PGSEA

March 24, 2012

GOLUBmcs

Molecular Concepts prepared at VAI from data created by Golub et al.

Description

386 molecular concepts generated at VAI. The data these concepts were generate from is available from http://www.broad.mit.edu/cmap/.

Usage

```
data(GOLUBmcs)
```

Format

a list of "smc" objects

Details

These concepts were generated using the limma BioConductor package. The code used for generation of these concepts is available upon request.

Source

```
http://www.broad.mit.edu/cmap/
```

```
data(GOLUBmcs)
str(GOLUBmcs[1:4])
```

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PGSEA Parametric Gene Set Enrichment Analys	sis
---	-----

Description

This package contains functions for an exploratory parametric analysis of gene expression data. This type of analysis can assist in determining of lists of genes, such as those deregulated in defined experimental systems, are similarly deregulated in other data sets.

This function subsets the data based on lists of genes, computes a summary statistic for each gene list, and returns the results in a convenient form.

Usage

```
PGSEA(exprs, cl, range = c(25, 500), ref = NULL, center = TRUE, p.value = 0.005,
```

Arguments

exprs	matrix expression data, a numeric matrix, eSet, or ExpressionSet
cl	gene set list - "GeneSetCollection" or list of "SMC" objects
range	a 2 element vector describing the min and max length of concepts to analyze
enforceRange	boolean - if TRUE, the expression matrix must contain data for the proper number of genes as set by the range argument to return a significant result. (this argument is used for data that contains NA's)
ref	a vector containing the index of reference samples from which to make comparisons. Defaults to NULL (internally referenced samples)
center	boolean - median center gene expression matrix columns prior to analysis. Can be helpful if 'ref' is used
p.value	numeric p.value threshold or NA to return all data or TRUE to return a matrix of p.values
weighted	boolean - weight results by the size of each gene list
	extra arguments passed along to FUN

Details

Gene expression values are separated into subsets based on the lists of genes contained in the cl argument. This can be a "GeneSetCollection" or a list of "SMC" (Simple Molecular Concept) objects. For example, readGmt can be used to produce a 'smc' object list from a simple tab-delimited text file. The gene expression values from each of these gene lists is extracted and a summary statistic is computed for each subset (or region in the case of chromosomal bands/arms).

The expression data must have the same identifiers as the list of genes being tested. If they are not, the expression data can be converted using the aggregateExprs function, that can use a current annotation environment to convert and condense the gene expression data.

By default the method set out by Kim and Volsky http://www.biomedcentral.com/1471-2105/6/144 is applied to the gene set. If weighted==FALSE than the default t.test function is used.

The function is set up to perform the analysis on individual samples. For convenient method to analyze groups of samples, see the "Limma User's Guide" for more information on how to see up a contrast matrix and perform a linear model fit. The coefficients of the fit can then be used a input into the PGSEA function.

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This package has not been extensively tested beyond a set of well defined curated pathways using the Affymetrix platform and significance values represent approximations. Any results should be confirmed by additional gene set testing methodologies.

Value

If p.value is set to a number, a matrix of results that pass at that significance is returned, of size <number of samples> x <number of molecular concepts>.

If p.value is set to NA, all results are returned.

If p.value is set to TRUE, then a list is returned that consists of the PGSEA results as well as their p.values.

Note

```
http://www.biomedcentral.com/1471-2105/6/144
```

Author(s)

Kim SY, Volsky DJ., kyle.furge@vai.org and karl.dykema@vai.org

References

PGSEA: Parametric Analysis of Gene Set Enrichment

Examples

```
datadir <- system.file("extdata", package = "PGSEA")
sample <- readGmt(file.path(datadir, "sample.gmt"))
data(nbEset)
pg <- PGSEA(nbEset, cl=sample, ref=1:5)
print(pg[,-c(1:5)])</pre>
```

VAIgsc

Molecular Concepts (Gene Sets) prepared at VAI

Description

A few gene sets compiled at VAI. We have found useful in our analysis.

Usage

```
data(VAIgsc)
```

Format

The format is: chr "VAIgsc"

Source

Various sources... See individual objects for PMID, GEO accession, etc...

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Examples

```
data(VAIgsc)
summary(VAIgsc)
details(VAIgsc[[1]])
```

VAImcs

Molecular Concepts prepared at VAI

Description

A few gene sets compiled at VAI. We have found useful in our analysis.

Usage

```
data(VAImcs)
```

Format

```
a list of "smc" objects
```

Source

See individual concepts for PMID or other source information.

