Package ‘preprocessCore’

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**Title** A collection of pre-processing functions

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**Imports** stats

**Description** A library of core preprocessing routines.

**License** LGPL (>= 2)

**URL** https://github.com/bmbolstad/preprocessCore

**Collate**

- normalize.quantiles.R
- quantile_extensions.R
- rma.background.correct.R
- rcModel.R
- colSummarize.R
- subColSummarize.R
- plmr.R
- plmd.R

**LazyLoad** yes

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colSummarize

Summarize the column of matrices

Description

Compute column wise summary values of a matrix.

Usage

colSummarizeAvg(y)
colSummarizeAvgLog(y)
colSummarizeBiweight(y)
colSummarizeBiweightLog(y)
colSummarizeLogAvg(y)
colSummarizeLogMedian(y)
colSummarizeMedian(y)
colSummarizeMedianLog(y)
colSummarizeMedianpolish(y)
colSummarizeMedianpolishLog(y)

Arguments

y A numeric matrix

Details

This groups of functions summarize the columns of a given matrices.

- colSummarizeAvg: Take means in column-wise manner
- colSummarizeAvgLog: Log2 transform the data and then take means in column-wise manner
- colSummarizeBiweight: Summarize each column using a one step Tukey Biweight procedure
- colSummarizeBiweightLog: Log2 transform the data and then summarize each column using a one step Tukey Biweight procedure
- colSummarizeLogAvg: Compute the mean of each column and then log2 transform it
- colSummarizeLogMedian: Compute the median of each column and then log2 transform it
- colSummarizeMedian: Compute the median of each column
- colSummarizeMedianLog: Log2 transform the data and then summarize each column using the median
normalize.quantiles

- colSummarizeMedianpolish: Use the median polish to summarize each column, by also using a row effect (not returned)
- colSummarizeMedianpolishLogLog2: transform the data and then use the median polish to summarize each column, by also using a row effect (not returned)

Value

A list with following items:

- Estimates: Summary values for each column.
- StdErrors: Standard error estimates.

Author(s)

B. M. Bolstad <bmb@bmbolstad.com>

Examples

```r
y <- matrix(10+rnorm(100),20,5)

colSummarizeAvg(y)
colSummarizeAvgLog(y)
colSummarizeBiweight(y)
colSummarizeBiweightLog(y)
colSummarizeLogAvg(y)
colSummarizeLogMedian(y)
colSummarizeMedian(y)
colSummarizeMedianLog(y)
colSummarizeMedianpolish(y)
colSummarizeMedianpolishLog(y)
```

**normalize.quantiles  Quantile Normalization**

Description

Using a normalization based upon quantiles, this function normalizes a matrix of probe level intensities.

Usage

`normalize.quantiles(x, copy=TRUE, keep.names=FALSE)`
Arguments

x  
A matrix of intensities where each column corresponds to a chip and each row is a probe.

copy  
Make a copy of matrix before normalizing. Usually safer to work with a copy, but in certain situations not making a copy of the matrix, but instead normalizing it in place will be more memory friendly.

keep.names  
Boolean option to preserve matrix row and column names in output.

Details

This method is based upon the concept of a quantile-quantile plot extended to n dimensions. No special allowances are made for outliers. If you make use of quantile normalization please cite Bolstad et al, Bioinformatics (2003).

This function will handle missing data (ie NA values), based on the assumption that the data is missing at random.

Note that the current implementation optimizes for better memory usage at the cost of some additional run-time.

Value

A normalized matrix.

Author(s)

Ben Bolstad, <bmbolstad.com>

References


See Also

normalize.quantiles.robust
normalize.quantiles.in.blocks

Quantile Normalization carried out separately within blocks of rows

Description
Using a normalization based upon quantiles this function normalizes the columns of a matrix such that different subsets of rows get normalized together.

Usage

normalize.quantiles.in.blocks(x, blocks, copy=TRUE)

Arguments

x A matrix of intensities where each column corresponds to a chip and each row is a probe.
copy Make a copy of matrix before normalizing. Usually safer to work with a copy
blocks A vector giving block membership for each each row

Details
This method is based upon the concept of a quantile-quantile plot extended to n dimensions. No special allowances are made for outliers. If you make use of quantile normalization either through rma or expresso please cite Bolstad et al, Bioinformatics (2003).

