others to perform the enrichment analysis for other organisms not supported by WebGestaltR. For other organisms, users need to provide the functional categories, interesting list and reference list (for ORA method). Because WebGestaltR does not perform the ID mapping for the other organisms, the above data should have the same ID type.
dataType	Type of data, either list, rnk or gmt. Could be list, rnk or matrix for <code>idToSymbol</code> .
inputGeneFile	The data file to be mapped.
inputGene	Or the input could be given as an R object. GMT file should be read with <code>readGmt</code> .

sourceIdType	The ID type of the data.
targetIdType	The ID type of the mapped data.
collapseMethod	The method to collapse duplicate IDs with scores. mean, median, min and max represent the mean, median, minimum and maximum of scores for the duplicate IDs.
mappingOutput	Boolean if the mapping output is written to file.
outputFileName	The output file name.
hostName	The server URL for accessing data. Mostly for development purposes.

Value

A list of mapped and unmapped IDs.

jaccardSim	<i>Jaccard Similarity</i>
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Description

Calculate Jaccard Similarity.

Usage

```
jaccardSim(idsInSet, score)
```

Arguments

idsInSet	A list of set names and their member IDs.
score	A vector of addible scores with the same length used to assign input preference; higher score has larger weight, i.e. $-\log P$.

Value

A list of similarity matrix `sim.mat` and input preference vector `ip.vec`.

Author(s)

Zhiao Shi, Yuxing Liao

listArchiveUrl	<i>List WebGestalt Servers</i>
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Description

List available WebGestalt servers.

Usage

```
listArchiveUrl()
```

Value

A data frame of available servers.

listGeneSet	<i>List Gene Sets</i>
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Description

List available gene sets for the given organism on WebGestalt server.

Usage

```
listGeneSet(organism = "hsapiens",
            hostName = "http://www.webgestalt.org/")
```

Arguments

organism	Currently, WebGestaltR supports 12 organisms. Users can use the function listOrganism to check available organisms. Users can also input others to perform the enrichment analysis for other organisms not supported by WebGestaltR. For other organisms, users need to provide the functional categories, interesting list and reference list (for ORA method). Because WebGestaltR does not perform the ID mapping for the other organisms, the above data should have the same ID type.
hostName	The server URL for accessing data. Mostly for development purposes.

Value

A data frame of available gene sets.

listIdType	<i>List ID Types</i>
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Description

List supported ID types for the given organism on WebGestalt server.

Usage

```
listIdType(organism = "hsapiens",  
           hostName = "http://www.webgestalt.org/")
```

Arguments

organism	Currently, WebGestaltR supports 12 organisms. Users can use the function <code>listOrganism</code> to check available organisms. Users can also input others to perform the enrichment analysis for other organisms not supported by WebGestaltR. For other organisms, users need to provide the functional categories, interesting list and reference list (for ORA method). Because WebGestaltR does not perform the ID mapping for the other organisms, the above data should have the same ID type.
hostName	The server URL for accessing data. Mostly for development purposes.

Value

A list of supported gene sets.

listOrganism	<i>List Organisms</i>
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Description

List supported organisms on WebGestalt server.

Usage

```
listOrganism(hostName = "http://www.webgestalt.org/")
```

Arguments

hostName	The server URL for accessing data. Mostly for development purposes.
----------	---

Value

A list of supported organisms.

listReferenceSet	<i>List Reference Sets</i>
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Description

List available reference sets for the given organism on WebGestalt server.

Usage

```
listReferenceSet(organism = "hsapiens",
  hostName = "http://www.webgestalt.org/")
```

Arguments

organism	Currently, WebGestaltR supports 12 organisms. Users can use the function <code>listOrganism</code> to check available organisms. Users can also input others to perform the enrichment analysis for other organisms not supported by WebGestaltR. For other organisms, users need to provide the functional categories, interesting list and reference list (for ORA method). Because WebGestaltR does not perform the ID mapping for the other organisms, the above data should have the same ID type.
hostName	The server URL for accessing data. Mostly for development purposes.

Value

A list of reference sets.

prepareGseaInput	<i>Prepare input for standard GSEA</i>
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Description

A helper to read files for performing standard GSEA.