Examples

```
data(VAImcs)
str(VAImcs)
```

aggregateExprs

Aggregate expression data

Description

This function removes duplicates row names from an expression set, summarizing them with a function of the users choice. The "absMax" function located in package "reb" we have found to be useful.

Usage

```
aggregateExprs(x, package = "hgu133plus2", using = "ENTREZID", FUN, ...)
```

Arguments

. . .

```
expression data - matrix, eSet, or ExpressionSet
Х
                  annotation package of expression data
package
using
                  format type that gene IDs are converted to
                  function by which to summarize duplicated values
FUN
                  extra parameters passed on to FUN
```

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Value

A matrix of expression data with the rows aggregated to a unique format chosen by the user. The new identifiers of the returned matrix are those specified with the "using" argument. To see possible values, use the ls() command illustrated below in the examples.

Author(s)

Kyle Furge <kyle.furge@vai.org> and Karl Dykema <karl.dykema@vai.org>

Examples

```
if (require(hgu95av2.db) & require(annaffy)) {
library(annaffy)
data(aafExpr)
class(exprs(aafExpr))
exprs(aafExpr)[1:4, 1:4]

#list possible values for the "using" argument
ls(pos=which(search()=="package:hgu95av2.db"))

convert <- aggregateExprs(exprs(aafExpr), "hgu95av2.db", FUN=mean, na.rm=TRUE)
convert[1:4,1:4]
}</pre>
```

convertSmc

Convert Entrez ID based "smc" object

Description

This function will convert the Entrez IDs of an smc object to the corresponding Entrez IDs from a different species. Data from the homologene project is downloaded and used within this function.

Usage

```
convertSmc(mcs, fromSpecies = "h", toSpecies = "r", hgX="./homologene.data")
```

Arguments

```
mcs a list of "smc" objects

fromSpecies character - a single letter describing the species to convert from ie, h=human, r= rat, etc..

toSpecies character - a single letter describing the species to convert to ie, h=human, r= rat, etc..

hgX character - file name of homologene data file
```

Details

This function will not work if you have not downloaded the homologene data file. Please use this command to do so: download.file("ftp://ftp.ncbi.nih.gov/pub/HomoloGene/current/homologene.data",destfile="homolog

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Value

```
a list of converted "smc" objects
```

Author(s)

Karl Dykema karl.dykema@vai.org

Examples

```
## Not run:
download.file("ftp://ftp.ncbi.nih.gov/pub/HomoloGene/current/homologene.data",destfile="f
datadir <- system.file("extdata", package = "PGSEA")
sample <- readGmt(file.path(datadir, "sample.gmt"))
converted <- convertSmc(sample[1:2],"h","r")
str(converted)</pre>
```

editSmc

End(Not run)

Edit "smc" objects

Description

This function will edit a single or list of "smc" objects.

Usage

```
editSmc(smcList, attName = "creator", newAtt = "changed!!")
```

Arguments

```
smcList a list of "smc" objects
```

attName character - which slot to change

newAtt character - what to change the slot to

Value

```
a list of edited "smc" objects
```

Author(s)

Karl Dykema < karl.dykema@vai.org

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Examples

```
datadir <- system.file("extdata", package = "PGSEA")
sample <- readGmt(file.path(datadir, "sample.gmt"))
str(sample[1:2])

temp <- editSmc(sample[1:2], "creator", "Joe Smith")
str(temp)</pre>
```

go2smc

Gene Ontology 2 "smc"

Description

This function creates "smc" objects from the "GO" Bioconductor library.

Usage

```
go2smc(min = 50, max = 200, organism="human")
```

Arguments

```
min numeric - minimum length of ids to be included
max numeric - maximum length of ids to be included
organism character - organism
```

Value

```
a list of "smc" objects
```

Author(s)

Karl Dykema < karl.dykema@vai.org>

```
if(require(GO)){
mcs <- go2smc()[1:2]
str(mcs)
}</pre>
```

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kegg2smc

KEGG pathway to "smc"

Description

This function creates "smc" objects from the "KEGG" Bioconductor library.

