Package ‘arrayQualityMetrics’

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Title Quality metrics report for microarray data sets
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Description This package generates microarray quality metrics reports for data in Bioconductor microarray data containers (ExpressionSet, NChannelSet, AffyBatch). One and two color array platforms are supported.

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biocViews Microarray, QualityControl, OneChannel, TwoChannel, ReportWriting

Collate classes.R affyspecific.r annotateSvg.R arrayQualityMetrics.r boxplot.r density.r globalParameters.R heatmap.r makeColors.R maplot.r meansd.r outlier.R pca.r prepdata.r probesmap.r spatial.r writereport.r XYfromGAL.r

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addXYfromGAL  

**Computing the coordinates of the spots on a slide**

**Description**

From the coordinates of the blocks of a microarray slide and the Row and Column locations of the spots within the blocks, addXYfromGAL computes the X and Y coordinates of the spots of a slide.

**Usage**

```r
addXYfromGAL(x, gal.file, nBlocks, skip, ...)
```

**Arguments**

- `x` is an `AnnotatedDataFrame` representing the featureData of an object.
- `gal.file` name of the file .gal that contains the coordinates of the blocks.
- `nBlocks` number of blocks on the slide.
- `skip` number of header lines to skip when reading the gal.file.
- `...` Arguments that get passed on to `read.table`.

**Value**

The object `x` of class `AnnotatedDataFrame` will be returned with two added columns: X and Y corresponding to the absolute position of the probes on the array.

**Author(s)**

Audrey Kauffmann, Wolfgang Huber. Maintainer: <kauffmann@bergonie.org>

aqm.writereport  

**Write a quality report**

**Description**

`aqm.writereport` produces a quality report (HTML document with figures) from a list of `aqmReportModule` objects.

**Usage**

```r
aqm.writereport(modules, arrayTable, reporttitle, outdir)
```

**Arguments**

- `modules` A list of `aqmReportModule` objects.
- `arrayTable` A data.frame with array (meta)data to be displayed in the report.
- `reporttitle`, `outdir`  
  Report title and output directory - as in `arrayQualityMetrics`. 
A side effect of this function is the creation of the HTML report.

Author(s)

Audrey Kauffmann, Wolfgang Huber

Class to contain all the information to render a quality report module.

Please see the vignette Advanced topics: Customizing arrayQualityMetrics reports and programmatic processing of the output.

Please see the manual page of the module generations functions, e.g. `aqm.boxplot`.

