Package ‘mi4p’

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Type Package

Title Multiple Imputation for Proteomics

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biocViews

Imports DAPAR, emmeans, foreach, imp4p, impute, limma, mice, stringr

Suggests Biobase, knitr, R.rsp, rmarkdown

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Description A framework for multiple imputation for proteomics is proposed by Marie Chion, Christine Carapito and Frederic Bertrand (2021) <arxiv:2108.07086>. It is dedicated to dealing with multiple imputation for proteomics.

License GPL (>= 2)

Encoding UTF-8

Classification/MSC 62J05, 62J07, 62J99, 92C42

VignetteBuilder knitr

RoxygenNote 7.1.1

URL https://mariechion.github.io/mi4p/,
https://github.com/mariechion/mi4p/

BugReports https://github.com/mariechion/mi4p/issues/

NeedsCompilation no

Repository CRAN

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R topics documented:

`mi4p-package` *The mi4p Package*

Description

A multiple imputation framework ...

Author(s)

This package has been written by Marie Chion, Christine Carapito and Frederic Bertrand. Maintainer: <frederic.bertrand@utt.fr>

References

M. Chion, Ch. Carapito and F. Bertrand (2021). *Accounting for multiple imputation-induced variability for differential analysis in mass spectrometry-based label-free quantitative proteomics*. arxiv:2108.07086. https://arxiv.org/abs/2108.07086.

`datasim` *A single simulated dataset*

Description

This dataset was simulated using the default values of the values of the options of the protdatasim function and the set.seed value set to 4619.

Format

A data frame with 200 observations on the following 11 variables.

id.obs a numeric vector

X1 a numeric vector

X2 a numeric vector

X3 a numeric vector

X4 a numeric vector

X5 a numeric vector

X6 a numeric vector

X7 a numeric vector

X8 a numeric vector

X9 a numeric vector

X10 a numeric vector

Author(s)

M. Chion, Ch. Carapito and F. Bertrand.

Source

We simulated the data.

References

M. Chion, Ch. Carapito and F. Bertrand (2021). *Accounting for multiple imputation-induced variability for differential analysis in mass spectrometry-based label-free quantitative proteomics*. arxiv:2108.07086. https://arxiv.org/abs/2108.07086.

Examples

```
data(datasim)
str(datasim)
```

---

eBayes.mod *MI-aware Modifed eBayes Function*

Description

Modified eBayes function to be used instead of the one in the limma package

Usage

```
eBayes.mod(
  fit,
  VarRubin,
  proportion = 0.01,
  stdev.coef.lim = c(0.1, 4),
  trend = FALSE,
  robust = FALSE,
  winsor.tail.p = c(0.05, 0.1)
)
```

Arguments

`fit`	an MArrayLM fitted model object produced by lmFit or contrasts.fit. For ebayes only, fit can alternatively be an unclassed list produced by lm.series, gls.series or mrlm containing components coefficients, stdev.unscaled, sigma and df.residual.
`VarRubin`	a variance-covariance matrix.
`proportion`	numeric value between 0 and 1, assumed proportion of genes which are differentially expressed
`stdev.coef.lim`	numeric vector of length 2, assumed lower and upper limits for the standard deviation of log2-fold-changes for differentially expressed genes
`trend`	logical, should an intensity-trend be allowed for the prior variance? Default is that the prior variance is constant.
`robust`	logical, should the estimation of df.prior and var.prior be robustified against outlier sample variances?
`winsor.tail.p`	numeric vector of length 1 or 2, giving left and right tail proportions of x to Winsorize. Used only when robust=TRUE.

Value

eBayes produces an object of class MArrayLM (see MArrayLM-class) containing everything found in `fit` plus the following added components:

t numeric matrix of moderated t-statistics.

p.value numeric matrix of two-sided p-values corresponding to the t-statistics.

lods numeric matrix giving the log-odds of differential expression (on the natural log scale).

s2.prior estimated prior value for sigma^2. A row-wise vector if covariate is non-NULL, otherwise a single value.

df.prior degrees of freedom associated with s2.prior. A row-wise vector if robust=TRUE, otherwise a single value.

df.total row-wise numeric vector giving the total degrees of freedom associated with the t-statistics for each gene. Equal to df.prior+df.residual or sum(df.residual), whichever is smaller.

s2.post row-wise numeric vector giving the posterior values for sigma^2.

var.prior column-wise numeric vector giving estimated prior values for the variance of the log2-fold-changes for differentially expressed gene for each constrast. Used for evaluating lods.

F row-wise numeric vector of moderated F-statistics for testing all contrasts defined by the columns of fit simultaneously equal to zero.

F.p.value row-wise numeric vector giving p-values corresponding to F.

The matrices t, p.value and lods have the same dimensions as the input object fit, with rows corresponding to genes and columns to coefficients or contrasts. The vectors s2.prior, df.prior, df.total, F and F.p.value correspond to rows, with length equal to the number of genes. The vector var.prior corresponds to columns, with length equal to the number of contrasts. If s2.prior or df.prior have length 1, then the same value applies to all genes.

s2.prior, df.prior and var.prior contain empirical Bayes hyperparameters used to obtain df.total, s2.post and lods.

Author(s)

Modified by M. Chion and F. Bertrand. Original by Gordon Smyth and Davis McCarthy

Examples

```
library(mi4p)
data(datasim)
datasim_imp <- multi.impute(data = datasim[,-1], conditions =
attr(datasim,"metadata")$Condition, method = "MLE")
VarRubin.matrix <- rubin2.all(datasim_imp[1:5,,],
attr(datasim,"metadata")$Condition)
set.seed(2016)
sigma2 <- 0.05 / rchisq(100, df=10) * 10
y <- datasim_imp[,,1]
design <- cbind(Intercept=1,Group=as.numeric(
attr(datasim,"metadata")$Condition)-1)
fit.model <- limma::lmFit(y,design)
eBayes.mod(fit=fit.model,VarRubin.matrix[[1]])
```

`formatLimmaResult` *Format a Result from Limma*

Description

It is not exported by DAPAR and has to be reproduced here.

Usage

```
formatLimmaResult(fit, conds, contrast)
```

Arguments

`fit`	Limma fit
`conds`	Condition vector
`contrast`	Contrast vector

Value

A list of two dataframes : logFC and P_Value. The first one contains the logFC values of all the comparisons (one column for one comparison), the second one contains the pvalue of all the comparisons (one column for one comparison). The names of the columns for those two dataframes are identical and correspond to the description of the comparison.

Author(s)

Adapted from the code of Samuel Wieczorek in the DAPAR package as it is an object that is not exported by the DAPAR package.

Examples

```
library(DAPAR)
set.seed(2016)
data(qData)
data(sTab)
contrast=1
sTab.old <- sTab
conds <- factor(sTab$Condition, levels = unique(sTab$Condition))
sTab <- sTab[unlist(lapply(split(sTab, conds), function(x) {
  x["Sample.name"]
})), ]
qData <- qData[, unlist(lapply(split(sTab.old, conds), function(x) {
  x["Sample.name"]
}))]
conds <- conds[order(conds)]
res.l <- NULL
design.matrix <- DAPAR::make.design(sTab)
contra <- DAPAR::make.contrast(design.matrix, condition = conds,
```

```
                                contrast)
cmtx <- limma::makeContrasts(contrasts = contra, levels = make.names(colnames(design.matrix)))
fit <- limma::eBayes(limma::contrasts.fit(limma::lmFit(qData,
                                                       design.matrix), cmtx))
res.l <- mi4p::formatLimmaResult(fit, conds, contrast)
```

---

hid.ebayes *MI-aware Modifed eBayes Function*

Description

Modified eBayes function to be used instead of the one, `.ebayes`, implemented in the limma package

Usage

```
hid.ebayes(
  fit,
  VarRubin,
  mod = TRUE,
  proportion = 0.01,
  stdev.coef.lim = c(0.1, 4),
  trend = FALSE,
  robust = FALSE,
  winsor.tail.p = c(0.05, 0.1)
)
```

Arguments

`fit`	an MArrayLM fitted model object produced by lmFit or contrasts.fit. For ebayes only, fit can alternatively be an unclassed list produced by lm.series, gls.series or mrlm containing components coefficients, stdev.unscaled, sigma and df.residual.
`VarRubin`	a variance-covariance matrix.
`mod`	TRUE (not used at the moment)
`proportion`	numeric value between 0 and 1, assumed proportion of genes which are differentially expressed
`stdev.coef.lim`	numeric vector of length 2, assumed lower and upper limits for the standard deviation of log2-fold-changes for differentially expressed genes
`trend`	logical, should an intensity-trend be allowed for the prior variance? Default is that the prior variance is constant.
`robust`	logical, should the estimation of df.prior and var.prior be robustified against outlier sample variances?
`winsor.tail.p`	numeric vector of length 1 or 2, giving left and right tail proportions of x to Winsorize. Used only when robust=TRUE.

Value

eBayes produces an object of class MArrayLM (see MArrayLM-class) containing everything found in `fit` plus the following added components:

t numeric matrix of moderated t-statistics.

p.value numeric matrix of two-sided p-values corresponding to the t-statistics.

lods numeric matrix giving the log-odds of differential expression (on the natural log scale).

s2.prior estimated prior value for sigma^2. A row-wise vector if covariate is non-NULL, otherwise a single value.

df.prior degrees of freedom associated with s2.prior. A row-wise vector if robust=TRUE, otherwise a single value.

df.total row-wise numeric vector giving the total degrees of freedom associated with the t-statistics for each gene. Equal to df.prior+df.residual or sum(df.residual), whichever is smaller.

s2.post row-wise numeric vector giving the posterior values for sigma^2.

var.prior column-wise numeric vector giving estimated prior values for the variance of the log2-fold-changes for differentially expressed gene for each constrast. Used for evaluating lods.

