Package 'DEqMS'

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Title a tool to perform statistical analysis of differential protein expression for quantitative proteomics data.

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Depends R(>= 3.5),graphics,stats,ggplot2,matrixStats,dplyr,limma(>= 3.34)

Suggests BiocStyle,knitr,rmarkdown,markdown,plyr,reshape2,utils,ggrepel,ExperimentHub,LSD

LazyLoad yes

Description DEqMS is developped on top of Limma. However, Limma assumes same prior variance for all genes. In proteomics, the accuracy of protein abundance estimates varies by the number of peptides/PSMs quantified in both label-free and labelled data. Proteins quantification by multiple peptides or PSMs are more accurate. DEqMS package is able to estimate different prior variances for proteins quantified by different number of PSMs/peptides, therefore achieving better accuracy. The package can be applied to analyze both label-free and labelled proteomics data.

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biocViews ImmunoOncology, Proteomics, MassSpectrometry, Preprocessing, DifferentialExpression, MultipleComparison,Normalization,Bayesian,ExperimentHubSoftware

VignetteBuilder knitr

BugReports https://github.com/yafeng/DEqMS/issues

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`equalMedianNormalization`
normalize to have equal medians in all samples

Description

This function is to normaliza out the differences of protein medians in different samples

Usage

```
equalMedianNormalization(dat)
```

Arguments

`dat`	an numeric data frame or matrix containing protein relative abundance in log2 scale

Value

a data frame or matrix with normalized protein relative abundance

Author(s)

Yafeng Zhu

Examples

```
library(ExperimentHub)
eh = ExperimentHub(localHub=TRUE)
query(eh, "DEqMS")
dat.psm = eh[["EH1663"]]

dat.psm.log = dat.psm
dat.psm.log[,3:12] =  log2(dat.psm[,3:12])
```

```
# use the 3 ctrl samples as reference channels to calculate log2 ratio
dat.gene = medianSummary(dat.psm.log,group_col = 2,ref_col =c(3,7,10))
dat.gene.nm = equalMedianNormalization(dat.gene)
```

`medianSummary` *summarize peptide/PSM intensity into protein level relative abundance estimate by taking the median*

Description

This function is to calculate proteins'relative abundance by median method

Usage

```
medianSummary(dat,group_col=2,ref_col)
```

Arguments

`dat`	an data frame with peptide/psm intensities in log2 scale
`group_col`	the column by which peptides/psm intensity are grouped. Usually the gene/protein id column. Default is 2
`ref_col`	an integer vector indicating the column(s) used as denominator to calcualte relative petide ratio.

Value

a data frame containing protein relative abundance estimate in log2 scale

Author(s)

Yafeng Zhu

Examples

```
library(ExperimentHub)
eh = ExperimentHub(localHub=TRUE)
query(eh, "DEqMS")
dat.psm = eh[["EH1663"]]

dat.psm.log = dat.psm
dat.psm.log[,3:12] =  log2(dat.psm[,3:12])
# use the 3 ctrl samples as reference channels to calculate log2 ratio
dat.gene = medianSummary(dat.psm.log,group_col = 2,ref_col =c(3,7,10))
```

`medianSweeping` *summarize peptide/PSM intensity into protein level relative abundance estimate by median sweeping method*

Description

This function is to calculate proteins'relative abundance by median sweeping method

Usage

```
medianSweeping(dat,group_col=2)
```

Arguments

`dat`	an data frame with peptide/PSM intensities in log2 scale
`group_col`	the column by which peptides/PSM intensity are grouped. Usually the gene/protein id column. Default is 2

Value

a data frame with protein relative abundance estimate in log2 scale

Author(s)

Yafeng Zhu

Examples

```
library(ExperimentHub)
eh = ExperimentHub(localHub=TRUE)
query(eh, "DEqMS")
dat.psm = eh[["EH1663"]]

dat.psm.log = dat.psm
dat.psm.log[,3:12] =  log2(dat.psm[,3:12])

dat.gene.nm = medianSweeping(dat.psm.log,group_col = 2)
```

