Package ‘preprocessCore’

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Title A collection of pre-processing functions
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Maintainer Ben Bolstad <bmb@bmbolstad.com>
Imports stats
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    subColSummarize.R plmr.R plmd.R

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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.

- colSummarizeAvgTake means in column-wise manner
- colSummarizeAvgLoglog2 transform the data and then take means in column-wise manner
- colSummarizeBiweightSummarize each column using a one step Tukey Biweight procedure
- colSummarizeBiweightLoglog2 transform the data and then summarize each column using a one step Tukey Biweight procedure
- colSummarizeLogAvgCompute the mean of each column and then log2 transform it
- colSummarizeLogMedianCompute the median of each column and then log2 transform it
- colSummarizeMedianCompute the median of each column
- colSummarizeMedianLoglog2 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

```r
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 functions 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
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

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

Examples

### 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)
pre.norm <- cbind(x,y)

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

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

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:

<table>
<thead>
<tr>
<th>Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Estimates</td>
<td>The parameter estimates.Stored in column effect then row effect order</td>
</tr>
<tr>
<td>Weights</td>
<td>The final weights used</td>
</tr>
<tr>
<td>Residuals</td>
<td>The residuals</td>
</tr>
<tr>
<td>StdErrors</td>
<td>Standard error estimates. Stored in column effect then row effect order</td>
</tr>
<tr>
<td>WasSplit</td>
<td>An indicator variable indicating whether or not a row was split with separate row effects for each group</td>
</tr>
</tbody>
</table>

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)$Residuals,col=c(rep("red",3),rep("blue",3)),ylab="residuals",xlab="probe",main="Residual")
matplot(rcModelPLMd(y,group.labels=c(1,1,2,2,2))$Residuals,col=c(rep("red",3),rep("blue",3)),xlab="probe",ylab="residuals",main="Residual")

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 `rcModelPLMr` and `rcModelWPLMr` functions use the PLM-r fitting procedure. This adds column and row robustness to single element robustness.

The `rcModelPLMrc` and `rcModelWPLMrc` functions use the PLM-rc fitting procedure. This adds column robustness to single element robustness.

The `rcModelPLMrr` and `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

- `rcModelPLM`, `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)$Weights,xlab="row",ylab="col",main="PLM-r",zlim=c(0,1))
image(1:10,1:5,rcModelWPLMr(y)$Weights,xlab="row",ylab="col",main="PLM-rc",zlim=c(0,1))
```
rcModels

Fit row-column model to a matrix

Description

These functions fit row-column effect models to matrices.

```r
image(1:10,1:5,rcModelPLMr(y)$Weights,xlab="row",ylab="col",main="PLM-r",zlim=c(0,1))
matplot(y,type="l")

### An example where there is a row outlier
y <- outer(row.effects, col.effects,"+")
y[1,] <- 11+ rnorm(5)
y <- y + rnorm(50,sd=0.1)
par(mfrow=c(2,2))
image(1:10,1:5,rcModelPLMr(y)$Weights,xlab="row",ylab="col",main="PLM-r",zlim=c(0,1))
image(1:10,1:5,rcModelWPLMr(y,w)$Weights,xlab="row",ylab="col",main="PLM-r",zlim=c(0,1))
image(1:10,1:5,rcModelWPLMrc(y,w)$Weights,xlab="row",ylab="col",main="PLM-rc",zlim=c(0,1))
image(1:10,1:5,rcModelWPLMrr(y,w)$Weights,xlab="row",ylab="col",main="PLM-rr",zlim=c(0,1))
matplot(y,type="l")

### An example where there is a column outlier
y <- outer(row.effects, col.effects,"+")
w <- rep(1,50)
y[,4] <- 12 + rnorm(10)
y <- y + rnorm(50,sd=0.1)
par(mfrow=c(2,2))
image(1:10,1:5,rcModelPLMr(y,w)$Weights,xlab="row",ylab="col",main="PLM-r",zlim=c(0,1))
image(1:10,1:5,rcModelWPLMr(y,w)$Weights,xlab="row",ylab="col",main="PLM-r",zlim=c(0,1))
image(1:10,1:5,rcModelWPLMrc(y,w)$Weights,xlab="row",ylab="col",main="PLM-rc",zlim=c(0,1))
image(1:10,1:5,rcModelWPLMrr(y,w)$Weights,xlab="row",ylab="col",main="PLM-rr",zlim=c(0,1))
matplot(y,type="l")

### An example where there is both column and row outliers
y <- outer(row.effects, col.effects,"+")
w <- rep(1,50)
y[,4] <- 12 + rnorm(10)
y[1,] <- 11+ rnorm(5)
y <- y + rnorm(50,sd=0.1)
par(mfrow=c(2,2))
image(1:10,1:5,rcModelPLMr(y,w)$Weights,xlab="row",ylab="col",main="PLM-r",zlim=c(0,1))
image(1:10,1:5,rcModelWPLMr(y,w)$Weights,xlab="row",ylab="col",main="PLM-r",zlim=c(0,1))
image(1:10,1:5,rcModelWPLMrc(y,w)$Weights,xlab="row",ylab="col",main="PLM-rc",zlim=c(0,1))
image(1:10,1:5,rcModelWPLMrr(y,w)$Weights,xlab="row",ylab="col",main="PLM-rr",zlim=c(0,1))
matplot(y,type="l")
```
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
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 correction. 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


Description

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

Usage

```r
subColSummarizeAvg(y, group.labels)
subColSummarizeLog(y, group.labels)
subColSummarizeBiweight(y, group.labels)
subColSummarizeBiweightLog(y, group.labels)
subColSummarizeLogAvg(y, group.labels)
subColSummarizeMedian(y, group.labels)
subColSummarizeLogMedian(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.
subColSummarize

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.

- subColSummarizeAvgSummarize by taking mean
- subColSummarizeAvgLoglog2 transform the data and then take means in column-wise manner
- subColSummarizeBiweightUse a one-step Tukey Biweight to summarize columns
- subColSummarizeBiweightLoglog2 transform the data and then use a one-step Tukey Biweight to summarize columns
- subColSummarizeLogAvgSummarize by taking mean and then taking log2
- subColSummarizeLogMedianSummarize by taking median and then taking log2
- subColSummarizeMedianSummarize by taking median
- subColSummarizeMedianLoglog2 transform the data and then summarize by taking median
- subColSummarizeMedianpolishUse the median polish to summarize each column, by also using a row effect (not returned)
- subColSummarizeMedianpolishLoglog2 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

subColSummarizeMedianpolishLog(y,c(rep(1,10),rep(2,10)))
subColSummarizeMedianpolish(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, row.effects=row.effects)
rcModelWPLM(y, w, row.effects=row.effects)
```

\texttt{rcModelPLM}(y, \text{row.eff}ects=\text{row.eff}ects, \text{input.scale}=1.0) \\
\texttt{rcModelWPLM}(y, w, \text{row.eff}ects=\text{row.eff}ects, \text{input.scale}=1.0)
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