Usage

```
kegg2smc(min = 1, max = 284,organism="human")
```

Arguments

```
min numeric - minimum length of ids to be included
max numeric - maximum length of ids to be included
organism character - organism
```

Value

```
a list of "smc" objects
```

Author(s)

Karl Dykema < karl.dykema@vai.org> and Richard Birnie < richard.birnie@pro-curetherapeutics.com>

Examples

```
if(require(KEGG)){
mcs <- kegg2smc(min=20,max=284)
length(mcs)
str(mcs[[1]])
}</pre>
```

nbEset

Reduced Neuroblastoma data set

Description

Neuroblastoma Data set - reduced in size to comply with BioC package guidelines

Usage

```
data(nbEset)
```

Details

This dataset was retrieved from GEO http://www.ncbi.nlm.nih.gov/geo/query/acc.cgi?acc=GSE3960 and consists of five reference samples, and ten primary neuroblastoma tumors. Four of the five reference samples GSM2827, GSM2842, GSM2883, and GSM2895 came from a separate dataset, http://www.ncbi.nlm.nih.gov/geo/gds/gds_browse.cgi?gds=181

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Source

```
http://www.ncbi.nlm.nih.gov/geo/query/acc.cgi?acc=GSE3960
```

Examples

```
data(nbEset)
nbEset
```

readGmt

readGmt

Description

This function will read a "gmt" file into R, returning results as a list of SMC objects.

Usage

```
readGmt (fname)
```

Arguments

fname

File name of concepts in .gmt format

Details

The .gmt file format is a tab delimited file format used to store gene lists. These gene lists are stored row by row. The first column is the gene set name. The second column is a brief description, and every entry after that is a gene within that gene set.

Value

A list of SMC objects

Author(s)

Karl Dykema < karl.dykema@vai.org>

References

```
http://www.broad.mit.edu/gsea/doc/data_formats.html#gmt
```

See Also

```
writeGmt
```

```
datadir <- system.file("extdata", package = "PGSEA")
sample <- readGmt(file.path(datadir, "sample.gmt"))
str(sample)</pre>
```

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readSmc

Read SMC files

Description

This function reads in SMCs (simple molecular concepts) from individual text files.

Usage

```
readSmc(files)
```

Arguments

files

a character vector of file names

Value

A list of SMC objects

Author(s)

Kyle Furge <kyle.furge@vai.org> and Karl Dykema <karl.dykema@vai.org>

References

??

See Also

```
writeSmc
```

```
datadir <- system.file("extdata", package = "PGSEA")
sample <- readGmt(file.path(datadir, "sample.gmt"))
str(sample)
sample[[1]]@reference <- "fileName"

## Not run:
writeSmc(sample[[1]])
smc <- readSmc("fileName-0.txt")

## End(Not run)</pre>
```

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scanSmc

Scan through smc objects

Description

This function scans through smc objects and returns those with specified attributes.

Usage

```
scanSmc(smcList, scanSlot = "private", scanFor = "no")
```

Arguments

```
smcList list of "smc" objects
scanSlot character - which smc slot to investigate
scanFor character - what character string to look for
```

Value

a list of "smc" objects with the desired attribute

Author(s)

Karl Dykema < karl.dykema@vai.org>

Examples

```
datadir <- system.file("extdata", package = "PGSEA")
sample <- readGmt(file.path(datadir, "sample.gmt"))
sample[1:2] <- editSmc(sample[1:2], "creator", "Joe Smith")
scanned <- scanSmc(sample, "creator", "Joe Smith")
str(scanned)</pre>
```

smcPlot

Plot PGSEA results

Description

This basic function will plot results from PGSEA with easy altering of margins, colors, and text.