`medpolishSummary` *summarize peptide/PSM intensity into protein level relative abundance estimate by Turkey median polish procedure*

Description

This function is to calculate proteins'relative abundance by Turkey median polish

Usage

```
medpolishSummary(dat,group_col=2)
```

Arguments

`dat`	an data frame containing peptide/psm intensities in log2 scale
`group_col`	the column by which peptides/psm intensity are grouped. Usually the gene/protein column. Default is 2

Value

a data frame containing protein relative abundance estimate in log2 scale

Author(s)

Yafeng Zhu

Examples

```
library(ExperimentHub)
eh = ExperimentHub(localHub=TRUE)
query(eh, "DEqMS")
dat.psm = eh[["EH1663"]]

dat.psm.log = dat.psm
dat.psm.log[,3:12] =  log2(dat.psm[,3:12])

dat.gene = medpolishSummary(dat.psm.log,group_col=2)
```

outputResult *output the DEqMS analysis results in a data frame*

Description

This function is to generate DEqMS outputs in a data frame.

Usage

```
outputResult(fit, coef_col=1)
```

Arguments

fit	an list object produced by spectraCounteBayes function
coef_col	is an integer indicating the column of fit$coefficients for which corresponding t-statistics and p-values are extracted in the output

Value

a data frame object with the last three columns being: sca.t - Peptide or Spectra Count Adjusted posterior t-value sca.P.Value - Adjusted posterior p-value sca.adj - sca.P.Value adjusted by BH method

Author(s)

Yafeng Zhu

Examples

```
library(ExperimentHub)
eh = ExperimentHub(localHub=TRUE)
query(eh, "DEqMS")
dat.psm = eh[["EH1663"]]

dat.psm.log = dat.psm
dat.psm.log[,3:12] =  log2(dat.psm[,3:12])

dat.gene.nm = medianSweeping(dat.psm.log,group_col = 2)

psm.count.table = as.data.frame(table(dat.psm$gene)) # generate PSM count table
rownames(psm.count.table)=psm.count.table$Var1

cond = c("ctrl","miR191","miR372","miR519","ctrl",
"miR372","miR519","ctrl","miR191","miR372")

sampleTable <- data.frame(
row.names = colnames(dat.psm)[3:12],
cond = as.factor(cond)
)
```

```
gene.matrix = as.matrix(dat.gene.nm)
design = model.matrix(~cond,sampleTable)

fit1 <- eBayes(lmFit(gene.matrix,design))
# add PSM count for each gene
fit1$count <- psm.count.table[rownames(fit1$coefficients),2]

fit2 = spectraCounteBayes(fit1)

DEqMS.results = outputResult(fit2, coef_col=3)
```

---

peptideProfilePlot *plot log2 intensities of all peptides for one gene in different samples*

Description

This function is to plot log2 intensities of all peptides for one gene in different samples.

Usage

```
peptideProfilePlot(dat, col=2, gene)
```

Arguments

dat	a data frame with peptide/psm log2 intensities
col	an integer indicates the column number where the gene protein id is. default is 2, asumming the gene/protein is in the second column
gene	an character indicates the gene name/id to be plotted

Value

return a ggplot2 object

Author(s)

Yafeng Zhu

Examples

```
library(ExperimentHub)
eh = ExperimentHub(localHub=TRUE)
query(eh, "DEqMS")
dat.psm = eh[["EH1663"]]

dat.psm.log = dat.psm
dat.psm.log[,3:12] =  log2(dat.psm[,3:12])

peptideProfilePlot(dat.psm.log,col=2,gene="TGFBR2")
```

Residualplot *plot the residuals against the number of quantified peptides/PSMs.*

Description

This function is to plot the residuals of fit model on the vertical axis and the peptide or PSM count on the horizontal axis.