Value
From normalize.quantiles.use.target a normalized matrix.

Author(s)
Ben Bolstad, <bmb@bmbolstad.com>

References

See Also
normalize.quantiles
### Examples

```r
### setup the data
blocks <- c(rep(1,5),rep(2,5),rep(3,5))
par(mfrow=c(3,2))
x <- matrix(c(rexp(5,0.05),rnorm(5),rnorm(5,10)))
boxplot(x ~ blocks)
y <- matrix(c(-rexp(5,0.05),rnorm(5,10),rnorm(5)))
boxplot(y ~ blocks)
prenorm <- cbind(x,y)

### the in.blocks version
post.norm <- normalize.quantiles.in.blocks(prenorm,blocks)
boxplot(post.norm[,1] ~ blocks)
boxplot(post.norm[,2] ~ blocks)

### the usual version
post.norm <- normalize.quantiles(prenorm)
boxplot(post.norm[,1] ~ blocks)
boxplot(post.norm[,2] ~ blocks)
```

---

**normalize.quantiles.robust**

*Robust Quantile Normalization*

**Description**

Using a normalization based upon quantiles, this function normalizes a matrix of probe level intensities. Allows weighting of chips

**Usage**

```r
normalize.quantiles.robust(x,copy=TRUE,weights=NULL,
remove.extreme=c("variance","mean","both","none"),
n.remove=1,use.median=FALSE,use.log2=FALSE, keep.names=FALSE)
```

**Arguments**

- `x` A matrix of intensities, columns are chips, rows are probes
- `copy` Make a copy of matrix before normalizing. Usually safer to work with a copy
- `weights` A vector of weights, one for each chip
- `remove.extreme` If weights is null, then this will be used for determining which chips to remove from the calculation of the normalization distribution. See details for more info
- `n.remove` number of chips to remove
- `use.median` if TRUE use the median to compute normalization chip, otherwise uses a weighted mean
normalize.quantiles.target

use.log2  work on log2 scale. This means we will be using the geometric mean rather than ordinary mean
keep.names Boolean option to preserve matrix row and column names in output.

Details
This method is based upon the concept of a quantile-quantile plot extended to n dimensions. Note that the matrix is of intensities not log intensities. The function performs better with raw intensities.
Choosing variance will remove chips with variances much higher or lower than the other chips, mean removes chips with the mean most different from all the other means, both removes first extreme variance and then an extreme mean. The option none does not remove any chips, but will assign equal weights to all chips.
Note that this function does not handle missing values (ie NA). Unexpected results might occur in this situation.

Value
a matrix of normalized intensities

Note
This function is still experimental.

Author(s)
Ben Bolstad, <bmb@bmbolstad.com>

See Also
normalize.quantiles

normalize.quantiles.target

Quantile Normalization using a specified target distribution vector

Description
Using a normalization based upon quantiles, these function normalizes the columns of a matrix based upon a specified normalization distribution

Usage
normalize.quantiles.use.target(x,target,copy=TRUE,subset=NULL)
normalize.quantiles.determine.target(x,target.length=NULL,subset=NULL)
**Arguments**

- **x**: A matrix of intensities where each column corresponds to a chip and each row is a probe.
- **copy**: Make a copy of matrix before normalizing. Usually safer to work with a copy.
- **target**: A vector containing datapoints from the distribution to be normalized to.
- **target.length**: number of datapoints to return in target distribution vector. If NULL then this will be taken to be equal to the number of rows in the matrix.
- **subset**: A logical variable indexing whether corresponding row should be used in reference distribution determination.

**Details**

This method is based upon the concept of a quantile-quantile plot extended to n dimensions. No special allowances are made for outliers. If you make use of quantile normalization either through `rma` or `expresso` please cite Bolstad et al, Bioinformatics (2003).

These functions will handle missing data (ie NA values), based on the assumption that the data is missing at random.

**Value**

From `normalize.quantiles.use.target` a normalized matrix.

**Author(s)**

Ben Bolstad, <bmb@bmbolstad.com>

**References**


**See Also**

`normalize.quantiles`
rcModelPLMd

Fit robust row-column models to a matrix

Description

These functions fit row-column effect models to matrices using PLM-d

Usage

rcModelPLMd(y, group.labels)

Arguments

y
A numeric matrix

group.labels
A vector of group labels. Of length ncol(y)

Details

This functions first tries to fit row-column models to the specified input matrix. Specifically the model

\[ y_{ij} = r_i + c_j + \epsilon_{ij} \]

with \( r_i \) and \( c_j \) as row and column effects respectively. Note that these functions treat the row effect as the parameter to be constrained using sum to zero.

