# Package 'mcr'

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Title Method Comparison Regression

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**Depends** R (>= 3.0.0), methods

Suggests RUnit, XML

Description This package provides regression methods to quantify the relation between two measurement methods. In particular it addresses regression problems with errors in both variables and without repeated measurements. The package provides implementations of Deming regression, weighted Deming regression, and Passing-Bablok regression following the CLSI EP09-A3 recommendations for analytical method comparison and bias estimation using patient samples.

**License** GPL (>= 3)

Collate ``mcrMisc.r" ``mcLinReg.r" ``mcDeming.r" ``mcWDeming.r"

``mcPaBaLarge.r" ``mcPaBa.r" ``mcCalcCI.r" ``mcCalcTstar.r"

``mcBootstrap.r" ``MCResultMethods.r" ``MCResult.r"

 $``MCResultAnalyticalMethods.r"\ ``MCResultAnalytical.r"$ 

``MCResultJackknifeMethods.r" ``MCResultJackknife.r"

``MCResultResamplingMethods.r" ``MCResultResampling.r"

``MCResultBCaMethods.r" ``MCResultBCa.r" ``mcrInterface.r"

``mcrCompareFit.r" ``mcrIncludeLegend.r" ``zzz.r"

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# Description

mcr-package

Method Comparison Regression. This package provides regression methods to quantify the relation between two measurement methods. In particular it addresses regression problems with errors in both variables and without repeated measurements. The package provides implementations of Deming regression, weighted Deming regression, and Passing-Bablok regression following the CLSI EP09-A3 recommendations for analytical method comparison and bias estimation using patient samples.

Method Comparison Regression

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# **Details**

The main function for performing regression analysis is mcreg. Various functions for summarizing and plotting regression results are provided (see examples in mcreg).

For user site testing (installation verification) please use the test case suite provided with the package. The test case suite can be run by sourcing the 'runalltests.R' script in the 'unitTests' folder. It requires the XML and Runit packages.

calcDiff 5

Package: mcr
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### Author(s)

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#### References

CLSI EP09-A3 http://www.clsi.org

calcDiff Calculate difference between two numeric vectors that gives exactly zero for very small relative differences.

# Description

Calculate difference between two numeric vectors that gives exactly zero for very small relative differences.

### Usage

```
calcDiff(X, Y, EPS = 1e-12)
```

### Arguments

X first number
Y second number

EPS relative difference equivalent to zero

#### Value

difference

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compareFit

Graphical Comparison of Regression Parameters and Associated Confidence Intervals

#### **Description**

Graphical comparison of regression parameters (intercept and slope) and their associated 100(1-alpha)% confidence intervals for multiple fitted models of 'MCResult' sub-classes.

#### Usage

```
compareFit(...)
```

### **Arguments**

.. list of fitted models, i.e. objects of "MCResult" sub-classes.

#### **Examples**

```
library("mcr")
    data("creatinine", package="mcr")
    fit.lr <- mcreg(as.matrix(creatinine), method.reg="LinReg", na.rm=TRUE)
    fit.wlr <- mcreg(as.matrix(creatinine), method.reg="WLinReg", na.rm=TRUE)
    compareFit( fit.lr, fit.wlr )</pre>
```

creatinine

Comparison of blood and serum creatinine measurement

# Description

This data set gives the blood and serum preoperative creatinine measurements in 110 heart surgery patients.

### Usage

creatinine

#### **Format**

A data frame containing 110 observations with serum and plasma creatinin measurements in mg/dL for each sample.

includeLegend 7

# Description

Include legend in regression plot (function plot()) or in bias plot (function plotBias ()) with two or more lines.

#### Usage

```
includeLegend(models = list(), digits = 2, design = paste(1:2),
  place = c("topleft", "topright", "bottomleft", "bottomright"), colors,
  lty = rep(1, length(models)), lwd = rep(2, length(models)),
  box.lty = "blank", cex = 0.8, bg = "white", inset = c(0.01, 0.01),
  bias = FALSE, model.names = NULL, ...)
```

### **Arguments**

models	list of length n with Objects of class "MCResult".
digits	number of digits in Coefficients.
design	type of legend design. There are two possible designs: "1" and "2" (See example).
place	place for Legend: "topleft", "topright", "bottomleft" or "bottomright".
colors	vector of length n with color of regression lines.
lty	vector of length n with type of regression lines.
lwd	vector of length n with thickness of regression lines.
box.lty	box line-type
cex	numeric value representing the plotting symbol magnification factor
bg	the background-color of the legend box
inset	inset distance(s) from the margins as a fraction of the plot region when legend is placed by keyword.
bias	logical value. If bias = TRUE, it will be drawn a legend for $plotBias()$ function.
model.names	legend names for different models. If NULL the regression type will be used.
	other parameters of function legend().

### Value

Legend in plot.

#### See Also

```
\verb"plot.mcr", \verb"plotBias", \verb"plotResiduals", \verb"plotDifference", \verb"compareFit"
```

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#### **Examples**

```
#library("mcr")
data(creatinine,package="mcr")
x <- creatinine$serum.crea
y <- creatinine$plasma.crea
m1 <- mcreg(x,y,method.reg="Deming", mref.name="serum.crea",</pre>
                                         mtest.name="plasma.crea", na.rm=TRUE)
m2 <- mcreg(x,y,method.reg="WDeming", method.ci="jackknife",</pre>
                                          mref.name="serum.crea"
                                          mtest.name="plasma.crea", na.rm=TRUE)
plot(m1, XLIM=c(0.5,3), YLIM=c(0.5,3), Legend=FALSE,
                          Title="Deming vs. weighted Deming regression",
                          Points.pch=19,ci.area=TRUE, ci.area.col=grey(0.9),
                          identity=FALSE, Grid=FALSE, Sub="")
plot(m2, ci.area=FALSE, ci.border=TRUE, ci.border.col="red3",
                          reg.col="red3", Legend=FALSE, add=TRUE,
                          Points=FALSE, identity=FALSE, Grid=FALSE)
 includeLegend(place="topleft", models=list(m1, m2),
                          colors=c("darkblue", "red"), design="1", digits=2)
```

mc.analytical.ci

Analytical Confidence Interval

### Description

Calculate wald confidence intervals for intercept and slope given point estimates and standard errors.

#### Usage

```
mc.analytical.ci(b0, b1, se.b0, se.b1, n, alpha)
```

### Arguments

b0	point estimate of intercept.
b1	point estimate of slope.
se.b0	standard error of intercept.
se.b1	standard error of slope.
n	number of observations.
alpha	numeric value specifying the 100(1-alpha)% confidence level for the confidence interval (Default is 0.05).

#### Value

2x4 matrix of estimates and confidence intervals for intercept and slope.

mc.bootstrap 9

mc.bootstrap	Resampling estimation of regression parameters and standard errors.

# Description

Generate jackknife or (nested-) bootstrap replicates of a statistic applied to data. Only a nonparametric ballanced design is possible. For each sample calculate point estimations and standard errors for regression coefficients.