F row-wise numeric vector of moderated F-statistics for testing all contrasts defined by the columns of fit simultaneously equal to zero.

F.p.value row-wise numeric vector giving p-values corresponding to F.

The matrices t, p.value and lods have the same dimensions as the input object fit, with rows corresponding to genes and columns to coefficients or contrasts. The vectors s2.prior, df.prior, df.total, F and F.p.value correspond to rows, with length equal to the number of genes. The vector var.prior corresponds to columns, with length equal to the number of contrasts. If s2.prior or df.prior have length 1, then the same value applies to all genes.

s2.prior, df.prior and var.prior contain empirical Bayes hyperparameters used to obtain df.total, s2.post and lods.

Author(s)

Modified by M. Chion and F. Bertrand. Original by Gordon Smyth and Davis McCarthy

Examples

```
library(mi4p)
data(datasim)
datasim_imp <- multi.impute(data = datasim[,-1], conditions =
attr(datasim,"metadata")$Condition, method = "MLE")
VarRubin.matrix <- rubin2.all(datasim_imp[1:5,,],
attr(datasim,"metadata")$Condition)
set.seed(2016)
sigma2 <- 0.05 / rchisq(100, df=10) * 10
y <- datasim_imp[,,1]
design <- cbind(Intercept=1,Group=as.numeric(
attr(datasim,"metadata")$Condition)-1)
fit.model <- limma::lmFit(y,design)
hid.ebayes(fit=fit.model,VarRubin.matrix[[1]])
```

limmaCompleteTest.mod *Computes a hierarchical differential analysis*

Description

Modified version of the `limmaCompleteTest` function from the `DAPAR` package to return both the fit and the results.

Usage

```
limmaCompleteTest.mod(qData, sTab, comp.type = "OnevsOne")
```

Arguments

`qData`	A matrix of quantitative data, without any missing values.
`sTab`	A dataframe of experimental design (`pData()`).
`comp.type`	A string that corresponds to the type of comparison. Values are: 'anova1way', 'OnevsOne' and 'OnevsAll'; default is 'OnevsOne'.

Value

A list of two dataframes : logFC and P_Value. The first one contains the logFC values of all the comparisons (one column for one comparison), the second one contains the pvalue of all the comparisons (one column for one comparison). The names of the columns for those two dataframes are identical and correspond to the description of the comparison.

Author(s)

Adapted from Hélène Borges, Thomas Burger, Quentin Giai-Gianetto, Samuel Wieczorek

Examples

```
set.seed(2016)
data(qData)
data(sTab)
limma <- limmaCompleteTest.mod(qData, sTab, comp.type='OnevsOne')
```

meanImp_emmeans *Multiple Imputation Estimate*

Description

Computes the multiple imputation parameter estimate using the emmeans package.

Usage

```
meanImp_emmeans(ind, peptide = 1, tabdata, metacond)
```

Arguments

`ind`	index
`peptide`	name of the peptide
`tabdata`	dataset
`metacond`	a factor to specify the groups

Value

A vector.

References

M. Chion, Ch. Carapito and F. Bertrand (2021). *Accounting for multiple imputation-induced variability for differential analysis in mass spectrometry-based label-free quantitative proteomics*. arxiv:2108.07086. https://arxiv.org/abs/2108.07086.

Examples

```
library(mi4p)
data(datasim)
datasim_imp <- multi.impute(data = datasim[,-1], conditions =
attr(datasim,"metadata")$Condition, method = "MLE")
meanImp_emmeans(1,1,datasim_imp,attr(datasim,"metadata")$Condition)
```

`mi4limma` *Title*

Description

Title

Usage

```
mi4limma(qData, sTab, VarRubin, comp.type = "OnevsOne", robust = FALSE)
```

Arguments

`qData`	A matrix of quantitative data, without any missing values.
`sTab`	The data.frame which correspond to the pData function of MSnbase
`VarRubin`	A variance-covariance matrix
`comp.type`	A string that corresponds to the type of comparison. Values are: 'anova1way', 'OnevsOne' and 'OnevsAll'; default is 'OnevsOne'.
`robust`	logical, should the estimation of df.prior and var.prior be robustified against outlier sample variances? (as in limma's eBayes)

Value

A list of two dataframes : logFC and P_Value. The first one contains the logFC values of all the comparisons (one column for one comparison), the second one contains the pvalue of all the comparisons (one column for one comparison). The names of the columns for those two dataframes are identical and correspond to the description of the comparison.

References

M. Chion, Ch. Carapito and F. Bertrand (2021). *Accounting for multiple imputation-induced variability for differential analysis in mass spectrometry-based label-free quantitative proteomics*. arxiv:2108.07086. https://arxiv.org/abs/2108.07086.

Examples

```
set.seed(2016)
data(qData)
data(sTab)
fit.limma <- mi4limma(qData, sTab, diag(1,2))
```

`multi.impute` *Function to impute quantitative datasets*

Description

This function creates an array made of slices of imputed dataset. Imputation methods can be chosen from `c("pmm","midastouch","sample","cart","rf","mean","norm","norm.nob","norm.boot","norm.predict")`.

Usage

```
multi.impute(data, conditions, nb.imp = NULL, method, parallel = FALSE)
```

Arguments

`data`	Dataset to impute.
`conditions`	Vector with the condition values.
`nb.imp`	Number of imputed dataset to create.
`method`	Imputation method, choose from `c("pmm","midastouch","sample","cart","rf","mean","norm","r`
`parallel`	Use parallel computing?

Value

a numeric array of dim c(dim(data),nb.imp).

References

M. Chion, Ch. Carapito and F. Bertrand (2021). *Accounting for multiple imputation-induced variability for differential analysis in mass spectrometry-based label-free quantitative proteomics*. arxiv:2108.07086. https://arxiv.org/abs/2108.07086.

Examples

```
library(mi4p)
data(datasim)
multi.impute(data = datasim[,-1], conditions = attr(datasim,"metadata")$Condition, method = "MLE")
```

MVgen *Amputation of a dataset*

Description

This function is designed to ampute datasets.

Usage

```
MVgen(dataset, prop_NA)
```

Arguments

dataset	dataset to be amputed
prop_NA	desired proportion of missing values in the amputed dataset

Value

A dataset with missing values.

References

M. Chion, Ch. Carapito and F. Bertrand (2021). *Accounting for multiple imputation-induced variability for differential analysis in mass spectrometry-based label-free quantitative proteomics*. arxiv:2108.07086. https://arxiv.org/abs/2108.07086.

Examples

```
library(mi4p)
data(datasim)
datasim_amp <- MVgen(datasim, .2)
sum(is.na(datasim_amp))/prod(dim(datasim_amp))
```

norm.200.m100.sd1.vs.m200.sd1.list *A list of simulated datasets.*

Description

This list of 100 datasets was simulated using the default values of the options of the protdatasim function and the set.seed value set to 4619.