Usage

```
Residualplot(fit, xlab="log2(count)",
ylab="Variance(fitted - observed)", main="")
```

Arguments

fit	an object returned from spectraCounteBayes function
xlab	the title for x axis
ylab	the title for y axis
main	the title for the figure

Value

return a plot graphic

Author(s)

Yafeng Zhu

Examples

```
library(ExperimentHub)
eh = ExperimentHub(localHub=TRUE)
query(eh, "DEqMS")
dat.psm = eh[["EH1663"]]

dat.psm.log = dat.psm
dat.psm.log[,3:12] =  log2(dat.psm[,3:12])

dat.gene.nm = medianSweeping(dat.psm.log,group_col = 2)

psm.count.table = as.data.frame(table(dat.psm$gene)) # generate PSM count table
rownames(psm.count.table)=psm.count.table$Var1

cond = c("ctrl","miR191","miR372","miR519","ctrl",
"miR372","miR519","ctrl","miR191","miR372")

sampleTable <- data.frame(
row.names = colnames(dat.psm)[3:12],
```

```
cond = as.factor(cond)
)

gene.matrix = as.matrix(dat.gene.nm)
design = model.matrix(~cond,sampleTable)

fit1 <- eBayes(lmFit(gene.matrix,design))
# add PSM count for each gene
fit1$count <- psm.count.table[rownames(fit1$coefficients),2]

fit2 = spectraCounteBayes(fit1)

Residualplot(fit2,xlab="log2(PSM count)",main="TMT data PXD004163")
```

`spectraCounteBayes` *Peptide/Spectra Count Based Empirical Bayes Statistics for Differential Expression*

Description

This function is to calculate peptide/PSM count adjusted t-statistics, p-values.

Usage

```
spectraCounteBayes(fit, fit.method="loess", coef_col)
```

Arguments

`fit`	an list object produced by Limma `eBayes` function, it should have one additional attribute `$count`, which stored the peptide or PSM count quantified for the gene in label-free or isobaric labelled data.
`fit.method`	the method used to fit variance against the number of peptides/PSM count quantified. Two available methods: "loess","nls" and "spline". default "loess"."loess" uses `loess` and span = 0.75, "nls"" uses a explicit formula `y~a+b/x`. "spline" uses `smooth.spline` and "generalized cross-validation" for smoothing parameter computation. For "nls", independent variable x is peptide/PSM count, response y is pooled variance (`fit$sigma^2`). For "loess" and "spline" method, both x and y are log transformed before applying the two methods. In most of time, "loess" is sufficient. To quickly assess the fit model, use `VarianceScatterplot` and `Residualplot` functions.
`coef_col`	an integer vector indicating the column(s) of fit$coefficients for which the function is to be performed. if not specified, all coefficients are used.

Details

This function adjusts the T-statistics and p-values for quantitative MS proteomics experiment according to the number of peptides/PSMs used for quantification. The method is similar in nature to intensity-based Bayes method (Maureen A. Sartor et al BMC Bioinformatics 2006).

Value

a list object with the following components

count	Peptide or PSM count used for quantification
sca.t	Spectra Count Adjusted posterior t-value
sca.p	Spectra Count Adjusted posterior p-value
sca.dfprior	Spectra Count Adjusted prior degrees of freedom
sca.priorvar	Spectra Count Adjusted prior variance
sca.postvar	Spectra Count Adjusted posterior variance
model	fitted model
fit.method	The method used to fit the model

Author(s)

Yafeng Zhu

Examples

```
library(ExperimentHub)
eh = ExperimentHub(localHub=TRUE)
query(eh, "DEqMS")
dat.psm = eh[["EH1663"]]

dat.psm.log = dat.psm
dat.psm.log[,3:12] =  log2(dat.psm[,3:12])

dat.gene.nm = medianSweeping(dat.psm.log,group_col = 2)

psm.count.table = as.data.frame(table(dat.psm$gene)) # generate PSM count table
rownames(psm.count.table)=psm.count.table$Var1

cond = c("ctrl","miR191","miR372","miR519","ctrl",
"miR372","miR519","ctrl","miR191","miR372")

sampleTable <- data.frame(
row.names = colnames(dat.psm)[3:12],
cond = as.factor(cond)
)

gene.matrix = as.matrix(dat.gene.nm)
design = model.matrix(~cond,sampleTable)

fit1 <- eBayes(lmFit(gene.matrix,design))
# add PSM count for each gene
fit1$count <- psm.count.table[rownames(fit1$coefficients),2]

fit2 = spectraCounteBayes(fit1)
```