Usage

```
smcPlot(m, ff = NULL, skip = "NO", scale = c(-3, 3), na.color = par("bg"), marginal smcPlot(m, ff = NULL) skip = "NO", scale = c(-3, 3), na.color = par("bg"), marginal smcPlot(m, ff = NULL) skip = "NO", scale = c(-3, 3), na.color = par("bg"), marginal smcPlot(m, ff = NULL) skip = "NO", scale = c(-3, 3), na.color = par("bg"), marginal smcPlot(m, ff = NULL) skip = "NO", scale = c(-3, 3), na.color = par("bg"), marginal smcPlot(m, ff = NULL) skip = "NO", scale = c(-3, 3), na.color = par("bg"), marginal smcPlot(m, ff = NULL) skip = "NO", scale = c(-3, 3), na.color = par("bg"), marginal smcPlot(m, ff = NULL) skip = "NO", scale = c(-3, 3), na.color = par("bg"), marginal smcPlot(m, ff = NULL) skip = "NO", scale = c(-3, 3), na.color = par("bg"), marginal smcPlot(m, ff = NULL) skip = "NO", scale = c(-3, 3), na.color = par("bg"), marginal smcPlot(m, ff = NULL) skip = "NO", scale = c(-3, 3), na.color = par("bg"), marginal smcPlot(m, ff = NULL) skip = "NO", scale = c(-3, 3), marginal smcPlot(m, ff = NULL) skip = "NO", scale = c(-3, 3), marginal smcPlot(m, ff = NULL) skip = "NO", scale = c(-3, 3), marginal smcPlot(m, ff = NULL) skip = "NO", scale = c(-3, 3), marginal smcPlot(m, ff = NULL) skip = "NO", scale = c(-3, 3), marginal smcPlot(m, ff = NULL) skip = "NO", scale = c(-3, 3), marginal smcPlot(m, ff = NULL) skip = "NO", scale = c(-3, 3), marginal smcPlot(m, ff = NULL) skip = "NO", scale = c(-3, 3), marginal smcPlot(m, ff = NULL) skip = "NO", scale = c(-3, 3), marginal smcPlot(m, ff = NULL) skip = "NO", scale = c(-3, 3), marginal smcPlot(m, ff = NULL) skip = "NO", scale = c(-3, 3), marginal smcPlot(m, ff = NULL) skip = "NO", scale = c(-3, 3), marginal smcPlot(m, ff = NULL) skip = "NO", scale = c(-3, 3), marginal smcPlot(m, ff = NULL) skip = "NO", scale = c(-3, 3), marginal smcPlot(m, ff = NULL) skip = "NO", scale = c(-3, 3), marginal smcPlot(m, ff = NULL) skip = "NO", scale = c(-3, 3), marginal smcPlot(m, ff = NULL) skip = "NO", scale = c(-3, 3), marginal smcPlot(m, ff = NULL) skip = "NO", scale = c(-3, 3), marginal smcP
```

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Arguments

m	matrix - your results from PGSEA (or any other numeric matrix of data)
ff	factor - this factor corresponds to the subtypes of your samples and will control the column names
skip	character - which subtype(s) to skip from "ff"
scale	vector, length 2 - this vector sets the minimum and maximum values for the graph scale (at bottom of plot)
na.color	character - color to display in the result of an NA
margins	vector, length 4 - this vector gives the expansion values for the margins
r.cex	numeric - number giving the amount by which row names should be scaled relative to the default
c.cex	numeric - number giving the amount by which column names should be scaled relative to the default
show.grid	boolean - show grid outlines within plot?
cnames	boolean or character - vector of alternative column names
rnames	boolean or character - vector of alternative row names
grid.lty	numeric - line type of the grid lines
clust	boolean - want to cluster?
	additional graphical parameters passed along to the plotting function

Author(s)

Karl Dykema < karl.dykema@vai.org>

Examples

```
library(PGSEA)
datadir <- system.file("extdata", package = "PGSEA")
sample <- readGmt(file.path(datadir, "sample.gmt"))
data(nbEset)

pg <- PGSEA(nbEset, cl=sample, ref=1:5)
sub <- factor(c(rep(NA,5), rep("NeuroB",5), rep("NeuroB_MYC+",5))))
smcPlot(pg, sub, scale=c(-10,10), col=.rwb, margins=c(1,1,8,13))</pre>
```

writeGmt

writeGmt

Description

This function writes out SMC objects into .gmt file format

Usage

```
writeGmt(fname, cl)
```

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Arguments

fname name of the file to be written out cl list of SMC objects

Details

The .gmt file format is a tab delimited file format used to store gene lists. These gene lists are stored row by row. The first column is the gene set name. The second column is a brief description, and every entry after that is a gene within that gene set.

Author(s)

Kyle Furge <kyle.furge@vai.org> and Karl Dykema <karl.dykema@vai.org>

References

```
http://www.broad.mit.edu/gsea/doc/data_formats.html#gmt
```

See Also

readGmt

Examples

```
datadir <- system.file("extdata", package = "PGSEA")
sample <- readGmt(file.path(datadir, "sample.gmt"))
str(sample)

## Not run:
writeGmt(paste(datadir, "/output.gmt", sep=""), sample)
## End(Not run)</pre>
```

writeSmc

writeSmc

Description

This function will write out SMC objects to individual text files

Usage

```
writeSmc(x)
```

Arguments

Х

an object of class SMC

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Details

The file name is determined by the reference slot of the SMC object.

Author(s)

Kyle Furge <kyle.furge@vai.org> and Karl Dykema <karl.dykema@vai.org>

See Also

```
writeSmc
```

```
datadir <- system.file("extdata", package = "PGSEA")
sample <- readGmt(file.path(datadir, "sample.gmt"))
str(sample)
sample[[1]]@reference <- "fileName"

## Not run:
writeSmc(sample[[1]])

## End(Not run)</pre>
```

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