# Usage

```
mc.bootstrap(method.reg = c("LinReg", "WLinReg", "Deming", "WDeming", "PaBa",
   "PaBaLarge"), X, Y, error.ratio, nsamples = 1000, jackknife = TRUE,
   bootstrap = c("none", "bootstrap", "nestedbootstrap"), nnested = 25,
   iter.max = 30, threshold = 1e-08, NBins = 1e+06,
   slope.measure = c("radian", "tangent"))
```

# Arguments

Χ	Measurement values of reference method
Υ	Measurement values of test method
error.ratio	Ratio between squared measurement errors of reference- and test method, necessary for Deming regression. Default 1.
method.reg	Regression method. It is possible to choose between five regression types: "LinReg" - ordinary least square regression, "WLinReg" - weighted ordinary least square regression, "Deming" - Deming regression, "WDeming" - weighted Deming regression, "PaBa" - Passing-Bablok regression.
bootstrap	Bootstrap based confidence interval estimation method.
jackknife	Logical value. If TRUE - Jackknife based confidence interval estimation method.
nsamples	Number of bootstrap samples.
nnested	Number of nested bootstrap samples.
iter.max	maximum number of iterations for weighted Deming iterative algorithm.
threshold	Numerical tolerance for weighted Deming iterative algorithm convergence.
NBins	number of bins used when 'reg.method="PaBaLarge"' to classify each slope in one of 'NBins' bins of constant slope angle covering the range of all slopes.
slope.measure	angular measure of pairwise slopes used for exact PaBa regression (see mcreg for details).  "radian" - for data sets with even sample numbers median slope is calculated as average of two central slope angles.  "tangent" - for data sets with even sample numbers median slope is calculated as average of two central slopes (tan(angle)).

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# Value

glob.coef	Numeric vector of length two with global point estimations of intercept and slope.
glob.sigma	Numeric vector of length two with global estimations of standard errors of intercept and slope.
xmean	Global (weighted-)average of reference method values.
B0jack	Numeric vector with point estimations of intercept for jackknife samples. The i-th element contains point estimation for data set without i-th observation
B1jack	Numeric vector with point estimations of slope for jackknife samples. The i-th element contains point estimation for data set without i-th observation
В0	Numeric vector with point estimations of intercept for each bootstrap sample. The i-th element contains point estimation for i-th bootstrap sample.
B1	Numeric vector with point estimations of slope for each bootstrap sample. The i-th element contains point estimation for i-th bootstrap sample.
MX	Numeric vector with point estimations of (weighted-)average of reference method values for each bootstrap sample. The i-th element contains point estimation for i-th bootstrap sample.
sigmaB0	Numeric vector with estimation of standard error of intercept for each bootstrap sample. The i-th element contains point estimation for i-th bootstrap sample.
sigmaB1	Numeric vector with estimation of standard error of slope for each bootstrap sample. The i-th element contains point estimation for i-th bootstrap sample.
nsamples	Number of bootstrap samples.
nnested	Number of nested bootstrap samples.
cimeth	Method of confidence interval calculation (bootstrap).
npoints	Number of observations.

# Author(s)

Ekaterina Manuilova <ekaterina.manuilova@roche.com>, Fabian Model <fabian.model@roche.com>

# References

Efron, B., Tibshirani, R.J. (1993) *An Introduction to the Bootstrap*. Chapman and Hall. Carpenter, J., Bithell, J. (2000) Bootstrap confidence intervals: when, which, what? A practical guide for medical statisticians. *Stat Med*, **19** (**9**), 1141–1164.

mc.calc.bca

mc.calc.bca	Bias Corrected and Accelerated Resampling Confidence Interval

# Description

Calculate resampling BCa confidence intervals for intercept, slope or bias given a vector of bootstrap and jackknife point estimates.

### Usage

```
mc.calc.bca(Xboot, Xjack, xhat, alpha)
```

### Arguments

Xboot	vector of point estimates for bootstrap samples. The i-th element contains point estimate of the i-th bootstrap sample.
Xjack	vector of point estimates for jackknife samples. The i-th element contains point estimate of the dataset without i-th observation.
xhat	point estimate for the complete data set (scalar).
alpha	numeric value specifying the 100(1-alpha)% confidence level for the confidence interval (Default is 0.05).

# Value

a list with elements

est point estimate for the complete data set (xhat).

CI confidence interval for point estimate.

### References

Carpenter, J., Bithell, J. (2000) Bootstrap confidence intervals: when, which, what? A practical guide for medical statisticians. *Stat Med*, **19** (9), 1141–1164.

mc.calc.quant	Quantile Calculation for BCa

# Description

We are using the R default (SAS (type=3) seems bugged) quantile calculation instead of the quantile function described in Effron&Tibshirani.

#### Usage

```
mc.calc.quant(X, alpha)
```

mc.calc.quantile

#### **Arguments**

X numeric vector.

alpha probabilty

#### Value

alpha-quantile of vector X.

mc.calc.quantile

Quantile Method for Calculation of Resampling Confidence Intervals

# **Description**

Calculate bootstrap confidence intervals for intercept, slope or bias given the vector of bootstrap point estimates.

### Usage

```
mc.calc.quantile(Xboot, alpha)
```

### Arguments

Xboot vector of point estimates for bootstrap samples. The i-th element contains point

estimate of the i-th bootstrap sample.

alpha numeric value specifying the 100(1-alpha)% confidence level for the confidence

interval (Default is 0.05).

### Value

a list with elements

est median of bootstrap point estimates Xboot.

CI confidence interval for point estimate 'est', calculated as quantiles.

#### References

B. Efron and RJ. Tibshirani (1994) An Introduction to the Bootstrap. Chapman & Hall.

mc.calc.Student 13

mc.calc.Student	Student Method for Calculation of Resampling Confidence Intervals

# Description

Calculate bootstrap confidence intervals for intercept, slope or bias given a vector of bootstrap point estimates.

# Usage

```
mc.calc.Student(Xboot, xhat, alpha, npoints)
```

# Arguments

Xboot	vector of point estimates for each bootstrap sample. The i-th element contains the point estimate of the i-th bootstrap sample.
alpha	numeric value specifying the $100(1-alpha)\%$ confidence level for the confidence interval (Default is $0.05$ ).
xhat	global point estimate for which the confidence interval shall be computed.
npoints	number of points used for the regression analysis.

#### Value

a list with elements

est	the point estimate xhat
se	standard deviation computed from bootstrap point estimates Xboot
CI	Confidence interval for point estimate xhat, calculated as $xhat + / - qt(1 - alpha, n-2) * sd$ .

### References

Carpenter, J., Bithell, J. (2000) Bootstrap confidence intervals: when, which, what? A practical guide for medical statisticians. *Stat Med*, **19** (9), 1141–1164.

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mc.calc.tboot Bootstrap-t Method for Calculation of Resampling Confidence Intervals	mc.calc.tboot	
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# Description

Calculate resampling confidence intervals for intercept, slope or bias with t-Boot method given a vector of bootstrap point estimates and a vector of bootstrap standard deviations.