Audrey Kauffmann, Wolfgang Huber

Quality metrics for microarray experiments

Produce an array quality metrics report. This is the main function of the package.

```r
arrayQualityMetrics(expressionset,
    outdir = reporttitle,
    force = FALSE,
    do.logtransform = FALSE,
    intgroup = character(0),
    grouprep,
    spatial = TRUE,
    reporttitle = paste("arrayQualityMetrics report for", deparse(substitute(expressionset))),
    ...
)```
modulefunctions

Arguments

expressionset  a Bioconductor microarray dataset container. This can be an object of class ExpressionSet, AffyBatch, NChannelSet, ExpressionSetIllumina, RGL, MAList, MAList.

outdir the name of the directory in which the report is created; a character of length 1.

force if the directory named by outdir already exists, then, if force is TRUE, the directory is overwritten, otherwise an error is thrown; if the directory does not exist, the value of force is irrelevant; a logical of length 1.

do.logtransform indicates whether the data should be logarithm transformed before the analysis; a logical of length 1.

intgroup the name of the sample covariate(s) used to draw a colour side bar next to the heatmap. The first element of intgroup is also used define sample groups in other plots (boxplots, densities). intgroup should be a character vector, and its elements need to match the columns names of phenoData(expressionset). If its length is 0, then the plots are not decorated with sample covariate information.

grouprep deprecated. Use argument intgroup instead.

spatial indicates whether spatial plots should be made; a logical of length 1. This can be useful for large arrays (like Affymetrix hgu133Plus2) when CPU time and RAM resources of the machine would be limiting.

reporttitle title for the report (character of length 1).

... further arguments that will be passed on to the different module functions.

Details

See the arrayQualityMetrics vignette for examples of this function.

Value

A side effect of the function is the creation of directory named by outdir containing a HTML report QMreport.html and figures. The function also returns a list with R objects containing the report elements for subsequent programmatic processing.

Author(s)

Audrey Kauffmann and Wolfgang Huber.

modulefunctions Functions for computing quality report modules.

Description

These functions produce objects of class aqmReportModule representing the various modules of the quality report. Given a list of modules, the report is then rendered by the aqm.writereport function.

Most users will not call these functions directly, but will use the function arrayQualityMetrics, which in turns calls these functions. The function arguments can be provided through the ... argument of arrayQualityMetrics.
modulefunctions

Usage

aqm.boxplot(x, subsample=20000, outlierMethod = "KS", ...)  
aqm.density(x, ...)  
aqm.heatmap(x, ...)  
aqm.pca(x, ...)  
aqm.maplot(x, subsample=20000, Dthresh=0.15, maxNumArrays=8, nrColumns=4, ...)  
aqm.spatial(x, scale="rank", channels = c("M", "R", "G"), maxNumArrays=8, nrColumns=4, ...)  
aqm.meansd(x, ...)  
aqm.probesmap(x, ...)

# Affymetrix specific sections

aqm.pmmm(x, ...)  
aqm.rnadeg(expressionset, x, ...)  
aqm.rle(x, outlierMethod = "KS", ...)  
aqm.nuse(x, outlierMethod = "upperquartile", ...)

Arguments

x An object resulting from a call to prepdata(expressionset).
expressionset An object of class AffyBatch.
subsample For efficiency, some computations are performed not on the full set of features (which can be hundreds of thousands on some arrays), but on a randomly subset whose size is indicated by this number.
outlierMethod As in outliers.
Dthresh In maplot, the arrays with a Hoeffding D statistic larger than this value are called outliers. See also hoeffd.
scale, channels In aqm.spatial, scale determines the choice of the false colour scale in the spatial plots. If the value is "rank", then the colour is proportional to the ranks of the values; if it is "direct", then it is proportional to the values themselves. channels determines for which elements of x spatial plots are made.
maxNumArrays, nrColumns The parameter maxNumArrays determines the number of arrays for which a plot is produced. nrColumns determines the number of columns in the multi-panel plot. In aqm.maplot, first maxNumArrays is incremented to the next multiple of maxNumArrays. A value of +Inf is allowed. If this value is larger than or equal to the actual number of arrays in x, then plots are produced for all arrays. If it is smaller, then plots are shown for the maxNumArrays/2 with the worst values of Hoeffding’s D and for the maxNumArrays/2 best.
...

Will be ignored - the dots are formal arguments which permit that all of these functions can be called from arrayQualityMetrics with the same, overall set of arguments.

Details

For a simple example of the aqm.* functions, have a look at the source code of the aqm.pca function. Please see also the vignette Advanced topics: Customizing arrayQualityMetrics reports and programmatic processing of the output.
Value

An object of class `aqmReportModule`.

Author(s)

Audrey Kauffmann, Wolfgang Huber

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`outlierDetection`  
*Represents the results from applying an outlier detection criterion to the arrays.*

Description

The class is described in the vignette *Advanced topics: Customizing arrayQualityMetrics reports and programmatic processing of the output*.

Author(s)

Audrey Kauffmann, Wolfgang Huber

See Also

`outliers`

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`outliers`  
*Helper functions for outlier detection and reporting in arrayQualityMetrics*.

Description

For an overview of outlier detection, please see the corresponding section in the vignette *Advanced topics: Customizing arrayQualityMetrics reports and programmatic processing of the output*. These two functions are helper functions used by the different report generating functions, such as `aqm.boxplot`.

Usage

```r
outliers(exprs, method = c("KS", "sum", "upperquartile"))
boxplotOutliers(x, coef = 1.5)
```

Arguments

- `exprs`: A matrix whose columns correspond to arrays, rows to the array features.
- `method`: A character string specifying the summary statistic to be used for each column of `exprs`. See Details.
- `x`: A vector of real numbers.
- `coef`: A number is called an outlier if it is larger than the upper hinge plus `coef` times the interquartile range. Upper hinge and interquartile range are computed by `fivenum`. 
**Details**

*outliers*: with argument `method="KS"`, the function first computes for each column of `exprs` (i.e. for each array) the value of the `ks.test` test statistic between its distribution of intensities and the pooled distribution of intensities from all arrays. With "sum" and "upperquartile", it computes the sum or the 75 percent quantile. Subsequently, it calls `boxplotOutliers` on these values to identify the outlying arrays.

`boxplotOutliers` uses a criterion similar to that used in `boxplot.stats` to detect outliers in a set of real numbers. The main difference is that in `boxplotOutliers`, only the outliers to the right (i.e. extraordinarily large values) are detected.

**Value**

For outliers, an object of class `outlierDetection`. For `boxplotOutliers`, a list with two elements: `thresh`, the threshold against which `x` was compared, and `outliers`, an integer vector of indices.

**Author(s)**

Wolfgang Huber

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**Description**

`prepdata` computes summary statistics that are useful for all platforms; `prepaffy` computes Affymetrix-specific ones. These are helper functions used by `arrayQualityMetrics`.

**Usage**

```r
prepdata(expressionset, intgroup, do.logtransform)
prepaffy(expressionset, x)
```

**Arguments**

- `expressionset`: An object of class `ExpressionSet` for one colour non Affymetrix data, `AffyBatch` for Affymetrix data, `NChannelSet` for two colour arrays, or `BeadLevelList` for Illumina bead arrays.
- `intgroup`, `do.logtransform`: as in `arrayQualityMetrics`.
- `x`: A list, typically the result from a prior call to `prepdata`.

**Details**

See the vignette `Working with arrayQualityMetrics report sections`.

**Value**

A list with various derived quantities. In the case of `prepaffy`, the returned list is `x` with the additional elements appended.
Author(s)

Audrey Kauffmann, Wolfgang Huber
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