Package 'MetNorm'

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Type Package

Title Statistical Methods for Normalizing Metabolomics Data

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Author Alysha M De Livera

Maintainer Alysha M De Livera <alyshad@unimelb.edu.au>

Description Metabolomics data are inevitably subject to a component of unwanted variation, due to factors such as batch effects, matrix effects, and confounding biological variation. This package contains a collection of R functions which can be used to remove unwanted variation and obtain normalized metabolomics data.

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`MetNorm-package` *MetNorm*

Description

Statistical methods for normalizing metabolomics data

Details

Metabolomics data are inevitably subject to a component of unwanted variation, due to factors such as batch effects, matrix effects, and confounding biological variation. This package contains a collection of R fuctions which may be used to obtain normalized metabolomics data.

Author(s)

Alysha M De Livera

References

De Livera, A. M., Dias, D. A, De Souza, D., Rupasinghe, T., Pyke, J., Tull, D., Roessner, U., McConville, M., and Speed, T. P. (2012). Normalizing and integrating metabolomics data. Analytical chemistry, 84(24), 10768-76.

De Livera, A.M., Aho-Sysi, M., Jacob, L., Gagnon-Bartch, J., Castillo, S., Simpson, J.A., and Speed, T.P. (2014), Statistical methods for handling unwanted variation in metabolomics data

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`NormalizeRUVRand` *RUV-random normalized data*

Description

Given suitable controls, this function may be used to obtain a normalized metabolomics data matrix for downstream statistical analysis

Usage

```
NormalizeRUVRand(Y,ctl,k=NULL,lambda=NULL,plotk=TRUE)
```

Arguments

`Y`	A metabolomics data matrix with samples in rows and metabolites in columns
`ctl`	A logical vector indicating which metabolites should be used as negative controls
`k`	The number of factors of unwanted variation
`plotk`	A logical indicating whether a bargraph for the proportion of variance explained by the factors of unwanted variation needs to be plotted
`lambda`	The regularization parameter which depends on k. If not entered, it will be estimated. See DeLivera et al, 2014 for details.

Value

The result is an object of class `normdata`.

Author(s)

Alysha M De Livera and Laurent Jacob

References

De Livera, A. M., Dias, D. A, De Souza, D., Rupasinghe, T., Pyke, J., Tull, D., Roessner, U., McConville, M., and Speed, T. P. (2012). Normalizing and integrating metabolomics data. Analytical chemistry, 84(24), 10768-76.

De Livera, A.M., Aho-Sysi, M., Jacob, L., Gagnon-Bartch, J., Castillo, S., Simpson, J.A., and Speed, T.P. (2014), Statistical methods for handling unwanted variation in metabolomics data

Examples

```
data(UV)
Y<-data.matrix(UV[,-c(1:3)])

##Empirical controls
IS<-Y[,which(colnames(Y)=="IS")]
r<-numeric(dim(Y)[2])
for(j in 1:length(r)){
  r[j]<-cor(IS,Y[,j])
}
ctl<-logical(length(r))
ctl[which(r>round(quantile(r,0.7),2))]<-TRUE

## Not run:
ruv<-NormalizeRUVRand(Y=Y,ctl=ctl,k=3)
ruvclust<-NormalizeRUVRandClust(RUVRand=ruv,
                   maxIter=200,
                   nUpdate=100,
                   lambdaUpdate=TRUE,
                   p=2)
ruvclustY<-ruvclust$newY
pairs(princomp(ruvclustY,cor=TRUE)$scores[,c(1:3)],
      pch=as.numeric(UV[,2]), col=UV[,3],
      main="RUV random for clustering")

## End(Not run)
```

`NormalizeRUVRandClust` *RUV-random method for clustering*

Description

Given suitable controls and user input, this function may be used to obtain a normalized metabolomics data matrix suitable for clustering

Usage

```
NormalizeRUVRandClust(RUVRand,
                              maxIter,
                              nUpdate=maxIter+1,
                              lambdaUpdate=TRUE,
                              p=p,...)
```

Arguments

RUVRand	Output from NormalizeRUVRand
maxIter	Maximum number of iterations
nUpdate	Update the unwanted variation component every nUpdate iterations
lambdaUpdate	A logical indicating whether the regularization parameter needs to be updated
p	The number of clusters to be used in the k-means clustering
...	Other arguments for kmeans

Author(s)

Alysha M De Livera and Laurent Jacob

References

De Livera, A. M., Dias, D. A, De Souza, D., Rupasinghe, T., Pyke, J., Tull, D., Roessner, U., McConville, M., and Speed, T. P. (2012). Normalizing and integrating metabolomics data. Analytical chemistry, 84(24), 10768-76.

De Livera, A.M., Aho-Sysi, M., Jacob, L., Gagnon-Bartch, J., Castillo, S., Simpson, J.A., and Speed, T.P. (2014), Statistical methods for handling unwanted variation in metabolomics data

Examples

```
data(UV)
Y<-data.matrix(UV[,-c(1:3)])

##Empirical controls
IS<-Y[,which(colnames(Y)=="IS")]
r<-numeric(dim(Y)[2])
for(j in 1:length(r)){
  r[j]<-cor(IS,Y[,j])
}
ctl<-logical(length(r))
ctl[which(r>round(quantile(r,0.7),2))]<-TRUE

## Not run:
ruv<-NormalizeRUVRand(Y=Y,ctl=ctl,k=3)
ruvclust<-NormalizeRUVRandClust(RUVRand=ruv,
                  maxIter=200,
                  nUpdate=100,
                  lambdaUpdate=TRUE,
                  p=2)
ruvclustY<-ruvclust$newY
pairs(princomp(ruvclustY,cor=TRUE)$scores[,c(1:3)],
      pch=as.numeric(UV[,2]), col=UV[,3],
      main="RUV random for clustering")

## End(Not run)
```

normdata-class *Normalized data -class*

Description

A list containing the following components:

Slots/Components

`unadjY` The unadjusted data matrix

`newY` The normalized data matrix).

`UVcomp` The removed unwanted variation component

`ctl` A logical vector indicating the controls used in the model

`k` The number of factors of unwanted variation

`lambda` The regularization parameter

Author(s)

Alysha M De Livera

UV *Example data*

Description

A metabolomics dataset with samples run on different machines and settings

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