### Usage

```
mc.calc.tboot(Xboot, Sboot, xhat, shat, alpha)
```

# Arguments

×	(boot	vector of point estimates for bootstrap sample. The i-th element contains the point estimate for the i-th bootstrap sample.
S	Sboot	vector of standard deviations for each bootstrap sample. It schould be estimated with any analytical method or nonparametric with nested bootstrap.
×	hat	point estimate for the complete data set (scalar).
S	shat	estimate of standard deviation for the complete data set (scalar).
ā	alpha	numeric value specifying the 100(1-alpha)% confidence level for the confidence interval (Default is 0.05).

#### Value

#### a list with elements

est	point estimate for the complete data set (xhat).
se	estimate of standard deviation for the complete data set (shat).
CT	confidence interval for the point estimate.

### References

Carpenter, J., Bithell, J. (2000) Bootstrap confidence intervals: when, which, what? A practical guide for medical statisticians. *Stat Med*, **19** (9), 1141–1164.

mc.calcAngleMat 15

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mc.cal	cAngleMat	

Calculate Matrix of All Pair-wise Slope Angles

### **Description**

This version is implemented in C for computational efficiency.

### Usage

```
mc.calcAngleMat(X, Y, posCor = TRUE)
```

### **Arguments**

X measurement values of reference method.Y measurement values of test method.

posCor should algorithm assume positive correlation, i.e. symmetry around slope 1?

#### Value

Upper triangular matrix of slopes for all point combinations. Slopes in radian.

mc.calcAngleMat.R

Calculate Matrix of All Pair-wise Slope Angles

#### **Description**

This is a very slow R version. It should not be called except for debugging purposes.

# Usage

```
mc.calcAngleMat.R(X, Y, posCor = TRUE)
```

### **Arguments**

X measurement values of reference method.

Y measurement values of test method.

posCor should the algorithm assume positive correlation, i.e. symmetry around slope 1?

### Value

Upper triangular matrix of slopes for all point combinations. Slopes in radian.

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mc	calcl	innetCI	
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Jackknife Confidence Interval

#### **Description**

Calculate Jackknife confidence intervals for intercept, slope or bias given of vector of jackknife point estimates and global point estimate.

#### Usage

```
mc.calcLinnetCI(Xjack, xhat, alpha = 0.05)
```

### **Arguments**

Xjack vector of point estimates for jackknife samples. The i-th element contains point

estimate for the dataset without the i-th observation.

xhat point estimate for the complete data set (scalar).

alpha numeric value specifying the 100(1-alpha)% confidence level for the confidence

interval (Default is 0.05).

#### Value

a list with elements

est point estimate for the complete data set (scalar).

se standard deviation of point estimate calculated with Jackknife Method.

CI confidence interval for point estimate.

#### References

Linnet, K. (1993) Evaluation of Regression Procedures for Methods Comparison Studies. *CLIN. CHEM.* **39/3**, 424–432.

mc.calcTstar

Compute Resampling T-statistic.

### **Description**

Compute Resampling T-statistic. for Calculation of t-Bootstrap Confidence Intervals.

#### Usage

```
mc.calcTstar(.Object, x.levels, iter.max = 30, threshold = 1e-06)
```

mc.deming 17

### **Arguments**

.Object	object of class	"MCResultResampling".

x.levels a numeic vector of clinical desision points of interest.

iter.max maximal number of iterations for calculation of weighted deming regression.

threshold threshold for calculation of weighted deming regression.

#### Value

Tstar numeric vector containing resampling pivot statistic.

#### References

Carpenter J., Bithell J. Bootstrap confidence intervals: when, which, what? A practical guide for medical statisticians. Stat Med, 19 (9), 1141-1164 (2000).

mc.deming	Calculate Unweighted Deming Regression and Estimate Standard Er-
	rors

# Description

Calculate Unweighted Deming Regression and Estimate Standard Errors

### Usage

```
mc.deming(X, Y, error.ratio)
```

### Arguments

X measurement values of reference method.

Y measurement values of test method.

error.ratio ratio of measurement error of reference method to measurement error of test

method.

#### Value

a list with elements

b0 intercept. b1 slope.

se.b0 respective standard error of intercept.
se.b1 respective standard error of slope.
xw average of reference method values.

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#### References

Linnet K. Evaluation of Regression Procedures for Methods Comparison Studies. CLIN. CHEM. 39/3, 424-432 (1993).

Linnet K. Estimation of the Linear Relationship between the Measurements of two Methods with Proportional Errors. STATISTICS IN MEDICINE, Vol. 9, 1463-1473 (1990).

mc.linreg

Calculate ordinary linear Regression and Estimate Standard Errors

# Description

Calculate ordinary linear Regression and Estimate Standard Errors

### Usage

```
mc.linreg(X, Y)
```

### Arguments

X measurement values of reference method.

Y measurement values of test method.

### Value

a list with elements

b0 intercept.
b1 slope.
se.b0 respective standard error of intercept.
se.b1 respective standard error of slope.
xw average of reference method values.

#### References

Neter J., Wassermann W., Kunter M. Applied Statistical Models. Richard D. Irwing, INC., 1985.

mc.make.Clframe

mc	maka	CIframe
IIIC.	IIIAK 🖰	CITTAME

Returns Results of Calculations in Matrix Form

# Description

Returns Results of Calculations in Matrix Form

# Usage

```
mc.make.CIframe(b0, b1, se.b0, se.b1, CI.b0, CI.b1)
```

# Arguments

b0	point estimate for intercept.
b1	point estimate for slope.
se.b0	standard error of intercept estimate.
se.b1	standard error of slope estimate.
CI.b0	numeric vector of length 2 - confidence interval for intercept.
CI.b1	numeric vector of length 2 - confidence interval for slope.

### Value

2x4 matrix of estimates and confidence intervals for intercept and slope.

mc	paba

Passing-Bablok Regression

# Description

Passing-Bablok Regression

### Usage

```
mc.paba(angM, X, Y, alpha = 0.05, posCor = TRUE, calcCI = TRUE,
    slope.measure = c("radian", "tangent"))
```

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#### **Arguments**

angM	upper triangular matr	ix of slopes for all point	combinations. Slopes in radian.
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X measurement values of reference methodY measurement values of test method

alpha numeric value specifying the 100(1-alpha) confidence level

posCor should algorithm assume positive correlation, i.e. symmetry around slope 1?

calcCI should confidence intervals be computed?

slope.measure angular measure of pairwise slopes (see mcreg for details).

"radian" - for data sets with even sample numbers median slope is calculated

as average of two central slope angles.

"tangent" - for data sets with even sample numbers median slope is calculated

as average of two central slopes (tan(angle)).

### Value

Matrix of estimates and confidence intervals for intercept and slope. No standard errors provided by this algorithm.

mc.paba.LargeData

Passing-Bablok Regression for Large Datasets

### **Description**

This function represents an interface to a fast C-implementation of an adaption of the Passing-Bablok algorithm for large datasets. Instead of building the complete matrix of pair-wise slope values, a pre-defined binning of slope-values is used (Default NBins=1e06). This reduces the required memory dramatically and speeds up the computation.

