Package ‘dagLogo’
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Description Visualize significant conserved amino acid sequence pattern in groups based on probability theory.
License GPL (>=2)
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Description

We implement iceLogo by R to visualize significant conserved amino acid sequence pattern based on probability theory. Compare to iceLogo, dagLogo can also visualize significant sequence patterns by clustering the peptides by groups such as charge, chemistry, hydrophobicity and etc.

Details

Package: dagLogo
Type: Package
Version: 1.0
Date: 2013-09-31
License: GPL (>= 2)

DAG: Differential Amino acid Group

There are several differences between dagLogo from iceLogo:

1. The sequence patterns can be grouped by charge, chemistry, hydrophobicity and etc.
2. dagLogo accepts different length of aligned amino acid sequences.
3. Except Random, regional (called restricted in dagLogo) and terminal (called anchored) background model, the background sequence could be set to other regions of the genes in inputs and complementary set of the proteome.

Author(s)

Jianhong Ou, Julie Lihua Zhu
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Examples

data("seq.example")
data("proteome.example")
bg <- buildBackgroundModel(seq.example, proteome=proteome.example, permutationSize=10L)
t <- testDAU(seq.example, bg)
dagLogo(t)
Usage

buildBackgroundModel(dagPeptides, 
  bg=c("wholeGenome", "inputSet", "nonInputSet"), 
  model=c("any", "anchored"), 
  targetPosition=c("any", "Nterminus", "Cterminus"), 
  uniqueSeq=TRUE, 
  permutationSize=30L, 
  rand.seed=1, 
  replacement=FALSE, 
  proteome)

Arguments

dagPeptides  an object of dagPeptides, output of fetchSequence or formatSequence
bg           could be "wholeGenome", "inputSet" or "nonInputSet"
model        could be "any" or "anchored"
targetPosition could be "any", "Nterminus" or "Cterminus"
uniqueSeq    should the background sequence be unique?
permutationSize how many times should it samples
rand.seed     random seed
replacement   Should sampling be with replacement?
proteome      an object of Proteome, output of prepareProteome

Details

The background could be generated from wholeGenome, inputSet or nonInputSet. whole genome: randomly select subsequences from the whole genome with each subsequence containing amino acids with same width of input sequences. anchored whole genome: randomly select subsequences from the whole genome with each subsequence containing amino acids with same width of input sequences where the middle amino acids must contain anchor amino acid, e.g., K, which is specified by user. input set: same to whole genome, but only use protein sequence from input id and not including the site specified in input sequences anchored input set: same to anchored whole genome, but only use protein sequences from input id, and not including the site specified in input sequences. non-input set: whole genome - input set. anchored non-input set: whole genome - input set and the middle amino acids must contain anchor amino acid.

Value

an object of dagBackground which contains background and permutationSize.

Author(s)

Jianhong Ou, Alexey Stukalov, Julie Zhu

See Also

prepareProteome
Examples

data("seq.example")
data("proteome.example")
bg <- buildBackgroundModel(seq.example, proteome=proteome.example)

---

colorsets
retrieve color setting for logo

Description
retrieve prepared color setting for logo

Usage

colorsets(colorScheme=c("null", "classic", "charge", "chemistry", "hydrophobicity"))

Arguments

colorScheme could be 'null', 'charge', 'chemistry', 'classic' or 'hydrophobicity'

Value
A character vector of color scheme

Author(s)
Jianhong Ou

Examples

col <- colorsets("hydrophobicity")

---

dagBackground-class
Class "dagBackground"

Description
An object of class "dagBackground" represents background model.

Objects from the Class
Objects can be created by calls of the form new("dagBackground", background, permutationSize).