Format

The format is: List of 100 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 99.6 99.9 100.2 99.8 100.4 ... ..$ X2 : num [1:200] 97.4 101.3 100.3 100.2 101.7 ... ..$ X3 : num [1:200] 100.3 100.9 99.1 101.2 100.6 ... ..$ X4 : num [1:200] 99.4 99.2 98.5 99.1 99.5 ... ..$ X5 : num [1:200] 98.5 99.7 100 100.2 100.7 ... ..$ X6 : num [1:200] 200 199 199 200 199 ... ..$ X7 : num [1:200] 200 200 202 199 199 ... ..$ X8 : num [1:200] 202 199 200 199 201 ... ..$ X9 : num [1:200] 200 200 199 201 200 ... ..$ X10 : num [1:200] 200 198 200 201 199 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 100.3 97.6 100.1 99.3 101.1 ... ..$ X2 : num [1:200] 100.4 98.6 99.9 99.7 100.2 ... ..$ X3 : num [1:200] 100.4 101.3 99.1 100.2 100.3 ... ..$ X4 : num [1:200] 98.9 100.5 101 100.5 99.5 ... ..$ X5 : num [1:200] 101.5 99.7 98.1 99.5 100.2 ... ..$ X6 : num [1:200] 201 200 201 201 200 ... ..$ X7 : num [1:200] 200 200 201 200 199 ... ..$ X8 : num [1:200] 198 200 202 199 199 ... ..$ X9 : num [1:200] 200 201 198 200 200 ... ..$ X10 : num [1:200] 200 199 201 199 199 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 101 98.8 101 101.2 100.1 ... ..$ X2 : num [1:200] 101.1 100.6 98.8 100.8 99.9 ... ..$ X3 : num [1:200] 99.6 99.7 100.1 98.7 101.4 ... ..$ X4 : num [1:200] 100.3 100.6 100.1 99.5 97.4 ... ..$ X5 : num [1:200] 100.4 100.1 101 99.1 100.3 ... ..$ X6 : num [1:200] 202 200 200 200 202 ... ..$ X7 : num [1:200] 198 199 201 200 199 ... ..$ X8 : num [1:200] 202 201 200 201 198 ... ..$ X9 : num [1:200] 199 200 200 199 199 ... ..$ X10 : num [1:200] 199 199 201 201 199 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 98.4 98.5 100.5 98.7 101.4 ... ..$ X2 : num [1:200] 98.4 101.2 99.1 100.4 99.3 ... ..$ X3 : num [1:200] 99.8 100.3 98.4 99.6 101 ... ..$ X4 : num [1:200] 98.5 98.8 99.8 100.4 98.7 ... ..$ X5 : num [1:200] 100.9 99.5 100.5 100.5 99.3 ... ..$ X6 : num [1:200] 201 200 200 198 199 ... ..$ X7 : num [1:200] 201 200 201 202 200 ... ..$ X8 : num [1:200] 201 200 200 201 199 ... ..$ X9 : num [1:200] 201 198 201 201 198 ... ..$ X10 : num [1:200] 201 200 199 200 200 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 100.2 100.7 99.6 99.8 100.1 ... ..$ X2 : num [1:200] 100.8 98.7 101.1 101.8 99.9 ... ..$ X3 : num [1:200] 101.5 100.6 100.9 100.3 99.8 ... ..$ X4 : num [1:200] 97.3 99.1 100.2 98.4 98.4 ... ..$ X5 : num [1:200] 101 101 101 100 101 ... ..$ X6 : num [1:200] 201 201 198 200 199 ... ..$ X7 : num [1:200] 198 199 199 201 200 ... ..$ X8 : num [1:200] 199 197 199 199 199 ... ..$ X9 : num [1:200] 201 199 199 199 200 ... ..$ X10 : num [1:200] 201 199 199 200 197 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 98.6 100.7 100.1 99 101 ... ..$ X2 : num [1:200] 99.1 99.9 100.9 99.9 99.8 ... ..$ X3 : num [1:200] 99.4 100.3 100.6 100.7 98.6 ... ..$ X4 : num [1:200] 100 100.3 100.2 98.2 103.7 ... ..$ X5 : num [1:200] 100.7 99.1 100.8 100.4 99.5 ... ..$ X6 : num [1:200] 201 201 199 199 201 ... ..$ X7 : num [1:200] 201 199 202 202 202 ... ..$ X8 : num [1:200] 201 199 199 202 201 ... ..$ X9 : num [1:200] 200 199 200 202 200 ... ..$ X10 : num [1:200] 200 201 200 200 203

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198 ... ..$ X10 : num [1:200] 199 199 198 199 199 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 100.6 100 101.4 99.3 101.9 ... ..$ X2 : num [1:200] 101.4 98.1 101.2 101 99.5 ... ..$ X3 : num [1:200] 99 100.3 100.5 102.7 98.5 ... ..$ X4 : num [1:200] 99.5 99.3 99.4 100.7 100 ... ..$ X5 : num [1:200] 99.7 99.9 100 100.2 98.6 ... ..$ X6 : num [1:200] 199 201 198 201 199 ... ..$ X7 : num [1:200] 203 198 200 200 199 ... ..$ X8 : num [1:200] 200 201 199 201 201 ... ..$ X9 : num [1:200] 200 200 201 202 200 ... ..$ X10 : num [1:200] 200 198 201 201 200 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 101.8 100.4 100.5 99.5 100.8 ... ..$ X2 : num [1:200] 99.9 100.3 101.5 100.2 99.9 ... ..$ X3 : num [1:200] 100.5 98.9 99.5 100.3 101.1 ... ..$ X4 : num [1:200] 99.5 100.5 99.4 101.6 101 ... ..$ X5 : num [1:200] 100.9 100.1 99.2 99.2 99.1 ... ..$ X6 : num [1:200] 202 200 199 201 200 ... ..$ X7 : num [1:200] 199 201 200 198 201 ... ..$ X8 : num [1:200] 198 200 199 200 201 ... ..$ X9 : num [1:200] 202 199 202 200 200 ... ..$ X10 : num [1:200] 199 199 202 198 201 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 99.7 98.6 99.6 101.2 98.5 ... ..$ X2 : num [1:200] 99.9 97.7 100.1 100 99.2 ... ..$ X3 : num [1:200] 100 100 101 101 100 ... ..$ X4 : num [1:200] 100 101.5 99.9 100.9 99 ... ..$ X5 : num [1:200] 99.2 100.4 97.5 99.8 99.6 ... ..$ X6 : num [1:200] 199 199 199 200 199 ... ..$ X7 : num [1:200] 199 199 201 201 199 ... ..$ X8 : num [1:200] 201 199 201 200 200 ... ..$ X9 : num [1:200] 199 201 201 199 199 ... ..$ X10 : num [1:200] 201 200 201 199 199 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 100.3 99 99.8 102.2 100.5 ... ..$ X2 : num [1:200] 101.8 99.8 98.8 100.5 98.8 ... ..$ X3 : num [1:200] 100 101.6 100.9 99.7 98.2 ... ..$ X4 : num [1:200] 100 100.6 100.4 99.9 99.8 ... ..$ X5 : num [1:200] 99.5 100.8 99.3 101.6 99.3 ... ..$ X6 : num [1:200] 200 200 200 201 199 ... ..$ X7 : num [1:200] 200 200 201 200 199 ... ..$ X8 : num [1:200] 200 199 202 199 199 ... ..$ X9 : num [1:200] 201 201 200 200 200 ... ..$ X10 : num [1:200] 198 199 199 200 201 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 100.8 99.4 100.1 99.9 100.6 ... ..$ X2 : num [1:200] 100.2 98.2 99.7 99.8 100.8 ... ..$ X3 : num [1:200] 100 100 101 102 101 ... ..$ X4 : num [1:200] 99.7 99.2 99.9 100.3 100.3 ... ..$ X5 : num [1:200] 100.1 100.7 100 99.1 100.5 ... ..$ X6 : num [1:200] 201 201 198 199 201 ... ..$ X7 : num [1:200] 202 198 200 199 199 ... ..$ X8 : num [1:200] 200 200 199 201 200 ... ..$ X9 : num [1:200] 200 202 200 200 201 ... ..$ X10 : num [1:200] 200 201 200 200 199 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 100.3 99.6 100.6 100.6 99.4 ... ..$ X2 : num [1:200] 99.9 101.3 99.4 100.4 99.5 ... ..$ X3 : num [1:200] 100.1 99.4 100.5 100.5 101 ... ..$ X4 : num [1:200] 99.7 100.9 99.4 100.1 100 ... ..$ X5 : num [1:200] 99.5 100.2 100.9 101.3 100.1 ... ..$ X6 : num [1:200] 199 200 200 201 200 ... ..$ X7 : num [1:200] 200 198 199 199 201 ... ..$

X8 : num [1:200] 201 200 201 199 198 ... ..$ X9 : num [1:200] 202 200 200 200 200 ... ..$ X10 : num [1:200] 200 199 201 201 200 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 99.4 100.2 100.5 99.3 98.9 ... ..$ X2 : num [1:200] 99.7 100.4 101 101.4 101 ... ..$ X3 : num [1:200] 99.8 101.1 99.2 98.8 100.5 ... ..$ X4 : num [1:200] 99.2 99.5 98.7 99 100.5 ... ..$ X5 : num [1:200] 100.4 99.5 100.2 98.8 99.1 ... ..$ X6 : num [1:200] 199 198 198 199 200 ... ..$ X7 : num [1:200] 200 199 199 199 201 ... ..$ X8 : num [1:200] 201 199 200 202 201 ... ..$ X9 : num [1:200] 199 200 200 198 200 ... ..$ X10 : num [1:200] 201 200 199 200 199 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 101 99.4 100.3 99.4 100.6 ... ..$ X2 : num [1:200] 98.6 98.5 100.7 100.5 99.2 ... ..$ X3 : num [1:200] 99.4 98.2 99.8 100 101.8 ... ..$ X4 : num [1:200] 102 101 101 102 101 ... ..$ X5 : num [1:200] 100.7 101.6 99 99.2 98.8 ... ..$ X6 : num [1:200] 199 201 200 200 202 ... ..$ X7 : num [1:200] 200 200 199 198 199 ... ..$ X8 : num [1:200] 201 198 200 201 200 ... ..$ X9 : num [1:200] 200 200 200 200 199 ... ..$ X10 : num [1:200] 200 200 201 200 200 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 101.4 98.5 100.5 99.9 100.7 ... ..$ X2 : num [1:200] 100.4 100.3 98.7 100 99.6 ... ..$ X3 : num [1:200] 99.3 100 99.3 99.2 99.7 ... ..$ X4 : num [1:200] 98.6 100.3 100.4 100.7 99.4 ... ..$ X5 : num [1:200] 100.3 99.9 101.9 100.5 101.3 ... ..$ X6 : num [1:200] 200 199 200 199 200 ... ..$ X7 : num [1:200] 200 202 199 202 199 ... ..$ X8 : num [1:200] 199 201 200 200 200 ... ..$ X9 : num [1:200] 200 200 202 200 201 ... ..$ X10 : num [1:200] 201 201 201 201 200 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 98.7 99.9 101.9 99.4 100.7 ... ..$ X2 : num [1:200] 102.3 100.3 100.2 97.7 100 ... ..$ X3 : num [1:200] 99.7 98.8 100.1 100.1 100.7 ... ..$ X4 : num [1:200] 100 100.3 100.7 100.8 98.9 ... ..$ X5 : num [1:200] 100.2 100.3 99.7 99.5 100.6 ... ..$ X6 : num [1:200] 199 200 199 200 201 ... ..$ X7 : num [1:200] 199 198 200 200 201 ... ..$ X8 : num [1:200] 200 198 201 200 202 ... ..$ X9 : num [1:200] 201 200 201 200 199 ... ..$ X10 : num [1:200] 201 198 200 200 201 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 101.7 100.7 99.3 98 100.2 ... ..$ X2 : num [1:200] 99.2 100.8 99.9 100.3 99.7 ... ..$ X3 : num [1:200] 100.4 102.2 99.5 100.1 100.4 ... ..$ X4 : num [1:200] 97.4 101.6 99.5 100.8 99.7 ... ..$ X5 : num [1:200] 100.3 100.7 101.4 99.8 100.8 ... ..$ X6 : num [1:200] 200 199 201 198 200 ... ..$ X7 : num [1:200] 201 201 202 201 199 ... ..$ X8 : num [1:200] 201 202 200 203 201 ... ..$ X9 : num [1:200] 200 200 200 200 201 ... ..$ X10 : num [1:200] 201 200 201 200 201 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 100.6 100.8 101.2 100.6 99.6 ... ..$ X2 : num [1:200] 100.8 99.8 101.4 100.7 98.9 ... ..$ X3 : num [1:200] 99.9 100.9 99.1 99.8 100.9 ... ..$ X4 : num [1:200] 98.9 100.3 98.7 98.8 97.9 ... ..$ X5 : num [1:200] 101.2