#### Usage

```
mc.paba.LargeData(X, Y, NBins = 1e+06, alpha = 0.05, posCor = TRUE,
    calcCI = TRUE)
```

### Arguments

X	(numeric) vector containing measurement values of reference method
Υ	(numeric) vector containing measurement values of test method
NBins	(integer) value specifying the number of bins used to classify slope-values
alpha	(numeric) value specifying the $100 (1\mbox{-alpha})\%$ confidence level for confidence intervals
posCor	(logical) should algorithm assume positive correlation, i.e. symmetry around slope $1$ ?
calcCI	(logical) should confidence intervals be computed?

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#### Value

Matrix of estimates and confidence intervals for intercept and slope. No standard errors provided by this algorithm.

#### Author(s)

Andre Schuetzenmeister <andre.schuetzenmeister@roche.com> (partly re-using code of function 'mc.paba')

### **Examples**

```
library("mcr")
  data(creatinine,package="mcr")

# remove any NAs
  crea <- na.omit(creatinine)

# call the approximative Passing-Bablok algorithm (Default NBins=1e06)
  res1 <- mcreg(x=crea[,1], y=crea[,2], method.reg="PaBaLarge", method.ci="analytical")
  getCoefficients(res1)

# now increase the number of bins and see whether this makes a difference
  res2 <- mcreg(x=crea[,1], y=crea[,2], method.reg="PaBaLarge", method.ci="analytical", NBins=1e07)
  getCoefficients(res2)
  getCoefficients(res1)-getCoefficients(res2)</pre>
```

mc.wdemingConstCV

Calculate Weighted Deming Regression

#### **Description**

Calculate weighted deming regression with iterative algorithm suggested by Linnet. This algorithm is avalaible only for positive values. But even in this case there is no guarantee that the algorithm always converges.

#### Usage

```
mc.wdemingConstCV(X, Y, error.ratio, iter.max = 30, threshold = 1e-06)
```

# **Arguments**

X measurement values of reference method.Y measurement values of test method.

error.ratio ratio between squared measurement errors of reference- and test method, neces-

sary for Deming regression (Default is 1).

iter.max maximal number of iterations.

threshold threshold value.

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#### Value

a list with elements

b0 intercept.b1 slope.

xw average of reference method values.

iter number of iterations.

#### References

Linnet K. Evaluation of Regression Procedures for Methods Comparison Studies. CLIN. CHEM. 39/3, 424-432 (1993).

Linnet K. Estimation of the Linear Relationship between the Measurements of two Methods with Proportional Errors. STATISTICS IN MEDICINE, Vol. 9, 1463-1473 (1990).

mc.wlinreg Calculate Weighted Ordinary Linear Regression and Estimate Standard Errors

# Description

The weights of regression are taken as reverse squared values of the reference method, that's why it is impossible to achieve the calculations for zero values.

### Usage

```
mc.wlinreg(X, Y)
```

#### **Arguments**

X measurement values of reference method.
Y measurement values of test method.

#### Value

a list with elements.

b0 intercept.b1 slope.

se.b0 respective standard error of intercept. se.b1 respective standard error of slope.

xw weighted average of reference method values.

#### References

Neter J., Wassermann W., Kunter M. Applied Statistical Models. Richard D. Irwing, INC., 1985.

mcreg

Comparison of Two Measurement Methods Using Regression Analysis

#### Description

mcreg is used to compare two measurement methods by means of regression analysis. Available methods comprise ordinary and weighted linear regression, Deming and weighted Deming regression and Passing-Bablok regression. Point estimates of regression parameters are computed together with their standard errors and confidence intervals.

### Usage

```
mcreg(x, y = NULL, error.ratio = 1, alpha = 0.05, mref.name = NULL,
  mtest.name = NULL, sample.names = NULL, method.reg = c("PaBa", "LinReg",
  "WLinReg", "Deming", "WDeming", "PaBaLarge"), method.ci = c("bootstrap",
  "jackknife", "analytical", "nestedbootstrap"),
  method.bootstrap.ci = c("quantile", "Student", "BCa", "tBoot"),
  nsamples = 999, nnested = 25, rng.seed = NULL,
  rng.kind = "Mersenne-Twister", iter.max = 30, threshold = 1e-06,
  na.rm = FALSE, NBins = 1e+06, slope.measure = c("radian", "tangent"))
```

#### **Arguments**

Х measurement values of reference method, or two column matrix. measurement values of test method. y mref.name name of reference method (Default "Method1"). mtest.name name of test Method (Default "Method2"). names of cases (Default "S##"). sample.names ratio between squared measurement errors of reference and test method, neceserror.ratio sary for Deming regression (Default 1). alpha value specifying the 100(1-alpha)% confidence level for confidence intervals (Default is 0.05). method.reg regression method. It is possible to choose between five regression methods: "LinReg" - ordinary least square regression. "WLinReg" - weighted ordinary least square regression. "Deming" - Deming regression. "WDeming" - weighted Deming regression. "PaBa" - Passing-Bablok regression. "PaBaLarge" - approximative Passing-Bablok regression for large datasets, operating on NBins classes of constant slope angle which each slope is classified to instead of building the complete triangular matrix of all N\*N/2 slopes. method.ci method of confidence interval calculation. The function contains four basic methods for calculation of confidence intervals for regression coefficients. "analytical" - with parametric method.

"jackknife" - with leave one out resampling.

"bootstrap" - with ordinary non-parametric bootstrap resampling.

"nested bootstrap" - with ordinary non-parametric bootstrap resampling.

#### method.bootstrap.ci

bootstrap based confidence interval estimation method.

nsamples number of bootstrap samples.

nnested number of nested bootstrap samples.

rng. seed integer number that sets the random number generator seed for bootstrap sam-

pling. If set to NULL currently in the R session used RNG setting will be used.

rng.kind type of random number generator for bootstrap sampling. Only used when

rng.seed is specified, see set.seed for details.

iter.max maximum number of iterations for weighted Deming iterative algorithm.

threshold numerical tolerance for weighted Deming iterative algorithm convergence.

na.rm remove measurement pairs that contain missing values (Default is FALSE).

number of bins used when 'reg.method="PaBaLarge"' to classify each slope in one of 'NBins' bins covering the range of all slopes

slope.measure angular measure of pairwise slopes used for exact PaBa regression (see below

for details).

"radian" - for data sets with even sample numbers median slope is calculated

as average of two central slope angles.

"tangent" - for data sets with even sample numbers median slope is calculated

as average of two central slopes (tan(angle)).

#### **Details**

**NBins** 

The regression analysis yields regression coefficients 'Inercept' and 'Slope' of the regression Testmethod = Intercept + Slope\*Referencemethod. There are methods for computing the systematical bias between reference and test method at a decision point Xc, Bias(Xc) = Intercept + (Slope - 1)\*Xc, accompanied by its corresponding standard error and confidence interval. One can use plotting method plotBias for a comprehensive view of the systematical bias.

Weighted regression for heteroscedastic data is available for linear and Deming regression and implemented as a data point weighting with the inverted squared value of the reference method. Therefore calculation of weighted regression (linear and Deming) is available only for positive values (>0). Passing-Bablok regression is only available for non-negative values (>=0).

Confidence intervals for regression parameters and bias estimates are calculated either by using analytical methods or by means of resampling methods ("jackknife", "bootstrap", "nested bootstrap"). An analytical method is available for all types of regression except for weighted Deming. For Passing-Bablok regression the option "analytical" calculates confidence intervals for the regression parameters according to the non-parametric approach given in the original reference.