Next the residuals for each row are compared to the group variable. In cases where there appears to be a significant relationship, the row-effect is "split" and separate row-effect parameters, one for each group, replace the single row effect.

Value

A list with following items:

- Estimates: The parameter estimates. Stored in column effect then row effect order
- Weights: The final weights used
- Residuals: The residuals
- StdErrors: Standard error estimates. Stored in column effect then row effect order
- WasSplit: An indicator variable indicating whether or not a row was split with separate row effects for each group

Author(s)

B. M. Bolstad <bmb@bmbolstad.com>

See Also

rcModelPLM, rcModelPLMr
Examples

col.effects <- c(10,11,10.5,12,9.5)
row.effects <- c(seq(-0.5,-0.1,by=0.1),seq(0.1,0.5,by=0.1))

y <- outer(row.effects, col.effects,"+")
y <- y + rnorm(50, sd=0.1)
rcModelPLMd(y, group.labels=c(1,1,2,2,2))

row.effects <- c(4,3,2,1,-1,-2,-3,-4)
col.effects <- c(8,9,10,11,12,10)

y <- outer(row.effects, col.effects,"+") + rnorm(48,0,0.25)
y[8,4:6] <- c(11,12,10)+ 2.5 + rnorm(3,0,0.25)
y[5,4:6] <- c(11,12,10)-2.5 + rnorm(3,0,0.25)

rcModelPLMd(y, group.labels=c(1,1,1,2,2,2))

par(mfrow=c(2,2))
matplot(y, type="l", col=c(rep("red",3), rep("blue",3)), ylab="residuals", xlab="probe", main="Observed Data")
matplot(rcModelPLM(y)$Residuals, col=c(rep("red",3), rep("blue",3)), ylab="residuals", xlab="probe", main="Residuals (PLM)"
matplot(rcModelPLMd(y, group.labels=c(1,1,2,2,2))$Residuals, col=c(rep("red",3), rep("blue",3)), xlab="probe",ylab="residuals", main="Residuals (PLM-d)"

rcModelPLMr

Fit robust row-column models to a matrix

Description

These functions fit row-column effect models to matrices using PLM-r and variants

Usage

rcModelPLMr(y)
rcModelPLMrr(y)
rcModelPLMrc(y)
rcModelWPLMr(y, w)
rcModelWPLMrr(y, w)
rcModelWPLMrc(y, w)

Arguments

y A numeric matrix
w A matrix or vector of weights. These should be non-negative.
Details

These functions fit row-column models to the specified input matrix. Specifically the model

\[ y_{ij} = r_i + c_j + \epsilon_{ij} \]

with \( r_i \) and \( c_j \) as row and column effects respectively. Note that these functions treat the row effect as the parameter to be constrained using sum to zero.

The \texttt{rcModelPLMr} and \texttt{rcModelWPLMr} functions use the PLM-r fitting procedure. This adds column and row robustness to single element robustness.

The \texttt{rcModelPLMrC} and \texttt{rcModelWPLMrC} functions use the PLM-rc fitting procedure. This adds column robustness to single element robustness.

The \texttt{rcModelPLMrr} and \texttt{rcModelWPLMrr} functions use the PLM-rr fitting procedure. This adds row robustness to single element robustness.

Value

A list with following items:

- **Estimates**: The parameter estimates. Stored in column effect then row effect order
- **Weights**: The final weights used
- **Residuals**: The residuals
- **StdErrors**: Standard error estimates. Stored in column effect then row effect order

Author(s)

B. M. Bolstad <bmb@bmbolstad.com>

See Also

\texttt{rcModelPLM}, \texttt{rcModelPLMd}

Examples

```r
col.effects <- c(10,11,10.5,12,9.5)
row.effects <- c(seq(-0.5,-0.1,by=0.1),seq(0.1,0.5,by=0.1))

y <- outer(row.effects, col.effects,"+")
w <- runif(50)

rcModelPLMr(y)
rcModelWPLMr(y, w)

### An example where there no or only occasional outliers
y <- y + rnorm(50,sd=0.1)
par(mfrow=c(2,2))
image(1:10,1:5,rcModelPLMr(y)$Weights,xlab="row",ylab="col",main="PLM-r",zlim=c(0,1))
image(1:10,1:5,rcModelWPLMrC(y)$Weights,xlab="row",ylab="col",main="PLM-rc",zlim=c(0,1))
```
rcModels