100.5 100.7 98.6 100.1 ... ..$ X6 : num [1:200] 200 200 201 200 200 ... ..$ X7 : num [1:200] 201 199 202 200 200 ... ..$ X8 : num [1:200] 200 199 200 201 199 ... ..$ X9 : num [1:200] 200 201 200 200 203 ... ..$ X10 : num [1:200] 200 201 200 199 200 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 100 99.9 100.1 101.8 100.9 ... ..$ X2 : num [1:200] 99.9 100.9 98.7 100.6 100.2 ... ..$ X3 : num [1:200] 97.4 99.9 99.7 98.2 99.9 ... ..$ X4 : num [1:200] 101 98.5 99.8 100.4 101.5 ... ..$ X5 : num [1:200] 101.3 99.7 99.2 101.2 99.5 ... ..$ X6 : num [1:200] 199 199 199 200 200 ... ..$ X7 : num [1:200] 199 200 202 199 198 ... ..$ X8 : num [1:200] 199 200 201 199 197 ... ..$ X9 : num [1:200] 201 200 198 200 199 ... ..$ X10 : num [1:200] 200 199 200 201 200 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 101.5 99.7 99.7 99.9 100.9 ... ..$ X2 : num [1:200] 100.3 100.8 99.2 99.1 100 ... ..$ X3 : num [1:200] 100.8 98.8 98.7 100.5 99.6 ... ..$ X4 : num [1:200] 101.1 100.1 100.7 99.9 100.5 ... ..$ X5 : num [1:200] 97.4 100.3 100.9 101.6 99.3 ... ..$ X6 : num [1:200] 199 201 198 199 199 ... ..$ X7 : num [1:200] 199 201 200 201 200 ... ..$ X8 : num [1:200] 201 201 199 200 198 ... ..$ X9 : num [1:200] 202 199 199 201 202 ... ..$ X10 : num [1:200] 200 203 201 199 199 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 98.6 99.8 98.7 98.5 99.7 ... ..$ X2 : num [1:200] 102 97.7 99.6 99.2 96.4 ... ..$ X3 : num [1:200] 99.9 101.3 100.1 99.6 99.1 ... ..$ X4 : num [1:200] 98.9 99 99.1 98.6 99.2 ... ..$ X5 : num [1:200] 99.3 99.2 100.2 100.4 100.3 ... ..$ X6 : num [1:200] 202 200 201 201 201 ... ..$ X7 : num [1:200] 201 200 200 199 199 ... ..$ X8 : num [1:200] 200 200 200 200 199 ... ..$ X9 : num [1:200] 201 200 199 200 202 ... ..$ X10 : num [1:200] 201 201 200 200 201 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 99.7 101.3 99.8 100.2 100.2 ... ..$ X2 : num [1:200] 100.3 98.3 99.2 100.6 100.3 ... ..$ X3 : num [1:200] 98.5 97.9 101 98.2 98.7 ... ..$ X4 : num [1:200] 100.2 98.8 100.8 99.6 100.5 ... ..$ X5 : num [1:200] 99.1 98.7 99.5 100.8 99.4 ... ..$ X6 : num [1:200] 201 201 199 201 199 ... ..$ X7 : num [1:200] 201 199 202 200 200 ... ..$ X8 : num [1:200] 200 199 202 200 199 ... ..$ X9 : num [1:200] 200 200 202 201 200 ... ..$ X10 : num [1:200] 199 200 201 200 200 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 99.1 99.6 100.4 101.8 99.3 ... ..$ X2 : num [1:200] 98.9 99.5 100.7 100.4 100.2 ... ..$ X3 : num [1:200] 101.9 99.8 98.6 99.4 101.3 ... ..$ X4 : num [1:200] 100.8 101.9 99.9 101.4 100.2 ... ..$ X5 : num [1:200] 101.6 99.2 99.6 98.9 101.8 ... ..$ X6 : num [1:200] 200 200 200 200 200 ... ..$ X7 : num [1:200] 201 199 200 201 201 ... ..$ X8 : num [1:200] 200 201 199 200 201 ... ..$ X9 : num [1:200] 201 200 200 200 201 ... ..$ X10 : num [1:200] 201 200 202 200 199 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 102 100 101 100 101 ... ..$ X2 : num [1:200] 100.3 100.8 99.7 99.6 101 ... ..$ X3 : num [1:200] 99.7 99.6

101.4 101.9 101 ... ..$ X4 : num [1:200] 100 99.6 99.2 98.6 100.1 ... ..$ X5 : num [1:200] 98.9 100.3 99.8 100.7 98.8 ... ..$ X6 : num [1:200] 200 199 199 201 200 ... ..$ X7 : num [1:200] 199 201 201 199 201 ... ..$ X8 : num [1:200] 199 201 201 201 201 ... ..$ X9 : num [1:200] 200 200 198 199 200 ... ..$ X10 : num [1:200] 199 199 201 200 201 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 100.6 99.2 99.8 99.9 98.6 ... ..$ X2 : num [1:200] 99.6 100.5 100.6 99.6 100.5 ... ..$ X3 : num [1:200] 100.6 100.1 99.5 100.8 99.8 ... ..$ X4 : num [1:200] 101.2 100.1 100.7 99.1 100.4 ... ..$ X5 : num [1:200] 101.4 100.2 100.2 99.9 100.1 ... ..$ X6 : num [1:200] 200 199 200 200 200 ... ..$ X7 : num [1:200] 199 199 201 200 201 ... ..$ X8 : num [1:200] 200 200 200 201 199 ... ..$ X9 : num [1:200] 200 200 201 199 200 ... ..$ X10 : num [1:200] 201 200 201 200 201 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 100.7 101.3 99.1 99.3 98.8 ... ..$ X2 : num [1:200] 101.8 100.8 99.2 100.5 98.9 ... ..$ X3 : num [1:200] 99.2 98.1 100.4 100.2 97.9 ... ..$ X4 : num [1:200] 99.5 99.8 99.8 99.8 99.2 ... ..$ X5 : num [1:200] 99.9 99.8 98.6 98.7 99.1 ... ..$ X6 : num [1:200] 199 198 200 199 200 ... ..$ X7 : num [1:200] 199 200 201 200 199 ... ..$ X8 : num [1:200] 199 200 200 200 200 ... ..$ X9 : num [1:200] 200 200 202 199 199 ... ..$ X10 : num [1:200] 199 198 199 200 201 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 98.8 101.2 100.5 98.1 99.2 ... ..$ X2 : num [1:200] 100.1 99.7 99.7 100 100.6 ... ..$ X3 : num [1:200] 100.7 98.4 100.3 100.1 99.8 ... ..$ X4 : num [1:200] 100.3 99.8 99 99 100 ... ..$ X5 : num [1:200] 99.8 100.8 101.3 100.4 101.6 ... ..$ X6 : num [1:200] 200 200 200 199 200 ... ..$ X7 : num [1:200] 201 199 201 199 200 ... ..$ X8 : num [1:200] 200 198 199 201 199 ... ..$ X9 : num [1:200] 200 200 200 200 200 ... ..$ X10 : num [1:200] 201 201 199 200 202 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 99.4 100.6 99.9 98.2 99.9 ... ..$ X2 : num [1:200] 98.6 97.6 101 100 100.6 ... ..$ X3 : num [1:200] 99.7 98.1 100.9 100.4 99 ... ..$ X4 : num [1:200] 99.1 99 99.7 99.8 100.2 ... ..$ X5 : num [1:200] 99 101.2 99.5 99.1 100.9 ... ..$ X6 : num [1:200] 199 198 201 200 201 ... ..$ X7 : num [1:200] 200 199 200 201 201 ... ..$ X8 : num [1:200] 200 199 200 201 202 ... ..$ X9 : num [1:200] 200 200 202 201 201 ... ..$ X10 : num [1:200] 199 200 199 200 200 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 101.5 98.6 100 101 98.9 ... ..$ X2 : num [1:200] 99.3 99.5 100.9 99.7 99.2 ... ..$ X3 : num [1:200] 101.7 100.1 97.5 99.1 99.5 ... ..$ X4 : num [1:200] 100.5 99.6 99.1 100.3 100.2 ... ..$ X5 : num [1:200] 99.7 99.2 98.9 100.1 99.4 ... ..$ X6 : num [1:200] 199 200 201 200 199 ... ..$ X7 : num [1:200] 201 199 199 201 200 ... ..$ X8 : num [1:200] 199 199 199 200 201 ... ..$ X9 : num [1:200] 201 199 202 199 199 ... ..$ X10 : num [1:200] 199 200 199 199 200 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 99.6 97.8 100.8 101.8 100.3 ... ..$ X2 :