Slots
background Object of class "list" records the background model
permutationSize code"integer" permutation size of background
**dagHeatmap**

plot heatmap for test results

**Description**
plot heatmap for test results

**Usage**
dagHeatmap(testDAUresults, type=c("diff", "zscore"), ...)

**Arguments**
- `testDAUresults`: output of `testDAU`, should be an object of `testDAUresults`
- `type`: "diff" or "zscore"
- `...`: parameter could be passed to `pheatmap`

**Value**
one

**Author(s)**
Jianhong Ou

**Examples**
data("seq.example")
data("proteome.example")
bg <- buildBackgroundModel(seq.example, proteome=proteome.example, permutationSize=10)
t <- testDAU(seq.example, bg)
dagHeatmap(t)

---

**dagLogo**
plot sequence logo for test results

**Description**
plot sequence logo for test results

**Usage**
dagLogo(testDAUresults, type=c("diff", "zscore"), pvalueCutoff=0.05, namehash=NULL, font="Helvetica-Bold", textgp=gpar(), legend=FALSE, labelRelativeToAnchor=FALSE, labels=NULL)
Arguments

- `testDAUresults` output of `testDAU`, should be an object of `testDAUresults` type
- `type` "diff" or "zscore"
- `pvalueCutoff` pvalue cutoff for logo plot
- `namehash` the hash table to convert rownames of test results to a single letter to be plotted in the logo
- `font` font for logo symbol
- `textgp` text parameter
- `legend` plot legend or not, default false.
- `labelRelativeToAnchor` plot label relative to anchor or not, default false.
- `labels` the labels in each position.

Value

none

Author(s)

Jianhong Ou

See Also

- `nameHash`

Examples

```r
data("seq.example")
data("proteome.example")
bg <- buildBackgroundModel(seq.example, proteome=proteome.example, permutationSize=10)
t <- testDAU(seq.example, bg)
dagLogo(t)
```

Description

An object of class "dagPeptides" represents the information of peptides.

Objects from the Class

Objects can be created by calls of the form `new("dagPeptides", data, peptides, upstreamOffset, downstreamOffset)`.
Slots

data Object of class "data.frame" The details of the input sequences. It includes the columns: IDs, anchorAA (anchor Amino Acid), anchorPos (anchor Position), peptide (protein peptide), anchor, upstream, downstream (peptides in given upstream and downstream offset from anchor)

peptides code"matrix" The input peptides. Each column contains one peptide in that position

upstreamOffset "numeric" The upstream offset from anchor
downstreamOffset "numeric" The downstream offset from anchor
type "character" ID type of inputs

Description

the subset proteome of Escherichia coli

Usage

data(ecoli.proteome)

Format

An object of Proteome for Escherichia coli proteome. The format is: A list with one data frame and an character.

proteome 'data.frame': obs. of 4 variables
type 'character': "UniProt"

The format of proteome is

ENTREZ_GENE a character vector, records entrez gene id
SEQUENCE a character vector, peptide sequences
ID a character vector, Uniprot ID
LEN a character vector, length of peptides

Details

used in the examples Annotation data obtained by: library(UniProt.ws) taxId(UniProt.ws) <- 562 proteome <- prepareProteome(UniProt.ws, species="Escherichia coli")

Examples

data(ecoli.proteome)
head(ecoli.proteome@proteome)
ecoli.proteome@type
fetchSequence

fetch sequence by id

Description

fetch amino acid sequence by given identifiers via biomaRt or proteome prepared by `prepareProteome`

Usage

fetchSequence(IDs, type="entrezgene", anchorAA=NULL, anchorPos, mart, proteome, upstreamOffset, downstreamOffset)

Arguments

- **IDs**: A vector of Identifiers to retrieve peptides
- **type**: type of identifiers
- **anchorAA**: a vector of character, anchor Amino Acid
- **anchorPos**: a vector of character or numeric, anchor position, for example, K121. Or a vector of character with amino acid sequences. If AA sequences is used, the anchorAA must be the a vector of character with single AA for each.
- **mart**: an object of Mart
- **proteome**: an object of Proteome, output of `prepareProteome`
- **upstreamOffset**: an integer, upstream offset position
- **downstreamOffset**: an integer, downstream offset position

Value

return an object of `dagPeptides`

Author(s)