### Fit row-column model to a matrix

These functions fit row-column effect models to matrices.
Usage

rcModelPLM(y, row.effects=NULL, input.scale=NULL)
rcModelWPLM(y, w, row.effects=NULL, input.scale=NULL)
rcModelMedianPolish(y)

Arguments

y A numeric matrix
w A matrix or vector of weights. These should be non-negative.
row.effects If these are supplied then the fitting procedure uses these (and analyzes individual columns separately)
input.scale If supplied will be used rather than estimating the scale from the data

Details

These functions fit row-column models to the specified input matrix. Specifically the model

\[ y_{ij} = r_i + c_j + \epsilon_{ij} \]

with \( r_i \) and \( c_j \) as row and column effects respectively. Note that this functions treat the row effect as the parameter to be constrained using sum to zero (for rcModelPLM and rcModelWPLM) or median of zero (for rcModelMedianPolish).

The rcModelPLM and rcModelWPLM functions use a robust linear model procedure for fitting the model.

The function rcModelMedianPolish uses the median polish algorithm.

Value

A list with following items:

- Estimates The parameter estimates. Stored in column effect then row effect order
- Weights The final weights used
- Residuals The residuals
- StdErrors Standard error estimates. Stored in column effect then row effect order
- Scale Scale Estimates

Author(s)

B. M. Bolstad <bmb@bmbolstad.com>

See Also

rcModelPLMr, rcModelPLMd
Examples

col.effects <- c(10,11,10.5,12,9.5)
row.effects <- c(seq(-0.5,-0.1,by=0.1),seq(0.1,0.5,by=0.1))

y <- outer(row.effects, col.effects,"+")
w <- runif(50)

rcModelPLM(y)
rcModelWPLM(y, w)
rcModelMedianPolish(y)

y <- y + rnorm(50)

rcModelPLM(y)
rcModelWPLM(y, w)
rcModelMedianPolish(y)

rcModelPLM(y,row.effects=row.effects)
rcModelWPLM(y,w,row.effects=row.effects)

rcModelPLM(y,input.scale=1.0)
rcModelWPLM(y, w,input.scale=1.0)
rcModelPLM(y,row.effects=row.effects,input.scale=1.0)
rcModelWPLM(y,w,row.effects=row.effects,input.scale=1.0)

rma.background.correct

RMA Background Correction

Description

Background correct each column of a matrix

Usage

rma.background.correct(x, copy=TRUE)

Arguments

x A matrix of intensities where each column corresponds to a chip and each row is a probe.
copy
Make a copy of matrix before background correcting. Usually safer to work with a copy, but in certain situations not making a copy of the matrix, but instead background correcting it in place will be more memory friendly.

Details
Assumes PMs are a convolution of normal and exponential. So we observe X+Y where X is background and Y is signal. bg.adjust returns E[Y|X+Y, Y>0] as our background corrected PM.

Value
A RMA background corrected matrix.

Author(s)
Ben Bolstad, <bmbolstad.com>

References

subColSummarize
Summarize columns when divided into groups of rows

Description
These functions summarize columns of a matrix when the rows of the matrix are classified into different groups

Usage
subColSummarizeAvg(y, group.labels)
subColSummarizeAvgLog(y, group.labels)
subColSummarizeBiweight(y, group.labels)
subColSummarizeBiweightLog(y, group.labels)
subColSummarizeLogAvg(y, group.labels)
subColSummarizeMedian(y, group.labels)
subColSummarizeMedianLog(y, group.labels)
subColSummarizeMedianpolish(y, group.labels)
subColSummarizeMedianpolishLog(y, group.labels)
convert.group.labels(group.labels)

Arguments
y A numeric matrix
group.labels A vector to be treated as a factor variable. This is used to assign each row to a group. NA values should be used to exclude rows from consideration
Details

These functions are designed to summarize the columns of a matrix where the rows of the matrix are assigned to groups. The summarization is by column across all rows in each group.