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2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 99 99.1 99.9 98.8 100.4 ... ..$ X2 : num [1:200] 100.4 100 99.5 99.4 100.9 ... ..$ X3 : num [1:200] 100 101.4 100.9 99.8 98.3 ... ..$ X4 : num [1:200] 100.3 98 100.6 100.7 99.7 ... ..$ X5 : num [1:200] 100 100 100 101 100 ... ..$ X6 : num [1:200] 201 199 199 201 199 ... ..$ X7 : num [1:200] 199 200 199 202 200 ... ..$ X8 : num [1:200] 200 202 201 198 201 ... ..$ X9 : num [1:200] 199 200 199 198 199 ... ..$ X10 : num [1:200] 200 201 200 199 198 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 98.4 100.4 99.8 99.1 99.5 ... ..$ X2 : num [1:200] 100.2 100.2 99.9 100.9 100.8 ... ..$ X3 : num [1:200] 99.6 98.9 99.5 98.6 98.1 ... ..$ X4 : num [1:200] 100.6 100.3 99.8 99.1 101.3 ... ..$ X5 : num [1:200] 99.1 101.4 99.2 99 99.7 ... ..$ X6 : num [1:200] 200 199 200 200 200 ... ..$ X7 : num [1:200] 199 201 200 199 200 ... ..$ X8 : num [1:200] 200 201 199 200 201 ... ..$ X9 : num [1:200] 199 199 201 201 199 ... ..$ X10 : num [1:200] 201 201 200 201 201 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 100.3 100.3 98.8 99.4 100.5 ... ..$ X2 : num [1:200] 98.1 99.1 98.8 98 100.8 ... ..$ X3 : num [1:200] 100 101 101 100 101 ... ..$ X4 : num [1:200] 100.1 99.8 100.6 101.6 101.5 ... ..$ X5 : num [1:200] 101.7 99.2 99.7 100.3 100.7 ... ..$ X6 : num [1:200] 200 201 200 200 200 ... ..$ X7 : num [1:200] 199 199 199 200 200 ... ..$ X8 : num [1:200] 200 201 199 200 200 ... ..$ X9 : num [1:200] 200 201 200 201 200 ... ..$ X10 : num [1:200] 198 201 200 200 198 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 99.5 99.7 99.2 100.3 99.7 ... ..$ X2 : num [1:200] 101.3 100.8 99.6 98.6 101 ... ..$ X3 : num [1:200] 100 100 99 101 101 ... ..$ X4 : num [1:200] 100 101.3 100.8 98.9 98.2 ... ..$ X5 : num [1:200] 99.3 100.3 100.3 99.8 99.6 ... ..$ X6 : num [1:200] 199 199 200 201 200 ... ..$ X7 : num [1:200] 200 199 200 200 200 ... ..$ X8 : num [1:200] 199 200 200 201 200 ... ..$ X9 : num [1:200] 198 202 200 200 200 ... ..$ X10 : num [1:200] 202 201 200 201 200 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 98.4 102.3 99 99 101.1 ... ..$ X2 : num [1:200] 99.8 99.4 99.1 101.4 100 ... ..$ X3 : num [1:200] 100.2 99.8 100.2 100.8 98.5 ... ..$ X4 : num [1:200] 97.7 101 99.4 99.6 99.2 ... ..$ X5 : num [1:200] 101 100 101 100 101 ... ..$ X6 : num [1:200] 201 200 199 199 201 ... ..$ X7 : num [1:200] 200 199 201 201 201 ... ..$ X8 : num [1:200] 199 201 202 199 201 ... ..$ X9 : num [1:200] 197 200 199 199 199 ... ..$ X10 : num [1:200] 201 200 200 199 199 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 100.7 98.1 99.3 100.7 99.8 ... ..$ X2 : num [1:200] 99.7 100.6 99.6 99.7 99.6 ... ..$ X3 : num [1:200] 100.8 100.9 100.2 99.6 101.9 ... ..$ X4 : num [1:200] 100.5 100 99.8 98.6 99.5 ... ..$ X5 : num [1:200] 101 100.5 100.5 101.9 99.3 ... ..$ X6 : num [1:200] 201 198 201 198 201 ... ..$ X7 : num [1:200] 200 200 198 199 199 ... ..$ X8 : num [1:200] 199 198 200 199 200 ... ..$ X9 : num [1:200] 200 201 202 200 201 ... ..$ X10 : num [1:200] 198 199 199 200 201 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $

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[1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 99.8 100.7 100.3 99 99.7 ... ..$ X2 : num [1:200] 101.3 100.7 101.6 100.5 99.5 ... ..$ X3 : num [1:200] 98.2 99.3 101.3 100.1 100.6 ... ..$ X4 : num [1:200] 98.9 99.6 98.8 98.9 100.2 ... ..$ X5 : num [1:200] 99.3 99.7 99.8 98.7 99.5 ... ..$ X6 : num [1:200] 199 200 199 200 200 ... ..$ X7 : num [1:200] 200 201 201 199 198 ... ..$ X8 : num [1:200] 199 200 201 199 201 ... ..$ X9 : num [1:200] 200 199 199 201 202 ... ..$ X10 : num [1:200] 202 202 201 198 198 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 99.4 101.6 98.9 101 101.2 ... ..$ X2 : num [1:200] 99.8 99.1 100.4 98.8 100.8 ... ..$ X3 : num [1:200] 100.1 100.3 100.5 99.6 100.4 ... ..$ X4 : num [1:200] 98.4 100.8 99.8 99.2 98.2 ... ..$ X5 : num [1:200] 98.8 100.9 100.6 99.8 101.5 ... ..$ X6 : num [1:200] 199 199 200 199 201 ... ..$ X7 : num [1:200] 198 201 200 198 199 ... ..$ X8 : num [1:200] 198 199 200 202 200 ... ..$ X9 : num [1:200] 199 198 201 200 200 ... ..$ X10 : num [1:200] 201 201 201 199 200 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 98.4 100.3 99.4 100.2 102.2 ... ..$ X2 : num [1:200] 100.8 99.7 99.7 100.6 101.6 ... ..$ X3 : num [1:200] 100.2 100.1 99.5 99.9 100.1 ... ..$ X4 : num [1:200] 99.7 98.9 101 100.9 100.4 ... ..$ X5 : num [1:200] 99.4 101.6 99.7 100.3 100 ... ..$ X6 : num [1:200] 199 200 201 199 200 ... ..$ X7 : num [1:200] 201 200 199 200 200 ... ..$ X8 : num [1:200] 201 200 202 201 199 ... ..$ X9 : num [1:200] 200 201 200 200 201 ... ..$ X10 : num [1:200] 200 200 202 202 199 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 99.6 101.1 101.7 100.2 101.1 ... ..$ X2 : num [1:200] 98.9 101.7 100.1 99.8 101.1 ... ..$ X3 : num [1:200] 99.9 100.6 99.6 100.4 100.1 ... ..$ X4 : num [1:200] 99.8 99.8 98.3 98.8 100.6 ... ..$ X5 : num [1:200] 97.7 99.8 99.1 99.8 98 ... ..$ X6 : num [1:200] 199 199 200 201 201 ... ..$ X7 : num [1:200] 200 200 200 200 200 ... ..$ X8 : num [1:200] 199 200 201 199 200 ... ..$ X9 : num [1:200] 200 201 200 200 199 ... ..$ X10 : num [1:200] 202 200 199 201 200 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 98.6 99.6 100.3 99.3 101 ... ..$ X2 : num [1:200] 101.1 100.3 98.6 99.6 99.1 ... ..$ X3 : num [1:200] 99.4 98.6 100.3 99.7 100.6 ... ..$ X4 : num [1:200] 99.3 100 99.3 99.5 99.4 ... ..$ X5 : num [1:200] 99.4 99.9 98.9 100.6 100.3 ... ..$ X6 : num [1:200] 201 200 201 199 200 ... ..$ X7 : num [1:200] 201 201 199 200 200 ... ..$ X8 : num [1:200] 199 200 200 203 199 ... ..$ X9 : num [1:200] 201 200 199 201 200 ... ..$ X10 : num [1:200] 199 201 200 201 200 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 100.1 99.5 100.1 100.6 100.3 ... ..$ X2 : num [1:200] 99.7 100.8 101 101.4 98.4 ... ..$ X3 : num [1:200] 100.8 98.7 99.6 100.6 101.4 ... ..$ X4 : num [1:200] 101.5 99.4 101.2 99.8 99.2 ... ..$ X5 : num [1:200] 100.5 99.5 97.5 101.6 99.7 ... ..$ X6 : num [1:200] 200 200 201 200 201 ... ..$ X7 : num [1:200] 199 199 200 200 199 ... ..$ X8 : num [1:200] 199 202 200 202 200 ... ..$ X9 : num [1:200] 201 201 200 201 200 ... ..$ X10 : num [1:200] 201