Jianhong Ou, Alexey Stukalov, Julie Zhu

See Also

`formatSequence`

Examples

if(interactive()){
  mart <- useMart("ensembl", "dmelanogaster_gene_ensembl")
  dat <- read.csv(system.file("extdata", "dagLogoTestData.csv", package="dagLogo"))
  seq <- fetchSequence(as.character(dat$entrez_geneid[1:5]),
                      anchorPos=as.character(dat$NCBI_site[1:5]),
                      mart=mart,
                      upstreamOffset=7,
                      downstreamOffset=7)
  ## sample: use sequence as anchorPos
  sequences <- seq@peptides
  sequences[, 8] <- "k"
formatSequence

sequences <- apply(sequences, 1, paste, collapse="")
seq <- fetchSequence(as.character(seq@data$IDs),
                     anchorAA="k",
                     anchorPos=sequences,
                     mart=mart,
                     upstreamOffset=7,
                     downstreamOffset=7)
## sample: use sequence as anchorPos 2
sequences <- cbind(seq@peptides[, 1:8], "+", seq@peptides[, 9:15])
seq <- fetchSequence(as.character(seq@data$IDs),
                     anchorAA="+",
                     anchorPos=sequences,
                     mart=mart,
                     upstreamOffset=7,
                     downstreamOffset=7)

formatSequence

prepare an object of dagPeptides from sequences

Description

prepare an object of dagPeptides from sequences

Usage

formatSequence(seq, proteome, upstreamOffset, downstreamOffset)

Arguments

seq a vector of character, amino acid sequences
proteome an object of Proteome, output of prepareProteome
upstreamOffset an integer, upstream offset position
downstreamOffset an integer, downstream offset position

Value

return an object of dagPeptides, which is a list contains: data, peptides, upstreamOffset, downstreamOffset and type information

Author(s)

Jianhong Ou, Julie Zhu

See Also

fetchSequence
Examples

```r
if(interactive()){
  dat <- unlist(read.delim(system.file("extdata", "grB.txt", package="dagLogo"),
               header=F, as.is=TRUE))
  proteome <- prepareProteome(fasta=system.file("extdata", "HUMAN.fasta",
                                    package="dagLogo"))
  seq <- formatSequence(dat, proteome)
}
```

nameHash

convert group name to a single character

Description

convert group name to a single character to shown in a logo

Usage

```r
nameHash(nameScheme=c("classic", "charge", "chemistry", "hydrophobicity"))
```

Arguments

nameScheme could be "classic", "charge", "chemistry", "hydrophobicity"

Value

A character vector of name scheme

Author(s)

Jianhong Ou

Examples

```r
nameHash("charge")
```

prepareProteome

prepare proteome for background building

Description

prepare proteome from UniProt webserver or a fasta file

Usage

```r
prepareProteome(UniProt.ws, fasta, species="unknown")
```
**Proteome-class**

**Arguments**

- **UniProt.ws**  
  an object of UniProt.ws
- **fasta**  
  fasta file name or an object of AAStringSet
- **species**  
  an character to assign the species of the proteome

**Value**

an object of Proteome which contain protein sequence information

**Author(s)**

Jianhong Ou

**See Also**

`formatSequence, buildBackgroundModel`

**Examples**

```r
if(interactive()){
  library(UniProt.ws)
  UniProt.ws <- UniProt.ws(taxId=7227)
  proteome <- prepareProteome(UniProt.ws, species="Drosophila melanogaster")
}
```

**Proteome-class**  

*Class* "Proteome"

**Description**

An object of class "Proteome" represents proteome of a given species.

**Objects from the Class**

Objects can be created by calls of the form `new("Proteome", proteome, type, species)`.