Usage

```
prepareGseaInput(rankFile, gmtFile)
```

Arguments

rankFile	Path of the rnk file
gmtFile	Path of the GMT file

Value

a data frame to be used in `swGsea`

prepareInputMatrixGsea

Prepare Input Matrix for GSEA

Description

Prepare Input Matrix for GSEA

Usage

prepareInputMatrixGsea(rank, gmt)

Arguments

rank	A 2 column Data Frame of gene and score
gmt	3 column Data Frame of geneSet, description, and gene

Value

A matrix used for input to swGsea.

readGmt

Read GMT File

Description

Read GMT File

Usage

readGmt(gmtFile)

Arguments

gmtFile	The file path or URL of the GMT file.
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Value

A data frame with columns of "geneSet", "description", "gene".

swGsea

*Site Weighted Gene Set Enrichment Analysis***Description**

Performs site weighted gene set enrichment analysis or standard GSEA when likelihood/weight columns in `input_df` are 1 or 0, $p=1$, $q=1$ and `thresh_type="val"`.

Usage

```
swGsea(input_df, thresh_type = "percentile", thresh = 0.9,
       thresh_action = "exclude", min_set_size = 10, max_set_size = 500,
       max_score = "max", min_score = "min", psuedocount = 0.001,
       perms = 1000, p = 1, q = 1, nThreads = 1, rng_seed = 1,
       fork = FALSE)
```

Arguments

<code>input_df</code>	A data frame in which first column is name of item of interest (gene, protein, phosphosite, etc.), the second is the correlation of that item of interest with the phenotype (typically log ratio of expression for phenotype vs. normal), and the remaining columns are the scores for the likelihood that the item belongs in each set (one column per set).
<code>thresh_type</code>	The type of thresh. Use 'percentile' to include all scores over that percentile given in <code>thresh</code> (i.e., 0.9 would be all items in 90th percentile, or top 10 percent); 'list' to include a list of set lists where the set lists are in the same order as the corresponding set columns in the <code>input_df</code> ; 'val' to apply a single threshold value to all sets; or 'values' to use a vector of unique cutoffs for each set (needs to be in the same order as the sets are specified in the columns of <code>input_df</code>)
<code>thresh</code>	Depends on <code>thresh_type</code> . A list of lists of the items in each set (with same names as colnames of the scores); a numeric vector of threshold scores for each set (in the same order as the colnames of the scores in the <code>input_df</code>), or a single percentile value between 0 and 1 (i.e., if <code>thresh=0.9</code> , the 90th percentile of the score or the highest scoring 10 of of the items are included in the set for each scoring regimen) (<code>thresh="all"</code> is not supported at this time, as it doesn't result in a Kolgorov-Smirnoff statistic; this may be worked in as an alternate scoring method later on).
<code>thresh_action</code>	Either "include", "exclude (default)", or "adjust"; this specifies how to treat each set if it doesn't contain a minimum number of items or contains all of the items; this option cannot be used with predefined lists of items in sets (if the number of items in a given set doesn't meet requirements, that set will be skipped).
<code>min_set_size, max_set_size</code>	The minimum/maximum number of items each set needs for the analysis to proceed.

max_score, min_score	A optional numeric vector of minimum/maximum boundaries to clip scores for each set.
psuedocount	Psuedocount (pc) is used for rescaling set scores: $(score - min_score + pc)/(max_score - min_score)$ this is needed to prevent division by 0 if $max_score == min_score$ (in this case, all scores for items in set will be 1, which is equivalent to standard GSEA); it also allows users to adjust weights for scores that are close to the minimum for the scores in the set (unless $min_score == max_score$): as psuedocount value approaches 0, scaled minimum scores also approach 0; as psuedocount approaches infinity, scaled minimum scores approach the scaled maximum scores (which equal 1); this value must be larger than 0.
perms	The number of permutations.
p	The exponential scaling factor of the phenotype score (second column in input_df).
q	The exponential scaling factor of the likelihood score (weights).
nThreads	The number of threads to use in calculating permutaions.
rng_seed	Random seed.
fork	A boolean. Whether pass "fork" to type parameter of makeCluster on Unix-like machines.