199 200 199 200 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 99.6 99.7 100.5 99.5 99.9 ... ..$ X2 : num [1:200] 100.2 99.6 100.5 100.3 100.7 ... ..$ X3 : num [1:200] 100.1 99.4 98.3 99.2 100.2 ... ..$ X4 : num [1:200] 98.6 101.1 100.9 100.7 100.8 ... ..$ X5 : num [1:200] 101 100 100 100 100 ... ..$ X6 : num [1:200] 200 201 199 199 201 ... ..$ X7 : num [1:200] 201 202 200 199 199 ... ..$ X8 : num [1:200] 199 199 200 202 201 ... ..$ X9 : num [1:200] 199 199 200 200 199 ... ..$ X10 : num [1:200] 200 199 201 201 201 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 100.1 102.9 99.9 99.5 99.9 ... ..$ X2 : num [1:200] 101.5 101.8 99.5 99.2 99 ... ..$ X3 : num [1:200] 99.8 98.6 99.7 100 99.6 ... ..$ X4 : num [1:200] 101.8 101.1 99.2 100 98.5 ... ..$ X5 : num [1:200] 100.5 101.3 101 100.7 97.6 ... ..$ X6 : num [1:200] 198 200 200 199 200 ... ..$ X7 : num [1:200] 201 200 201 199 200 ... ..$ X8 : num [1:200] 198 201 198 200 200 ... ..$ X9 : num [1:200] 200 199 202 201 200 ... ..$ X10 : num [1:200] 200 199 198 200 200 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 100.7 100.2 99.5 101.7 100.4 ... ..$ X2 : num [1:200] 100.3 100.4 101.5 101 99.7 ... ..$ X3 : num [1:200] 100.4 100.1 98.2 101.9 100.5 ... ..$ X4 : num [1:200] 100.6 102.2 101.4 99.6 98.6 ... ..$ X5 : num [1:200] 101 100.6 97.5 99.6 100.9 ... ..$ X6 : num [1:200] 201 200 200 199 201 ... ..$ X7 : num [1:200] 199 200 200 201 200 ... ..$ X8 : num [1:200] 199 200 199 199 200 ... ..$ X9 : num [1:200] 200 199 201 200 199 ... ..$ X10 : num [1:200] 199 200 201 199 201 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 101 98.7 99.4 101.7 101.3 ... ..$ X2 : num [1:200] 99.3 100.7 98.5 100.9 101.7 ... ..$ X3 : num [1:200] 98.9 97.9 100.5 101 99.6 ... ..$ X4 : num [1:200] 98.9 100.4 99 99.9 100.8 ... ..$ X5 : num [1:200] 100.7 101.2 101.1 98.6 99.6 ... ..$ X6 : num [1:200] 202 198 199 199 200 ... ..$ X7 : num [1:200] 199 201 200 199 200 ... ..$ X8 : num [1:200] 200 200 200 199 200 ... ..$ X9 : num [1:200] 201 199 201 199 200 ... ..$ X10 : num [1:200] 201 199 199 200 199 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 101.4 100.1 100.5 99.9 98.9 ... ..$ X2 : num [1:200] 100 99.4 100.3 99.4 98.3 ... ..$ X3 : num [1:200] 100.1 101.1 99.7 99.9 98.9 ... ..$ X4 : num [1:200] 100.2 100.9 99.8 100 99.6 ... ..$ X5 : num [1:200] 98.5 99.5 99.5 98.9 99.9 ... ..$ X6 : num [1:200] 197 200 199 201 198 ... ..$ X7 : num [1:200] 199 200 200 198 200 ... ..$ X8 : num [1:200] 200 200 198 200 201 ... ..$ X9 : num [1:200] 200 200 200 199 200 ... ..$ X10 : num [1:200] 200 200 201 201 199 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 101.9 99.4 99.8 99.2 99.9 ... ..$ X2 : num [1:200] 101.9 98.2 99.6 99.7 101 ... ..$ X3 : num [1:200] 99.5 100.4 101.1 99 100 ... ..$ X4 : num [1:200] 100.6 99.5 100.5 99.9 98.6 ... ..$ X5 : num [1:200] 101.2 100 99.1 101.1 100.6 ... ..$ X6 : num [1:200] 201 197 199 199 199 ... ..$ X7 : num [1:200] 199 200 201 201 200 ... ..$ X8 : num [1:200] 200 200 199 199 200

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X4 : num [1:200] 98.9 100.2 100.7 99.8 100.8 ... ..$ X5 : num [1:200] 100 100 101 100 101 ... ..$ X6 : num [1:200] 200 201 202 199 200 ... ..$ X7 : num [1:200] 200 202 202 198 201 ... ..$ X8 : num [1:200] 200 201 200 198 199 ... ..$ X9 : num [1:200] 197 200 200 201 199 ... ..$ X10 : num [1:200] 199 198 199 198 200 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 100.5 100.3 98.4 100.1 100.8 ... ..$ X2 : num [1:200] 100.6 100.3 99.3 99.4 98.6 ... ..$ X3 : num [1:200] 98.9 99.8 98.9 100.1 98.6 ... ..$ X4 : num [1:200] 100.2 100.2 101 99.9 100.6 ... ..$ X5 : num [1:200] 98.2 99.6 99.6 99.7 100 ... ..$ X6 : num [1:200] 201 199 200 200 200 ... ..$ X7 : num [1:200] 200 201 200 200 200 ... ..$ X8 : num [1:200] 200 200 202 200 201 ... ..$ X9 : num [1:200] 200 202 199 200 201 ... ..$ X10 : num [1:200] 202 201 201 201 199 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 99.6 99.4 100.5 100.1 100.1 ... ..$ X2 : num [1:200] 100.2 101 98.9 99.9 101.1 ... ..$ X3 : num [1:200] 100 100 101 102 100 ... ..$ X4 : num [1:200] 98.7 99.8 98.8 100 102 ... ..$ X5 : num [1:200] 98.4 100.3 100.9 100.7 99.3 ... ..$ X6 : num [1:200] 199 201 200 200 200 ... ..$ X7 : num [1:200] 200 199 201 202 201 ... ..$ X8 : num [1:200] 198 199 200 199 201 ... ..$ X9 : num [1:200] 199 200 202 199 200 ... ..$ X10 : num [1:200] 200 201 199 200 198 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 100.5 100.5 99 99.3 101.8 ... ..$ X2 : num [1:200] 100 100 101 100 101 ... ..$ X3 : num [1:200] 99 101.6 101 99.7 100.9 ... ..$ X4 : num [1:200] 100.4 99.8 100.1 96.9 100.1 ... ..$ X5 : num [1:200] 99.7 99.8 100 99.8 99.2 ... ..$ X6 : num [1:200] 201 201 199 201 200 ... ..$ X7 : num [1:200] 199 201 201 200 200 ... ..$ X8 : num [1:200] 200 199 199 199 200 ... ..$ X9 : num [1:200] 202 200 199 200 199 ... ..$ X10 : num [1:200] 198 198 198 198 199 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 101.2 99.8 99.9 99.9 100.5 ... ..$ X2 : num [1:200] 101.1 99.6 99.4 100.7 100.7 ... ..$ X3 : num [1:200] 101.1 100.2 100.7 98.3 99.3 ... ..$ X4 : num [1:200] 100.9 100.7 100.3 100 99.5 ... ..$ X5 : num [1:200] 101.9 99.1 97.1 100.4 99 ... ..$ X6 : num [1:200] 200 201 200 201 201 ... ..$ X7 : num [1:200] 200 201 200 198 201 ... ..$ X8 : num [1:200] 201 199 200 199 200 ... ..$ X9 : num [1:200] 201 200 199 201 200 ... ..$ X10 : num [1:200] 199 200 201 201 200 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 100.6 98.6 101.3 99.6 101.2 ... ..$ X2 : num [1:200] 99.8 98.6 98.5 100.2 100.1 ... ..$ X3 : num [1:200] 99.4 100.8 100.7 101.4 98.9 ... ..$ X4 : num [1:200] 100.8 99.4 100.7 98.6 99.7 ... ..$ X5 : num [1:200] 100.4 101.1 99.5 100.8 100.2 ... ..$ X6 : num [1:200] 201 199 201 198 200 ... ..$ X7 : num [1:200] 201 199 200 200 198 ... ..$ X8 : num [1:200] 199 199 199 199 201 ... ..$ X9 : num [1:200] 201 199 199 202 200 ... ..$ X10 : num [1:200] 201 200 200 201 201 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 100.2 100.4 99.8 100.4 99.6 ... ..$ X2 : num [1:200] 98 100.1 99.5