The "jackknife" (or leave one out resampling) method was suggested by Linnet for calculating confidence intervals of regression parameters of Deming and weighted Deming regression. It is possible to calculate jackknife confidence intervals for all types of regression. Note that we do

not recommend this method for Passing-Bablok since it has a tendency of underestimating the variability (jackknife is known to yield incorrect estimates for errors of quantiles).

The bootstrap method requires additionally choosing a value for method.bootstrap.ci. If bootstrap is the method of choice, "BCa", t-bootstrap ("tBoot") and simple "quantile" confidence intervals are recommended (See Efron B. and Tibshirani R.J.(1993), Carpenter J., Bithell J. (2000)). The "nestedbootstrap" method can be very time-consuming but is necessary for calculating t-bootstrap confidence intervals for weighted Deming or Passing-Bablok regression. For these regression methods there are no analytical solutions for computing standard errors, which therefore have to be obtained by nested bootstrapping.

Note that estimating resampling based confidence intervals for Passing-Bablok regressions can take very long for larger data sets due to the high computational complexity of the algorithm. To mitigate this drawback an adaption of the Passing-Bablok algorithm has been implemented ("PaBaLarge"), which yields approximative results. This approach does not build the complete upper triangular matrix of all 'n\*(n-1)/2' slopes. It subdivides the range of slopes into 'NBins' classes, and sorts each slope into one of these bins. The remaining steps are the same as for the exact "PaBa" algorithm, except that these are performed on the binned slopes instead of operating on the matrix of slopes.

Our implementation of exact Passing-Bablok regression ("PaBa") provides two alternative metrics for regression slopes which can result in different regression estimates. As a robust regression method PaBa is essentially invariant to the parameterization of regression slopes, however in the case of an even number of all pairwise slopes the two central slopes are averaged to estimate the final regression slope. In this situation using an angle based metric (slope.measure="radian") will result in a regression estimate that is geometrically centered between the two central slopes, whereas the tangent measure (slope.measure="tangent") proposed in Passing and Bablok (1983) will be geometrically biased towards a higher slope. See below for a pathological example. Note that the difference between the two measures is neglectable for data sets with reasonable sample size (N>20) and correlation.

### Value

"MCResult" object containing regression results. The function getCoefficients or printSummary can be used to obtain or print a summary of the results. The function getData allows to see the original data. An S4 object of class "MCResult" containing at least the following slots:

data measurement data in wide format, one pair of observations per sample. Includes

samples ID, reference measurement, test measurement.

para numeric matrix with estimates for slope and intercept, corresponding standard

deviations and confidence intervals.

mnames character vector of length two containing names of analytical methods.

regmeth type of regression type used for parameter estimation. cimeth method used for calculation of confidence intervals.

error.ratio ratio between squared measurement errors of reference and test method, neces-

sary for Deming regression.

alpha confidence level using for calculation of confidence intervals.

#### Author(s)

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#### References

Bland, J. M., Altman, D. G. (1986) Statistical methods for assessing agreement between two methods of clinical measurement. *Lancet*, **i**: 307–310.

Linnet, K. (1993) Evaluation of Regression Procedures for Methods Comparison Studies. *CLIN. CHEM.* **39/3**, 424–432.

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Looney, S. W. (2010) Statistical Methods for Assessing Biomarkers. *Methods in Molecular Biology*, vol. **184**: *Biostatistical Methods*. Human Press INC.

Passing, H., Bablok, W. (1983) A new biometrical procedure for testing the equality of measurements from two different analytical methods. Application of linear regression procedures for method comparison studies in clinical chemistry, Part I. *J Clin Chem Clin Biochem*. Nov; **21(11)**:709–20.

Efron, B., Tibshirani, R.J. (1993) An Introduction to the Bootstrap. Chapman and Hall.

Carpenter, J., Bithell, J. (2000) Bootstrap confidence intervals: when, which, what? A practical guide for medical statisticians. *Stat Med*, **19** (9), 1141–1164.

CLSI EP9-A2. Method Comparison and Bias Estimation Using Patient Samples; Approved Guideline.

#### See Also

 $\verb|plotDifference|, \verb|plot.mcr|, \verb|getResiduals|, \verb|plotResiduals|, \verb|calcResponse|, \verb|calcBias|, \verb|plotBias|, \verb|compareFit|$ 

# Examples

```
library("mcr")
data(creatinine,package="mcr")
x <- creatinine$serum.crea
v <- creatinine$plasma.crea</pre>
# Deming regression fit.
# The confidence intercals for regression coefficients
# are calculated with analytical method
model1<- mcreg(x,y,error.ratio=1,method.reg="Deming", method.ci="analytical",</pre>
               mref.name = "serum.crea", mtest.name = "plasma.crea", na.rm=TRUE)
# Results
printSummary(model1)
getCoefficients(model1)
plot(model1)
# Deming regression fit.
# The confidence intervals for regression coefficients
# are calculated with bootstrap (BCa) method
model2<- mcreg(x,y,error.ratio=1,method.reg="Deming",</pre>
               method.ci="bootstrap", method.bootstrap.ci = "BCa",
               mref.name = "serum.crea", mtest.name = "plasma.crea", na.rm=TRUE)
compareFit(model1, model2)
```

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MCResult-class

Class "MCResult"

#### **Description**

Result of a method comparison.

#### **Objects from the Class**

Object is typically created by a call to function mcreg. Object can be directly constructed by calling newMCResult or new("MCResult", data, para, mnames, regmeth, cimeth, error.ratio, alpha, weight).

#### **Slots**

```
data: Object of class "data.frame" ~~

para: Object of class "matrix" ~~

mnames: Object of class "character" ~~

regmeth: Object of class "character" ~~

cimeth: Object of class "character" ~~

error.ratio: Object of class "numeric" ~~

alpha: Object of class "numeric" ~~

weight: Object of class "numeric" ~~
```

### Methods

```
calcBias signature(.0bject = "MCResult"): ...
calcCUSUM signature(.0bject = "MCResult"): ...
calcResponse signature(.0bject = "MCResult"): ...
getCoefficients signature(.0bject = "MCResult"): ...
getData signature(.0bject = "MCResult"): ...
getErrorRatio signature(.0bject = "MCResult"): ...
```

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```
getRegmethod signature(.Object = "MCResult"): ...
getResiduals signature(.Object = "MCResult"): ...
getWeights signature(.Object = "MCResult"): ...
plot signature(x = "MCResult"): ...
plotBias signature(x = "MCResult"): ...
plotDifference signature(.Object = "MCResult"): ...
plotResiduals signature(.Object = "MCResult"): ...
printSummary signature(.Object = "MCResult"): ...
```

#### Author(s)

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### **Examples**

```
showClass("MCResult")
```

MCResult.calcBias

Systematical Bias Between Reference Method and Test Method

### Description

Calculate systematical bias between reference and test methods at the decision point Xc as Bias(Xc) = Intercept + (Slope - 1) \* Xc with corresponding confidence intervals.

# Usage