Details

The formula for weighting is as follows

$$\frac{s_j^q |r_j|^p}{\sum s^q |r|^p}$$

Where r is log ratio score, s is likelihood score, j is the index of the gene.

Value

A list of `Enrichment_Results`, `Items_in_Set` and `Running_Sums`.

Enrichment_Results A data frame with row names of gene set and columns of "ES", "NES", "p_val", "fdr".

Items_in_Set A list of one-column data frames. Describes genes and their ranks in each set.

Running_Sums Running sum scores along genes sorted by ranked scores, with gene sets as columns.

Author(s)

Eric Jaehnig

WebGestaltR *WebGestaltR: The R interface for enrichment analysis with WebGestalt.*

Description

Main function for enrichment analysis

Usage

```
WebGestaltR(enrichMethod = "ORA", organism = "hsapiens",
  enrichDatabase = "geneontology_Biological_Process",
  enrichDatabaseFile = NULL, enrichDatabaseType = NULL,
  enrichDatabaseDescriptionFile = NULL, interestGeneFile = NULL,
  interestGene = NULL, interestGeneType = NULL,
  collapseMethod = "mean", referenceGeneFile = NULL,
  referenceGene = NULL, referenceGeneType = NULL,
  referenceSet = NULL, minNum = 10, maxNum = 500,
  sigMethod = "fdr", fdrMethod = "BH", fdrThr = 0.05, topThr = 10,
  reportNum = 20, perNum = 1000, isOutput = TRUE,
  outputDirectory = getwd(), projectName = NULL,
  dagColor = "continuous", setCoverNum = 10,
  networkConstructionMethod = NULL, neighborNum = 10,
  highlightType = "Seeds", highlightSeedNum = 10, nThreads = 1,
  hostName = "http://www.webgestalt.org/", ...)
```

```
WebGestaltRBatch(interestGeneFolder = NULL, enrichMethod = "ORA",
  isParallel = FALSE, nThreads = 3, ...)
```

Arguments

enrichMethod	Enrichment methods: ORA, GSEA or NTA.
organism	Currently, WebGestaltR supports 12 organisms. Users can use the function <code>listOrganism</code> to check available organisms. Users can also input others to perform the enrichment analysis for other organisms not supported by WebGestaltR. For other organisms, users need to provide the functional categories, interesting list and reference list (for ORA method). Because WebGestaltR does not perform the ID mapping for the other organisms, the above data should have the same ID type.
enrichDatabase	The functional categories for the enrichment analysis. Users can use the function <code>listGeneSet</code> to check the available functional databases for the selected organism. Users can also input others to provide a custom functional databases not supported by WebGestaltR for the selected organism.
enrichDatabaseFile	If users set <code>organism</code> as others or set <code>enrichDatabase</code> as others, users need to provide a GMT file as the functional category for enrichment analysis. The

extension of the file should be gmt and the first column of the file is the category ID, the second one is the external link for the category. Genes annotated to the category are from the third column. All columns are separated by tabs.

enrichDatabaseType

If users set `enrichDatabase` as others, WebGestaltR will also perform ID mapping for the supplied GMT file. Thus, users need to set the ID type of the genes in the `enrichDatabaseFile`. If users set `organism` as others, users do not need to set this ID type because WebGestaltR will not perform ID mapping for other organisms. The supported ID types of WebGestaltR for the selected organism can be found by the function `listIdType`.

enrichDatabaseDescriptionFile

Users can also provide a description file for the custom `enrichDatabaseFile`. The extension of the description file should be `des`. The description file contains two columns: the first column is the category ID that should be exactly the same as the category ID in the custom `enrichDatabaseFile` and the second column is the description of the category. All columns are separated by tabs.

interestGeneFile

If `enrichMethod` is ORA or NTA, the extension of the `interestGeneFile` should be `txt` and the file can only contain one column: the interesting gene list. If `enrichMethod` is GSEA, the extension of the `interestGeneFile` should be `rnk` and the file should contain two columns separated by tab: the gene list and the corresponding scores.