99.6 99.7 ... ..$ X3 : num [1:200] 100.9 100.1 99.7 100.2 98.8 ... ..$ X4 : num [1:200] 97.5 100.3 100.6 99.7 100.5 ... ..$ X5 : num [1:200] 101 101 101 100 102 ... ..$ X6 : num [1:200] 202 199 199 200 201 ... ..$ X7 : num [1:200] 201 203 200 199 199 ... ..$ X8 : num [1:200] 199 199 199 201 199 ... ..$ X9 : num [1:200] 200 199 200 199 201 ... ..$ X10 : num [1:200] 199 199 201 199 201 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 101 100.2 99.5 99.9 101.3 ... ..$ X2 : num [1:200] 100.2 100.5 99.4 100.2 100.6 ... ..$ X3 : num [1:200] 99.8 100.1 99.4 100.4 100.1 ... ..$ X4 : num [1:200] 99.1 99 99.1 100.9 100.4 ... ..$ X5 : num [1:200] 99 99.9 98.9 100.3 99.4 ... ..$ X6 : num [1:200] 200 201 198 200 200 ... ..$ X7 : num [1:200] 199 200 201 199 201 ... ..$ X8 : num [1:200] 200 199 201 200 200 ... ..$ X9 : num [1:200] 201 201 200 201 199 ... ..$ X10 : num [1:200] 200 201 199 201 201 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 101 99.8 98.7 99.8 99.2 ... ..$ X2 : num [1:200] 100.4 100.3 99.8 100.3 99.5 ... ..$ X3 : num [1:200] 98.9 100.4 98.6 99.5 100.2 ... ..$ X4 : num [1:200] 100.4 100.7 100 99.8 100.2 ... ..$ X5 : num [1:200] 100.2 99.9 99.7 99.3 100.6 ... ..$ X6 : num [1:200] 200 200 201 200 198 ... ..$ X7 : num [1:200] 201 201 197 199 199 ... ..$ X8 : num [1:200] 200 201 199 200 199 ... ..$ X9 : num [1:200] 199 198 200 200 199 ... ..$ X10 : num [1:200] 200 201 199 200 202 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 100.8 100.2 101.2 99.4 98.9 ... ..$ X2 : num [1:200] 99.4 99.5 98.8 100.5 100.4 ... ..$ X3 : num [1:200] 98.9 99.7 99.7 99.2 101 ... ..$ X4 : num [1:200] 100.6 98.9 99.6 100.3 101 ... ..$ X5 : num [1:200] 102.2 99.6 99.7 100.2 101 ... ..$ X6 : num [1:200] 200 200 200 201 199 ... ..$ X7 : num [1:200] 199 200 199 200 200 ... ..$ X8 : num [1:200] 199 201 200 200 200 ... ..$ X9 : num [1:200] 202 198 199 200 200 ... ..$ X10 : num [1:200] 201 200 200 201 202 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 $:'data.frame': 200 obs. of 11 variables: ..$ id.obs: int [1:200] 1 2 3 4 5 6 7 8 9 10 ... ..$ X1 : num [1:200] 100.3 98.1 100.4 100.6 99.7 ... ..$ X2 : num [1:200] 100.8 99.3 100 97.5 99.8 ... ..$ X3 : num [1:200] 101.1 97.9 99.4 102 101.1 ... ..$ X4 : num [1:200] 98.2 98.9 100.9 101.8 100.8 ... ..$ X5 : num [1:200] 100.4 98.3 102 98.5 98.8 ... ..$ X6 : num [1:200] 200 200 202 200 199 ... ..$ X7 : num [1:200] 199 201 201 198 200 ... ..$ X8 : num [1:200] 201 200 200 202 200 ... ..$ X9 : num [1:200] 202 199 201 199 200 ... ..$ X10 : num [1:200] 199 198 200 202 198 ... ..- attr(*, "metadata")='data.frame': 10 obs. of 3 variables: .. ..$ Sample.name: chr [1:10] "X1" "X2" "X3" "X4" ... .$ Condition : Factor w/ 2 levels "A","B": 1 1 1 1 1 2 2 2 2 2 .. ..$ Bio.Rep : int [1:10] 1 2 3 4 5 6 7 8 9 10 [list output truncated]

Author(s)

M. Chion, Ch. Carapito and F. Bertrand.

Source

We simulated the data.

References

M. Chion, Ch. Carapito and F. Bertrand (2021). *Accounting for multiple imputation-induced variability for differential analysis in mass spectrometry-based label-free quantitative proteomics*. arxiv:2108.07086. https://arxiv.org/abs/2108.07086.

Examples

```
data(norm.200.m100.sd1.vs.m200.sd1.list)
str(norm.200.m100.sd1.vs.m200.sd1.list)
```

---

proj_matrix *Variance-Covariance Matrix Projection*

Description

Use a projection of the given variance-covariance matrix.

Usage

```
proj_matrix(VarRubin.matrix, metadata)
```

Arguments

VarRubin.matrix	A variance-covariance matrix.
metadata	Metadata of the experiment.

Value

A list of variance-covariance matrices.

References

M. Chion, Ch. Carapito and F. Bertrand (2021). *Accounting for multiple imputation-induced variability for differential analysis in mass spectrometry-based label-free quantitative proteomics*. arxiv:2108.07086. https://arxiv.org/abs/2108.07086.

Examples

```
library(mi4p)
data(datasim)
datasim_imp <- multi.impute(data = datasim[,-1], conditions =
attr(datasim,"metadata")$Condition, method = "MLE")
VarRubin.matrix <- rubin2.all(datasim_imp[1:5,,],
attr(datasim,"metadata")$Condition)
proj_matrix(VarRubin.matrix, attr(datasim,"metadata"))
```

`protdatasim` *Data simulation function*

Description

Function to simulate benchmark datasets.

Usage

```
protdatasim(
  iii = 1,
  nobs = 200,
  nobs1 = 10,
  ng1 = 5,
  ng2 = 5,
  mg1 = 100,
  mg2 = 200,
  dispg1 = 1,
  dispg2 = 1
)
```

Arguments

`iii`	A parameter useful to loop over for simulated lists of datasets. It has no effect.
`nobs`	Number of peptides
`nobs1`	Number of peptides with differential expressions between the two conditions
`ng1`	Number of biological replicates in condition A
`ng2`	Number of biological replicates in condition B
`mg1`	Mean in condition A
`mg2`	Mean in condition B
`dispg1`	Dispersion in condition A
`dispg2`	Dispersion in condition B

Value

A data frame with the simulated and attribute metadata.

References

M. Chion, Ch. Carapito and F. Bertrand (2021). *Accounting for multiple imputation-induced variability for differential analysis in mass spectrometry-based label-free quantitative proteomics*. arxiv:2108.07086. https://arxiv.org/abs/2108.07086.

Examples

```
data_sim <- protdatasim()
attr(data_sim,"metadata")

norm.200.m100.sd1.vs.m200.sd1_list <- lapply(1:100, protdatasim)
attr(norm.200.m100.sd1.vs.m200.sd1_list[[1]],"metadata")
```

---

qData — *Extract of the abundances of Exp1_R25_pept dataset*

Description

The data frame `qData` contains the first 500 rows of six columns that are the quantitation of peptides for the six replicates. They were obtained using the code `exprs(Exp1_R25_pept)[1:500,]`.

Format

The format is: num [1:500, 1:6] 24.8 24.7 24.6 NA 24.5 ... - attr(*, "dimnames")=List of 2 ..$: chr [1:500] "0" "1" "2" "3" ... ..$: chr [1:6] "Intensity_C_R1" "Intensity_C_R2" "Intensity_C_R3" "Intensity_D_R1" ...

Details

The `DAPARdata`'s `Exp1_R25_pept` dataset is the final outcome of a quantitative mass spectrometry-based proteomic analysis of two samples containing different concentrations of 48 human proteins (UPS1 standard from Sigma-Aldrich) within a constant yeast background (see Giai Gianetto et al. (2016) for details). It contains the abundance values of the different human and yeast peptides identified and quantified in these two conditions. The two conditions represent the measured abundances of peptides when respectively 25 fmol and 10 fmol of UPS1 human proteins were mixed with the yeast extract before mass spectrometry analyses. This results in a concentration ratio of 2.5. Three technical replicates were acquired for each condition.

Source

The `DAPARdata` package.

References

Cox J., Hein M.Y., Luber C.A., Paron I., Nagaraj N., Mann M. Accurate proteome-wide label-free quantification by delayed normalization and maximal peptide ratio extraction, termed MaxLFQ. Mol Cell Proteomics. 2014 Sep, 13(9):2513-26.

Giai Gianetto, Q., Combes, F., Ramus, C., Bruley, C., Coute, Y., Burger, T. (2016). Calibration plot for proteomics: A graphical tool to visually check the assumptions underlying FDR control in quantitative experiments. Proteomics, 16(1), 29-32.

Examples

```
data(qData)
str(qData)
pairs(qData)
```

rubin1.all *First Rubin rule (all peptide)*

Description

Computes the first Rubin's rule for all the peptide.

Usage

```
rubin1.all(
  data,
  metacond,
  funcmean = meanImp_emmeans,
  is.parallel = FALSE,
  verbose = FALSE
)
```

Arguments

`data`	dataset
`metacond`	a factor to specify the groups
`funcmean`	function that should be used to compute the mean
`is.parallel`	should parallel computing be used?
`verbose`	should messages be displayed?

Value

A vector of estimated parameters.

References

M. Chion, Ch. Carapito and F. Bertrand (2021). *Accounting for multiple imputation-induced variability for differential analysis in mass spectrometry-based label-free quantitative proteomics*. arxiv:2108.07086. https://arxiv.org/abs/2108.07086.