```
MCResult.calcBias(.Object, x.levels, type = c("absolute", "proportional"),
    percent = TRUE, alpha = 0.05, ...)
```

### **Arguments**

.Object	object of class "MCResult".
type	One can choose between absolute (default) and proportional bias (Bias (Xc)/Xc).
percent	logical value. If percent = TRUE the proportional bias will be calculated in percent.
x.levels	a numeric vector with decision points for which bias schould be calculated.
alpha	numeric value specifying the $100(1-alpha)\%$ confidence level of the confidence interval (Default is $0.05$ ).
	further parameters

#### Value

response and corresponding confidence interval for each decision point from x.levels.

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#### See Also

plotBias

#### **Examples**

MCResult.calcCUSUM

Calculate CUSUM Statistics According to Passing & Bablok (1983)

### Description

Calculate CUSUM Statistics According to Passing & Bablok (1983)

# Usage

```
MCResult.calcCUSUM(.Object)
```

#### **Arguments**

.0bject of class "MCResult".

### Value

A list containing the following elements:

nPos sum of positive residuals nNeg sum of negative residuals

cusum a cumulative sum of vector with scores ri for each point, sorted increasing by

distance of points to regression line.

max.cumsum Test statistics of linearity test

#### References

Passing, H., Bablok, W. (1983) A new biometrical procedure for testing the equality of measurements from two different analytical methods. Application of linear regression procedures for method comparison studies in clinical chemistry, Part I. *J Clin Chem Clin Biochem*. Nov; **21(11)**:709–20.

MCResult.calcResponse Calculate Response with Confidence Interval.

#### **Description**

 ${\bf Calculate\ Response\ } Intercept + Slope * Refrence method\ {\bf with\ Corresponding\ Confidence\ Interval}$ 

#### Usage

```
MCResult.calcResponse(.Object, x.levels, alpha, ...)
```

#### **Arguments**

```
.Object object of class "MCResult".

x.levels a numeric vector with points for which response schould be calculated.

alpha numeric value specifying the 100(1-alpha)% confidence level of the confidence interval (Default is 0.05).

... further parameters
```

### Value

response and corresponding confidence interval for each point in vector x.levels.

#### See Also

calcBias

### **Examples**

MCResult.getCoefficients

Get Regression Coefficients

# Description

Get Regression Coefficients

# Usage

```
MCResult.getCoefficients(.Object)
```

# Arguments

.Object

object of class "MCResult".

#### Value

Regression parameters in matrix form. Rows: Intercept, Slope. Cols: EST, SE, LCI, UCI.

 ${\tt MCResult.getData}$ 

Get Data

# Description

Get Data

#### Usage

```
MCResult.getData(.Object)
```

# Arguments

.Object

object of class "MCResult".

#### Value

Measurement data in matrix format. First column contains reference method (X), second column contains test method (Y).

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MCResult.getErrorRatio

Get Error Ratio

### **Description**

Get Error Ratio

### Usage

```
MCResult.getErrorRatio(.Object)
```

# **Arguments**

.Object

Object of class "MCResult"

#### Value

Error ratio. Only relevant for Deming type regressions.

MCResult.getFitted

Get Fitted Values.

### **Description**

This funcion computes fitted values for a 'MCResult'-object. Depending on the regression method and the error ratio, a projection onto the regression line is performed accordingly. For each point  $(x_i; y_i) = 1,...,n$  the projected point  $(x_h = 1,...,n]$  is computed.

### Usage

```
MCResult.getFitted(.Object)
```

#### **Arguments**

.Object

object of class "MCResult".

#### Value

fitted values as data frame.

#### See Also

plotResiduals getResiduals

MCResult.getRegmethod Get Regression Method

### **Description**

Get Regression Method

### Usage

```
MCResult.getRegmethod(.Object)
```

### **Arguments**

.0bject of class "MCResult".

#### Value

Name of the statistical method used for the regression analysis.

MCResult.getResiduals Get Regression Residuals

### Description

This function returnes residuals in x-direction (x-xhat), in y-direction(y-yhat) and optimized residuals. The optimized residuals correspond to distances between data points and the regression line which were optimized for regression coefficients estimation. In case of Passing-Bablok Regression orthogonal residuals will be returned as optimized residuals. The residuals in x-direction are interesting for regression types which assume errors in both variables (deming, weighted deming, Passing-Bablok), particularily for checking of model assumptions.

### Usage

```
MCResult.getResiduals(.Object)
```

### **Arguments**

.0bject of class "MCResult".

### Value

residuals as data frame.

#### See Also

plotResiduals

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MCResult.getWeights Get Weights of Data Points

#### **Description**

Get Weights of Data Points

#### Usage

```
MCResult.getWeights(.Object)
```

### Arguments

. Object of class "MCResult"

#### Value

Weights of data points.

MCResult.initialize MCResult Object Initialization

# Description

MCResult Object Initialization

#### Usage

```
MCResult.initialize(.Object, data = data.frame(X = NA, Y = NA),
  para = matrix(NA, ncol = 4, nrow = 2), mnames = c("unknown", "unknown"),
  regmeth = "unknown", cimeth = "unknown", error.ratio = 0,
  alpha = 0.05, weight = 1)
```

### Arguments

.Object	object of class "MCResult"

data measurement data in matrix format. First column reference method (x), second

column test method (y).

para regression parameters in matrix form. Rows: Intercept, Slope. Cols: EST, SE,

LCI, UCI.

mnames names of reference and test method.

regmeth name of statistical method used for regression.

cimeth name of statistical method used for computing confidence intervals.

error.ratio ratio between standard deviation of reference and test method.

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alpha numeric value specifying the 100(1-alpha)% confidence level of confidence in-

tervals (Default is 0.05).

weight weights to be used for observations

#### Value

MCResult object with initialized parameter.

MCResult.plot Scatter Plot Method X vs. Method Y

# Description

Plot method X (reference) vs. method Y (test) with (optional) line of identity, regression line and confidence bounds for response.

### Usage