interestGene

Users can also use an R object as the input. If `enrichMethod` is ORA or NTA, `interestGene` should be an R vector object containing the interesting gene list. If `enrichMethod` is GSEA, `interestGene` should be an R `data.frame` object containing two columns: the gene list and the corresponding scores.

interestGeneType

The ID type of the interesting gene list. The supported ID types of WebGestaltR for the selected organism can be found by the function `listIdType`. If the organism is others, users do not need to set this parameter.

collapseMethod

The method to collapse duplicate IDs with scores. `mean`, `median`, `min` and `max` represent the mean, median, minimum and maximum of scores for the duplicate IDs.

referenceGeneFile

For the ORA method, the users need to upload the reference gene list. The extension of the `referenceGeneFile` should be `txt` and the file can only contain one column: the reference gene list.

referenceGene

For the ORA method, users can also use an R object as the reference gene list. `referenceGene` should be an R vector object containing the reference gene list.

referenceGeneType

The ID type of the reference gene list. The supported ID types of WebGestaltR for the selected organism can be found by the function `listIdType`. If the organism is others, users do not need to set this parameter.

referenceSet

Users can directly select the reference set from existing platforms in WebGestaltR and do not need to provide the reference set through `referenceGeneFile`. All

existing platforms supported in WebGestaltR can be found by the function `listReferenceSet`. If `referenceGeneFile` and `referenceGene` are NULL, WebGestaltR will use the `referenceSet` as the reference gene set. Otherwise, WebGestaltR will use the user supplied reference set for enrichment analysis.

<code>minNum</code>	WebGestaltR will exclude the categories with the number of annotated genes less than <code>minNum</code> for enrichment analysis. The default is 10.
<code>maxNum</code>	WebGestaltR will exclude the categories with the number of annotated genes larger than <code>maxNum</code> for enrichment analysis. The default is 500.
<code>sigMethod</code>	Two methods of significance are available in WebGestaltR: <code>fdr</code> and <code>top</code> . <code>fdr</code> means the enriched categories are identified based on the FDR and <code>top</code> means all categories are ranked based on FDR and then select top categories as the enriched categories. The default is <code>fdr</code> .
<code>fdrMethod</code>	For the ORA method, WebGestaltR supports five FDR methods: <code>holm</code> , <code>hochberg</code> , <code>hommel</code> , <code>bonferroni</code> , <code>BH</code> and <code>BY</code> . The default is <code>BH</code> .
<code>fdrThr</code>	The significant threshold for the <code>fdr</code> method. The default is 0.05.
<code>topThr</code>	The threshold for the <code>top</code> method. The default is 10.
<code>reportNum</code>	The number of enriched categories visualized in the final report. The default is 20. A larger <code>reportNum</code> may be slow to render in the report.
<code>perNum</code>	The number of permutations for the GSEA method. The default is 1000.
<code>isOutput</code>	If <code>isOutput</code> is TRUE, WebGestaltR will create a folder named by the <code>projectName</code> and save the results in the folder. Otherwise, WebGestaltR will only return an R <code>data.frame</code> object containing the enrichment results. If hundreds of gene list need to be analyzed simultaneously, it is better to set <code>isOutput</code> to FALSE. The default is TRUE.
<code>outputDirectory</code>	The output directory for the results.
<code>projectName</code>	The name of the project. If <code>projectName</code> is NULL, WebGestaltR will use time stamp as the project name.
<code>dagColor</code>	If <code>dagColor</code> is binary, the significant terms in the DAG structure will be colored by steel blue for ORA method or steel blue (positive related) and dark orange (negative related) for GSEA method. If <code>dagColor</code> is continuous, the significant terms in the DAG structure will be colored by the color gradient based on corresponding FDRs.
<code>setCoverNum</code>	The number of expected gene sets after set cover to reduce redundancy. It could get fewer sets if the coverage reaches 100%. The default is 10.
<code>networkConstructionMethod</code>	Network construction method for NTA. Either <code>Network_Retrieval_Prioritization</code> or <code>Network_Expansion</code> . Network Retrieval & Prioritization first uses random walk analysis to calculate random walk probabilities for the input seeds, then identifies the relationships among the seeds in the selected network and returns a retrieval sub-network. The seeds with the top random walk probabilities are highlighted in the sub-network. Network Expansion first uses random walk analysis to rank all genes in the selected network based on their network proximity to the input seeds and then return an expanded sub-network in which nodes are the input seeds and their top ranking neighbors and edges represent their relationships.