Examples

```
library(mi4p)
data(datasim)
datasim_imp <- multi.impute(data = datasim[,-1], conditions =
attr(datasim,"metadata")$Condition, method = "MLE")
rubin1.all(datasim_imp[1:5,,],funcmean = meanImp_emmeans,
attr(datasim,"metadata")$Condition)
```

`rubin1.one` *First Rubin rule (a given peptide)*

Description

Computes the first Rubin's rule for a given peptide.

Usage

```
rubin1.one(peptide, data, funcmean = meanImp_emmeans, metacond)
```

Arguments

`peptide`	peptide for which the variance-covariance matrix should be derived.
`data`	dataset
`funcmean`	function that should be used to compute the mean
`metacond`	a factor to specify the groups

Value

A vector of estimated parameters.

References

M. Chion, Ch. Carapito and F. Bertrand (2021). *Accounting for multiple imputation-induced variability for differential analysis in mass spectrometry-based label-free quantitative proteomics*. arxiv:2108.07086. https://arxiv.org/abs/2108.07086.

Examples

```
library(mi4p)
data(datasim)
datasim_imp <- multi.impute(data = datasim[,-1], conditions =
attr(datasim,"metadata")$Condition, method = "MLE")
rubin1.one(1,datasim_imp,funcmean = meanImp_emmeans,
attr(datasim,"metadata")$Condition)
```

rubin2.all — *Computes the 2nd Rubin's rule (all peptides)*

Description

Computes the total variance-covariance component in the 2nd Rubin's rule for all peptides.

Usage

```
rubin2.all(
  data,
  metacond,
  funcmean = meanImp_emmeans,
  funcvar = within_variance_comp_emmeans,
  is.parallel = FALSE,
  verbose = FALSE
)
```

Arguments

`data`	dataset
`metacond`	a factor to specify the groups
`funcmean`	function that should be used to compute the mean
`funcvar`	function that should be used to compute the variance
`is.parallel`	should parallel computing be used?
`verbose`	should messages be displayed?

Value

List of variance-covariance matrices.

References

M. Chion, Ch. Carapito and F. Bertrand (2021). *Accounting for multiple imputation-induced variability for differential analysis in mass spectrometry-based label-free quantitative proteomics*. arxiv:2108.07086. https://arxiv.org/abs/2108.07086.

Examples

```
library(mi4p)
data(datasim)
datasim_imp <- multi.impute(data = datasim[,-1], conditions =
attr(datasim,"metadata")$Condition, method = "MLE")
rubin2.all(datasim_imp[1:5,,],attr(datasim,"metadata")$Condition)
```

`rubin2bt.all` *2nd Rubin's rule Between-Imputation component (all peptides)*

Description

Computes the between-imputation component in the 2nd Rubin's rule for all peptides.

Usage

```
rubin2bt.all(
  data,
  funcmean = meanImp_emmeans,
  metacond,
  is.parallel = FALSE,
  verbose = FALSE
)
```

Arguments

`data`	dataset
`funcmean`	function that should be used to compute the mean
`metacond`	a factor to specify the groups
`is.parallel`	should parallel computing be used?
`verbose`	should messages be displayed?

Value

List of variance-covariance matrices.

References

M. Chion, Ch. Carapito and F. Bertrand (2021). *Accounting for multiple imputation-induced variability for differential analysis in mass spectrometry-based label-free quantitative proteomics*. arxiv:2108.07086. https://arxiv.org/abs/2108.07086.

Examples

```
library(mi4p)
data(datasim)
datasim_imp <- multi.impute(data = datasim[,-1], conditions =
attr(datasim,"metadata")$Condition, method = "MLE")
rubin2bt.all(datasim_imp[1:5,,],funcmean = meanImp_emmeans,
attr(datasim,"metadata")$Condition)
```

`rubin2bt.one` *2nd Rubin's rule Between-Imputation Component (a given peptide)*

Description

Computes the between-imputation component in the 2nd Rubin's rule for a given peptide.

Usage

```
rubin2bt.one(peptide, data, funcmean, metacond)
```

Arguments

`peptide`	peptide for which the variance-covariance matrix should be derived.
`data`	dataset
`funcmean`	function that should be used to compute the mean
`metacond`	a factor to specify the groups

Value

A variance-covariance matrix.

References

M. Chion, Ch. Carapito and F. Bertrand (2021). *Accounting for multiple imputation-induced variability for differential analysis in mass spectrometry-based label-free quantitative proteomics*. arxiv:2108.07086. https://arxiv.org/abs/2108.07086.

Examples

```
library(mi4p)
data(datasim)
datasim_imp <- multi.impute(data = datasim[,-1], conditions =
attr(datasim,"metadata")$Condition, method = "MLE")
rubin2bt.one(1,datasim_imp,funcmean = meanImp_emmeans,
attr(datasim,"metadata")$Condition)
```

`rubin2wt.all` *2nd Rubin's rule Within-Variance Component (all peptides)*

Description

Computes the within-variance component in the 2nd Rubin's rule for all peptides.

Usage

```
rubin2wt.all(
  data,
  funcvar = mi4p::within_variance_comp_emmeans,
  metacond,
  is.parallel = FALSE,
  verbose = TRUE
)
```

Arguments

`data`	dataset
`funcvar`	function that should be used to compute the variance
`metacond`	a factor to specify the groups
`is.parallel`	should parallel computing be used?
`verbose`	should messages be displayed?

Value

List of variance-covariance matrices.

References

M. Chion, Ch. Carapito and F. Bertrand (2021). *Accounting for multiple imputation-induced variability for differential analysis in mass spectrometry-based label-free quantitative proteomics*. arxiv:2108.07086. https://arxiv.org/abs/2108.07086.

Examples

```
library(mi4p)
data(datasim)
datasim_imp <- multi.impute(data = datasim[,-1],
conditions = attr(datasim,"metadata")$Condition, method = "MLE")
rubin2wt.all(datasim_imp[1:5,,],funcvar = within_variance_comp_emmeans,
attr(datasim,"metadata")$Condition)
```

rubin2wt.one *2nd Rubin's rule Within-Variance Component (a given peptide)*

Description

Computes the within-variance component in the 2nd Rubin's rule for a given peptide.

Usage

```
rubin2wt.one(peptide, data, funcvar, metacond)
```

Arguments

`peptide`	peptide for which the variance-covariance matrix should be derived.
`data`	dataset
`funcvar`	function that should be used to compute the variance
`metacond`	a factor to specify the groups

Value

A variance-covariance matrix.

References

M. Chion, Ch. Carapito and F. Bertrand (2021). *Accounting for multiple imputation-induced variability for differential analysis in mass spectrometry-based label-free quantitative proteomics*. arxiv:2108.07086. https://arxiv.org/abs/2108.07086.

Examples

```
library(mi4p)
data(datasim)
datasim_imp <- multi.impute(data = datasim[,-1], conditions =
attr(datasim,"metadata")$Condition, method = "MLE")
rubin2wt.one(1,datasim_imp,funcvar=within_variance_comp_emmeans,
attr(datasim,"metadata")$Condition)
```

sTab *Experimental design for the Exp1_R25_pept dataset*

Description

The data frame `sTab` contains the experimental design and gives few informations about the samples. They were obtained using the code `pData(Exp1_R25_pept)`.

Format

A data frame with 6 observations on the following 3 variables.

Sample.name a character vector

Condition a character vector

Bio.Rep a numeric vector

Details

The `DAPARdata`'s `Exp1_R25_pept` dataset is the final outcome of a quantitative mass spectrometry-based proteomic analysis of two samples containing different concentrations of 48 human proteins (UPS1 standard from Sigma-Aldrich) within a constant yeast background (see Giai Gianetto et al. (2016) for details). It contains the abundance values of the different human and yeast peptides identified and quantified in these two conditions. The two conditions represent the measured abundances of peptides when respectively 25 fmol and 10 fmol of UPS1 human proteins were mixed with the yeast extract before mass spectrometry analyses. This results in a concentration ratio of 2.5. Three technical replicates were acquired for each condition.

Source

The `DAPARdata` package.

References

Cox J., Hein M.Y., Luber C.A., Paron I., Nagaraj N., Mann M. Accurate proteome-wide label-free quantification by delayed normalization and maximal peptide ratio extraction, termed MaxLFQ. Mol Cell Proteomics. 2014 Sep, 13(9):2513-26.

Giai Gianetto, Q., Combes, F., Ramus, C., Bruley, C., Coute, Y., Burger, T. (2016). Calibration plot for proteomics: A graphical tool to visually check the assumptions underlying FDR control in quantitative experiments. Proteomics, 16(1), 29-32.

Examples

```
data(sTab)
str(sTab)
```

within_variance_comp_emmeans

Multiple Imputation Within Variance Component

Description

Computes the multiple imputation within variance component using the emmeans package.

Usage

```
within_variance_comp_emmeans(ind, peptide, data, metacond)
```

Arguments

ind	index
peptide	name of the peptide
data	dataset
metacond	a factor to specify the groups

Value

A variance-covariance matrix.

References

M. Chion, Ch. Carapito and F. Bertrand (2021). *Accounting for multiple imputation-induced variability for differential analysis in mass spectrometry-based label-free quantitative proteomics*. arxiv:2108.07086. https://arxiv.org/abs/2108.07086.

Examples

```
library(mi4p)
data(datasim)
datasim_imp <- multi.impute(data = datasim[,-1], conditions =
attr(datasim,"metadata")$Condition, method = "MLE")
within_variance_comp_emmeans(1,1,datasim_imp,
attr(datasim,"metadata")$Condition)
```

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