**Slots**

- **proteome**  
  Object of class "data.frame" the proteome of a given species, should include ids and peptide sequences.
- **type**  
  code"character" indicates how the object is prepared, could be "fasta" or "UniProt"
- **species**  
  "character" the species
proteome.example  

the subset proteome of fruit fly

Description

the subset proteome of fruit fly

Usage

data(proteome.example)

Format

An object of Proteome for fly subset proteome. The format is: A list with one data frame and an character.

proteome 'data.frame': 1406 obs. of 4 variables
type 'character': "UniProt"

The format of proteome is

ENTREZ_GENE a character vector, records entrez gene id
SEQUENCE a character vector, peptide sequences
ID a character vector, Uniprot ID
LEN a character vector, length of peptides

Details

used in the examples Annotation data obtained by: library(UniProt.ws) taxId(UniProt.ws) <- 7227 proteome <- prepareProteome(UniProt.ws) proteome@proteome <- proteome@proteome[sample(1:19902, 1406), ]

Examples

data(proteome.example)
head(proteome.example@proteome)
proteome.example@type

seq.example  

example object of dagPeptides

Description

example object of dagPeptides

Usage

data(seq.example)
testDAU

Format
An object of dagPeptides. The format is: A list.

data 'data.frame': 732 obs. of 7 variables
peptides 'matrix': amino acid in each position
upstreamOffset an integer, upstream offset position
downstreamOffset an integer, downstream offset position
type "character", type of identifiers

The format of data is
IDs a character vector, input identifiers
anchorAA a character vector, anchor amino acid provided in inputs
anchorPos a numeric vector, anchor position in the protein
peptide a character vector, peptide sequences
anchor a character vector, anchor amino acid in the protein
upstream a character vector, upstream peptides
downstream a character vector, downstream peptides

Details
used in the examples seq obtained by: mart <- useMart("ensembl", "dmelanogaster_gene_ensembl")
dat <- read.csv(system.file("extdata", "dagLogoTestData.csv", package="dagLogo")) seq <- fetchSequence(as.character(dat$entrez_geneid), anchorPos=as.character(dat$NCBI_site), mart=mart, upstreamOffset=7, downstreamOffset=7)

Examples
data(seq.example)
head(seq.example@peptides)
seq.example@upstreamOffset
seq.example@downstreamOffset

testDAU

DAU test

Description
Performs DAU test

Usage
testDAU(dagPeptides, dagBackground,
group=c("null", "classic", "charge", "chemistry", "hydrophobicity"),
bgNoise=NA)
Arguments

- **dagPeptides**: an object of `dagPeptides`, output of `fetchSequence` or `formatSequence`
- **dagBackground**: an object of `dagBackground`, output of `buildBackgroundModel`
- **group**: could be "null", "classic", "charge", "chemistry", "hydrophobicity"
- **bgNoise**: if it is not NA, test will use a background by Dirichlet(1)-distributed random frequencies with weight bg.noise. The value of bgNoise should be a number in the range of 0 to 1, eg. 0.05

Value

- an object of `testDAUresults` ready for plotting

Author(s)

Jianhong Ou, Alexey Stukalov, Julie Zhu

Examples

```r
data("seq.example")
data("proteome.example")
bg <- buildBackgroundModel(seq.example, proteome=proteome.example)
t <- testDAU(seq.example, bg, bgNoise=0.05)
```

Description

An object of class "testDAUresults" represents background model.

Objects from the Class

Objects can be created by calls of the form `new("dagBackground", group="character", difference="matrix", zscore="matrix", pvalue="matrix", background="matrix", motif="matrix", upstream="numeric", downstream="numeric")`

Slots

- **group**: Object of class "character" could be "null", "classic", "charge", "chemistry", "hydrophobicity"
- **difference**: code"matrix" the difference of inputs from background for each amino acid in each position
- **zscore**: code"matrix" z score for each amino acid in each position
- **pvalue**: code"matrix" pvalue for each amino acid in each position
- **background**: code"matrix" background frequencies for each amino acid in each position
- **motif**: code"matrix" inputs frequencies for each amino acid in each position
- **upstream**: "numeric" The upstream offset from anchor
- **downstream**: "numeric" The downstream offset from anchor
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