neighborNum	The number of neighbors to include in NTA Network Expansion method.
highlightType	The type of nodes to highlight in the NTA Network Expansion method, either Seeds or Neighbors.
highlightSeedNum	The number of top input seeds to highlight in NTA Network Retrieval & Prioritization method.
nThreads	The number of cores to use for GSEA and set cover, and in batch function.
hostName	The server URL for accessing data. Mostly for development purposes.
...	In batch function, passes parameters to WebGestaltR function. Also handles backward compatibility for some parameters in old versions.
interestGeneFolder	Run WebGestaltR for gene list files in the folder.
isParallel	If jobs are run parallelly in the batch.

Details

WebGestaltR function can perform three enrichment analyses: ORA (Over-Representation Analysis) and GSEA (Gene Set Enrichment Analysis), and NTA (Network Topology Analysis). Based on the user-uploaded gene list or gene list with scores, WebGestaltR function will first map the gene list to the entrez gene ids and then summarize the gene list based on the GO (Gene Ontology) Slim. After performing the enrichment analysis, WebGestaltR function also returns an user-friendly HTML report containing GO Slim summary and the enrichment analysis result. If functional categories have DAG (directed acyclic graph) structure or genes in the functional categories have network structure, those relationship can also be visualized in the report.

Value

The WebGestaltR function returns a data frame containing the enrichment analysis result and also outputs an user-friendly HTML report if isOutput is TRUE.

The WebGestaltRBatch function returns a list of enrichment results.

Examples

```
## Not run:
##### ORA example #####
geneFile <- system.file("extdata", "interestingGenes.txt", package="WebGestaltR")
refFile <- system.file("extdata", "referenceGenes.txt", package="WebGestaltR")
outputDirectory <- getwd()
enrichResult <- WebGestaltR(enrichMethod="ORA", organism="hsapiens",
  enrichDatabase="pathway_KEGG", interestGeneFile=geneFile,
  interestGeneType="genesymbol", referenceGeneFile=refFile,
  referenceGeneType="genesymbol", isOutput=TRUE,
  outputDirectory=outputDirectory, projectName=NULL)

##### GSEA example #####
rankFile <- system.file("extdata", "GeneRankList.rnk", package="WebGestaltR")
outputDirectory <- getwd()
enrichResult <- WebGestaltR(enrichMethod="GSEA", organism="hsapiens",
```

```

enrichDatabase="pathway_KEGG", interestGeneFile=rankFile,
interestGeneType="genesymbol", sigMethod="top", topThr=10, minNum=5,
outputDirectory=outputDirectory)

##### NTA example #####
enrichResult <- WebGestaltR(enrichMethod="NTA", organism="hsapiens",
  enrichDatabase="network_PPI_BIOGRID", interestGeneFile=geneFile,
  interestGeneType="genesymbol", sigMethod="top", topThr=10,
  outputDirectory=getwd(), highlightSeedNum=10,
  networkConstructionMethod="Network_Retrieval_Prioritization")

## End(Not run)

```

weightedSetCover	<i>Weighted Set Cover</i>
------------------	---------------------------

Description

Size constrained weighted set cover problem to find top N sets while maximizing the coverage of all elements.

Usage

```
weightedSetCover(idsInSet, costs, topN, nThreads = 4)
```

Arguments

idsInSet	A list of set names and their member IDs.
costs	A vector of the same length to add weights for penalty, i.e. $1/-\log P$.
topN	The number of sets (or less when it completes early) to return.
nThreads	The number of processes to use. In Windows, it fallbacks to 1.

Value

A list of topSets and coverage.

topSets A list of set IDs.

coverage The percentage of IDs covered in the top sets.

Author(s)

Zhiao Shi, Yuxing Liao

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