VarianceBoxplot *generate a boxplot of the variance*

Description

This function is to draw a boxplot of the variance of genes quantified by different number of peptides/PSMs. Red curve indicate DEqMS prior variance.

Usage

```
VarianceBoxplot(fit,n=20, xlab="count", ylab = "log(Variance)", main="")
```

Arguments

fit	an object returned from spectraCounteBayes function
n	set a number to plot only the genes with count value smaller or equal to n
xlab	the title for x axis
ylab	the title for y axis
main	the title for the figure

Value

return a plot graphic

Author(s)

Yafeng Zhu

Examples

```
library(ExperimentHub)
eh = ExperimentHub(localHub=TRUE)
query(eh, "DEqMS")
dat.psm = eh[["EH1663"]]

dat.psm.log = dat.psm
dat.psm.log[,3:12] =  log2(dat.psm[,3:12])

dat.gene.nm = medianSweeping(dat.psm.log,group_col = 2)

psm.count.table = as.data.frame(table(dat.psm$gene)) # generate PSM count table
rownames(psm.count.table)=psm.count.table$Var1

cond = c("ctrl","miR191","miR372","miR519","ctrl",
"miR372","miR519","ctrl","miR191","miR372")

sampleTable <- data.frame(
row.names = colnames(dat.psm)[3:12],
```

```
cond = as.factor(cond)
)

gene.matrix = as.matrix(dat.gene.nm)
design = model.matrix(~cond,sampleTable)

fit1 <- eBayes(lmFit(gene.matrix,design))
# add PSM count for each gene
fit1$count <- psm.count.table[rownames(fit1$coefficients),2]

fit2 = spectraCounteBayes(fit1)

VarianceBoxplot(fit2,xlab="PSM count",main="TMT data PXD004163")
```

`VarianceScatterplot` *generate a scatter plot of the variance*

Description

This function is to draw a scatter plot of the variance against the number of quantified peptides/PSMs.Red curve indicate DEqMS prior variance.

Usage

```
VarianceScatterplot(fit, xlab="log2(count)",
ylab = "log(Variance)", main="")
```

Arguments

`fit`	an object returned from `spectraCounteBayes` function
`xlab`	the title for x axis
`ylab`	the title for y axis
`main`	the title for the figure

Value

return a plot graphic

Author(s)

Yafeng Zhu

Examples

```
library(ExperimentHub)
eh = ExperimentHub(localHub=TRUE)
query(eh, "DEqMS")
dat.psm = eh[["EH1663"]]

dat.psm.log = dat.psm
dat.psm.log[,3:12] =  log2(dat.psm[,3:12])

dat.gene.nm = medianSweeping(dat.psm.log,group_col = 2)

psm.count.table = as.data.frame(table(dat.psm$gene)) # generate PSM count table
rownames(psm.count.table)=psm.count.table$Var1

cond = c("ctrl","miR191","miR372","miR519","ctrl",
"miR372","miR519","ctrl","miR191","miR372")

sampleTable <- data.frame(
row.names = colnames(dat.psm)[3:12],
cond = as.factor(cond)
)

gene.matrix = as.matrix(dat.gene.nm)
design = model.matrix(~cond,sampleTable)

fit1 <- eBayes(lmFit(gene.matrix,design))
# add PSM count for each gene
fit1$count <- psm.count.table[rownames(fit1$coefficients),2]

fit2 = spectraCounteBayes(fit1)

VarianceScatterplot(fit2,xlab="log2(PSM count)",main="TMT data PXD004163")
```

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