```
MCResult.plot(x, alpha = 0.05, xn = 20, equal.axis = FALSE, xlim = NULL, ylim = NULL, x.lab = x@mnames[1], y.lab = x@mnames[2], add = FALSE, draw.points = TRUE, points.col = "black", points.pch = 1, points.cex = 0.8, reg = TRUE, reg.col = NULL, reg.lty = 1, reg.lwd = 2, identity = TRUE, identity.col = NULL, identity.lty = 2, identity.lwd = 1, ci.area = TRUE, ci.area.col = NULL, ci.border = FALSE, ci.border.col = NULL, ci.border.lty = 2, ci.border.lwd = 1, add.legend = TRUE, legend.place = c("topleft", "topright", "bottomleft", "bottomright"), main = NULL, sub = NULL, add.cor = TRUE, cor.method = c("pearson", "kendall", "spearman"), add.grid = TRUE, ...)
```

#### **Arguments**

X	object of class "MCResult".
alpha	numeric value specifying the 100(1-alpha)% confidence bounds.
xn	number of points (default 20) for calculation of confidence bounds.
draw.points	logical value. If draw.points=TRUE, the data points will be drawn.
xlim	limits of the x-axis. If xlim=NULL the x-limits will be calculated automatically.
ylim	limits of the y-axis. If ylim=NULL the y-limits will be calculated automatically.
x.lab	label of x-axis. Default is the name of reference method.
y.lab	label of y-axis. Default is the name of test method.
equal.axis	logical value. If equal.axis=TRUE x-axis will be equal to y-axis.
add	logical value. If add=TRUE, the plot will be drawn in current graphical window.
points.col	Color of data points.
points.pch	Type of data points (see par()).

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points.cex	Size of data points (see par()).
reg	Logical value. If reg=TRUE, the regression line will be drawn.
reg.col	Color of regression line.
reg.lty	Type of regression line.
reg.lwd	The width of regression line.
identity	logical value. If identity=TRUE the identity line will be drawn.
identity.col	The color of identity line.
identity.lty	The type of identity line.
identity.lwd	the width of identity line.
ci.area	logical value. If ci.area=TRUE (default) the confidence area will be drawn.
ci.area.col	the color of confidence area.
ci.border	logical value. If ci.border=TRUE the confidence limits will be drawn.
ci.border.col	The color of confidence limits.
ci.border.lty	The line type of confidence limits.
ci.border.lwd	The line width of confidence limits.
add.legend	logical value. If add.legend=FALSE the plot will not have any legend.
legend.place	The position of legend: "topleft", "topright", "bottomleft", "bottomright".
main	String value. The main title of plot. If main=NULL it will include regression name.
sub	String value. The subtitle of plot. If $sub=NULL$ and $ci.border=TRUE$ or $ci.area=TRUE$ it will include the art of confidence bounds calculation.
add.cor	Logical value. If add.cor=TRUE the correlation coefficient will be shown.
cor.method	a character string indicating which correlation coefficient is to be computed. One of "pearson" (default), "kendall", or "spearman", can be abbreviated.
add.grid	Logical value. If add.grid=TRUE (default) the gridlines will be drawn.
	further graphical parameters

### See Also

 $\verb|plotBias|, \verb|plotResiduals|, \verb|plotDifference|, \verb|compareFit|, \verb|includeLegend||$ 

# **Examples**

```
library(mcr)
data(creatinine,package="mcr")
creatinine <- creatinine[complete.cases(creatinine),]
x <- creatinine$serum.crea
y <- creatinine$plasma.crea

m1 <- mcreg(x,y,method.reg="Deming", mref.name="serum.crea", mtest.name="plasma.crea", na.rm=TRUE)
m2 <- mcreg(x,y,method.reg="WDeming", method.ci="jackknife", mref.name="serum.crea",</pre>
```

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MCResult.plotBias

Plot Estimated Systematical Bias with Confidence Bounds

#### Description

This function plots the estimated systematical bias (Intercept + Slope \* Refrencemethod) - Referencemethod with confidence bounds, covering the whole range of reference method X or only part of it.

#### Usage

```
MCResult.plotBias(x, xn = 100, alpha = 0.05, add = FALSE, prop = FALSE, xlim = NULL, ylim = NULL, bias = TRUE, bias.lty = 1, bias.lwd = 2, bias.col = NULL, ci.area = TRUE, ci.area.col = NULL, ci.border = FALSE, ci.border.col = NULL, ci.border.lwd = 1, ci.border.lty = 2, zeroline = TRUE, zeroline.col = NULL, zeroline.lty = 2, zeroline.lwd = 1, main = NULL, sub = NULL, add.grid = TRUE, xlab = NULL, ylab = NULL, cut.point = NULL, cut.point.col = "red", cut.point.lwd = 2, cut.point.lty = 1, ...)
```

X	object of class "MCResult".
xn	# number of poits for drawing of confidence bounds/area.
add	logical value. If add=TRUE, the grafic will be drawn in current grafical window.
prop	a logical value. If prop=TRUE the proportional bias $(Slope-1)\ast Xc]/Xc$ will be drawn.
xlim	limits of the x-axis. If xlim=NULL the x-limits will be calculated automatically.
ylim	limits of the y-axis. If ylim=NULL the y-limits will be calculated automatically.
bias	logical value. If identity=TRUE the bias line will be drawn. If ci.bounds=FALSE and ci.area=FALSE the bias line will be drawn always.
bias.col	color of the bias line.
bias.lty	type of the bias line.

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bias.lwd	width of the bias line.
zeroline	logical value. If zeroline=TRUE the zero-line will be drawn.
zeroline.col	color of the zero-line.
zeroline.lty	type of the zero-line.
zeroline.lwd	width of the zero-line.
ci.area	logical value. If ci.area=TRUE (default) the confidence area will be drawn.
ci.border	logical value. If ci.border=TRUE the confidence limits will be drawn.
ci.area.col	color of the confidence area.
ci.border.col	color of the confidence limits.
ci.border.lty	line type of confidence limits.
ci.border.lwd	line width of confidence limits.
cut.point	numeric value. Decision level of interest.
cut.point.col	color of the confidence bounds at the required decision level.
cut.point.lty	line type of the confidence bounds at the required decision level.
cut.point.lwd	line width of the confidence bounds at the required decision level.
main	character string. The main title of plot. If main = NULL it will include regression name.
sub	character string. The subtitle of plot. If sub=NULL and ci.border=TRUE or ci.area=TRUE it will include the art of confidence bounds calculation.
add.grid	logical value. If grid=TRUE (default) the gridlines will be drawn.
xlab	label for the x-axis
ylab	label for the y-axis
alpha	numeric value specifying the $100(1-alpha)\%$ confidence level of confidence intervals (Default is $0.05$ ).
•••	further graphical parameters

#### See Also

```
calcBias, plot.mcr, plotResiduals, plotDifference, compareFit
```

# **Examples**

```
method.bootstrap.ci="BCa",mref.name="serum.crea",
                mtest.name="plasma.crea", na.rm=TRUE)
# Grafical comparison of systematical Bias of two models
plotBias(m1, zeroline=TRUE, zeroline.col="black", zeroline.lty=1,
                ci.area=TRUE,ci.border=FALSE, ci.area.col=grey(0.9),
                main = "Bias between serum and plasma creatinine",
                sub="Comparison of Jackknife and BCa-Bootstrap confidence bounds")
plotBias(m2, ci.area=FALSE, ci.border=TRUE, ci.border.lwd=2,
                ci.border.col="red",bias=FALSE ,add=TRUE)
includeLegend(place="topleft", models=list(m1, m2), lwd=c(10,2),
                lty=c(2,1),colors=c(grey(0.9),"red"), bias=TRUE,
                design="1", digits=4)
# Drawing of proportional bias
plotBias(m1, ci.area=FALSE, ci.border=TRUE)
plotBias(m1, ci.area=FALSE, ci.border=TRUE, prop=TRUE)
plotBias(m1, ci.area=FALSE, ci.border=TRUE, prop=TRUE, cut.point=0.6)
plotBias(m1, ci.area=FALSE, ci.border=TRUE, prop=TRUE, cut.point=0.6,
             xlim=c(0.4,0.8),cut.point.col="orange", cut.point.lwd=3, main ="")
```

MCResult.plotDifference

Bland-Altman Plot

## **Description**

Draw different Bland-Altman plot modifications (see parameter plot.type).

#### Usage