- `subColSummarizeAvgLog` transform the data and then take means in column-wise manner
- `subColSummarizeBiweightLog` transform the data and then use a one-step Tukey Biweight to summarize columns
- `subColSummarizeLogAvg` summarize by taking mean and then taking log2
- `subColSummarizeLogMedian` summarize by taking median and then taking log2
- `subColSummarizeMedianLog` transform the data and then summarize by taking median
- `subColSummarizeMedianpolish` use the median polish to summarize each column, by also using a row effect (not returned)
- `subColSummarizeMedianpolishLog` transform the data and then use the median polish to summarize each column, by also using a row effect (not returned)

Value

A matrix containing column summarized data. Each row corresponds to data column summarized over a group of rows.

Author(s)

B. M. Bolstad <bmb@bmbolstad.com>

Examples

```r
### Assign the first 10 rows to one group and the second 10 rows to the second group
y <- matrix(c(10+rnorm(50),20+rnorm(50)),20,5,byrow=TRUE)
subColSummarizeAvgLog(y,c(rep(1,10),rep(2,10)))
subColSummarizeLogAvg(y,c(rep(1,10),rep(2,10)))
subColSummarizeAvg(y,c(rep(1,10),rep(2,10)))
subColSummarizeBiweight(y,c(rep(1,10),rep(2,10)))
subColSummarizeBiweightLog(y,c(rep(1,10),rep(2,10)))
subColSummarizeMedianLog(y,c(rep(1,10),rep(2,10)))
subColSummarizeLogMedian(y,c(rep(1,10),rep(2,10)))
subColSummarizeMedian(y,c(rep(1,10),rep(2,10)))
```
subrcModels

Fit row-column model to a matrix

Description
These functions fit row-column effect models to matrices

Usage

```
subrcModelPLM(y, group.labels, row.effects=NULL, input.scale=NULL)
subrcModelMedianPolish(y, group.labels)
```

Arguments

- **y**: A numeric matrix
- **group.labels**: A vector to be treated as a factor variable. This is used to assign each row to a group. NA values should be used to exclude rows from consideration
- **row.effects**: If these are supplied then the fitting procedure uses these (and analyzes individual columns separately)
- **input.scale**: If supplied will be used rather than estimating the scale from the data

Details

These functions fit row-column models to the specified input matrix. Specifically the model

\[ y_{ij} = r_i + c_j + \epsilon_{ij} \]

with \( r_i \) and \( c_j \) as row and column effects respectively. Note that this functions treat the row effect as the parameter to be constrained using sum to zero (for `rcModelPLM` and `rcModelWPLM`) or median of zero (for `rcModelMedianPolish`).

The `rcModelPLM` and `rcModelWPLM` functions use a robust linear model procedure for fitting the model.

The function `rcModelMedianPolish` uses the median polish algorithm.

Value

A list with following items:

- **Estimates**: The parameter estimates. Stored in column effect then row effect order
- **Weights**: The final weights used
- **Residuals**: The residuals
- **StdErrors**: Standard error estimates. Stored in column effect then row effect order
- **Scale**: Scale Estimates
Author(s)
B. M. Bolstad <bmb@bmbolstad.com>

See Also
rcModelPLM

Examples

```r
y <- matrix(c(10+rnorm(50),20+rnorm(50)),20,5,byrow=TRUE)
subrcModelPLM(y,c(rep(1,10),rep(2,10)))
subrcModelMedianPolish(y,c(rep(1,10),rep(2,10)))

col.effects <- c(10,11,10.5,12,9.5)
row.effects <- c(seq(-0.5,-0.1,by=0.1),seq(0.1,0.5,by=0.1))

y <- outer(row.effects, col.effects,"+")
w <- runif(50)
rcModelPLM(y)
rcModelWPLM(y, w)
rcModelMedianPolish(y)

y <- y + rnorm(50)
rcModelPLM(y)
rcModelWPLM(y, w)
rcModelMedianPolish(y)

rcModelPLM(y,row.effects=row.effects)
rcModelWPLM(y,w,row.effects=row.effects)
rcModelPLM(y,input.scale=1.0)
rcModelWPLM(y, w,input.scale=1.0)
rcModelPLM(y,row.effects=row.effects,input.scale=1.0)
rcModelWPLM(y,w,row.effects=row.effects,input.scale=1.0)
```
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