```
MCResult.plotDifference(.Object, xlab = NULL, ylab = NULL,
  ref.line = TRUE, ref.line.col = "black", ref.line.lty = 1,
  ref.line.lwd = 1, bias.line.lty = 1, bias.line.lwd = 1,
  bias.line.col = "red", bias.text.col = NULL, bias.text.cex = 0.8,
  loa.line.lty = 2, loa.line.lwd = 1, loa.line.col = "red",
  loa.text.col = NULL, plot.type = 3, main = NULL, cex = 0.8,
  digits = 2, add.grid = TRUE, ylim = NULL, ...)
```

.Object	object of class "MCResult".
xlab	label for the x-axis
ylab	label for the y-axis
digits	number of decimal places for the difference of means and standard deviation appearing in the plot.

plot.type

confidence intervals.

	mean. 7 - difference plot $\operatorname{sqrt}(X^*Y)$ vs. Y/X with null-line and mean plus confidence intervals calculated with help of log-transformation. 8 - difference plot $0.5*(X+Y)$ vs. $(Y-X) / (0.5*(X+Y))$ with null-line.
main	plot title.
ref.line	logical value. If ref.line=TRUE (default), the reference line will be drawn.
ref.line.col	reference line color.
ref.line.lty	reference line type.
ref.line.lwd	reference line width.
bias.line.lty	line type for estimated bias.
bias.line.lwd	line width for estimated bias.
bias.line.col	color of the line for estimated bias.
bias.text.col	color of the label for estimated bias (defaults to the same as bias.line.col.)
bias.text.cex	The magnification to be used for the label for estimated bias
loa.line.lty	line type for estimated limits of agreement.
loa.line.lwd	line width for estimated limits of agreement.
loa.line.col	color of the line for estimated limits of agreement.
loa.text.col	color of the label for estimated limits of agreement (defaults to the same as loa.line.col.)
add.grid	logical value. If add.grid=TRUE (Default) gridlines will be drawn.
ylim	limits for the y-axis
cex	numeric value specifying the magnification factor used for points

Bland, J. M., Altman, D. G. (1986) Statistical methods for assessing agreement between two meth-

integer specifying a specific Bland-Altman plot modification (default is 3). Possible choices are: 1 - difference plot X vs. Y-X with null-line and mean plus

2 - difference plot X vs. (Y-X)/X (relative differences) with null-line and mean. 3 - difference plot 0.5\*(X+Y) vs. Y-X with null-line and mean plus confidence

4 - difference plot 0.5\*(X+Y) vs. (Y-X)/X (relative differences) with null-line. 5 - difference plot rank(X) vs. Y-X with null-line and mean plus confidence in-

6 - difference plot rank(X) vs. (Y-X)/X (relative differences) with null-line and

# See Also

. . .

References

 $\verb"plot.mcr", \verb"plotResiduals", \verb"plotDifference", \verb"plotBias", \verb"compareFit"$ 

further graphical parameters

ods of clinical measurement. Lancet, i: 307-310.

#### **Examples**

MCResult.plotResiduals

Plot Residuals of an MCResult Object

## **Description**

Plot Residuals of an MCResult Object

## Usage

```
MCResult.plotResiduals(.Object, res.type = c("optimized", "y", "x"),
    xaxis = c("yhat", "both", "xhat"), ref.line = TRUE,
    ref.line.col = "red", ref.line.lty = 2, ref.line.lwd = 1, main = NULL,
    xlab = NULL, ylab = NULL, add.grid = TRUE, ...)
```

.Object	object of type "MCResult".
res.type	If res.type="y" the difference between the test method and it's prediction will be drawn. If res.type="x" the reference method and it's prediction will be drawn. In case ordinary and weighted ordinary linear regression this difference will be zero.
xaxis	Values on the x-axis. One can choose from estimated values of x (xaxis="xhat"), y (xaxis="xhat") or the mean of estimated values of x and y (xaxis="both"). If res.type="optimized" the proper type of residuals for each regression will be drawn.
ref.line	logical value. If ref.line = TRUE (default), the reference line will be drawn.
ref.line.col	reference line color.
ref.line.lty	reference line type.
ref.line.lwd	reference line width.

```
xlab label for the x-axis
ylab label for the y-axis
add.grid logical value. If add
```

add.grid logical value. If add.grid = TRUE (default) the gridlines will be drawn.

main character string specifying the main title of the plot

... further graphical parameters

#### See Also

```
getResiduals, plot.mcr, plotDifference, plotBias, compareFit
```

## **Examples**

MCResult.printSummary Print Summary of a Regression Analysis

## **Description**

Print Summary of a Regression Analysis

## Usage

```
MCResult.printSummary(.Object)
```

## **Arguments**

```
.0bject of type "MCResult".
```

#### See Also

```
getCoefficients, getRegmethod
```

```
MCResultAnalytical-class Class \ "\texttt{MCResultAnalytical"}
```

## **Description**

Result of a method comparison based on analytical methods for computing confidence intervals.

#### **Objects from the Class**

```
Object is typically created by a call to function mcreg. Object can be directly constructed by calling newMCResultAnalytical or new("MCResultAnalytical", data, xmean, para, mnames, regmeth, cimeth, error.r
```

# Slots

```
xmean: Object of class "numeric" ~~
data: Object of class "data.frame" ~~
para: Object of class "matrix" ~~
mnames: Object of class "character" ~~
regmeth: Object of class "character" ~~
cimeth: Object of class "character" ~~
error.ratio: Object of class "numeric" ~~
alpha: Object of class "numeric" ~~
weight: Object of class "numeric" ~~
```

#### **Extends**

```
Class "MCResult", directly.
```

#### Methods

```
calcResponse signature(.Object = "MCResultAnalytical"): ...
printSummary signature(.Object = "MCResultAnalytical"): ...
```

#### Author(s)

Ekaterina Manuilova <ekaterina.manuilova@roche.com>, Andre Schuetzenmeister <andre.schuetzenmeister@roche.com> Fabian Model <fabian.model@roche.com>

#### **Examples**

```
showClass("MCResultAnalytical")
```

```
\begin{tabular}{ll} MCResultAnalytical.calcResponse \\ Caluculate\ Response \\ \end{tabular}
```

#### **Description**

Calculate predicted values for given values of the reference-method.

## Usage

```
MCResultAnalytical.calcResponse(.Object, x.levels, alpha = 0.05)
```

## Arguments

. Object of class 'MCResultAnalytical'

x.levels numeric vector specifying values of the reference method for which prediction

should be made

alpha significance level for confidence intervals

MCResultAnalytical.initialize

Initialize Method for 'MCResultAnalytical' Objects.

#### Description

Initialize Method for 'MCResultAnalytical' Objects.

#### Usage

```
MCResultAnalytical.initialize(.Object, data = data.frame(X = NA, Y = NA),
    xmean = 0, para = matrix(NA, ncol = 4, nrow = 2), mnames = c("unknown",
    "unknown"), regmeth = "unknown", cimeth = "analytical", error.ratio = 0,
    alpha = 0.05, weight = 1)
```

#### **Arguments**

. Object object to be initialized data empty data.frame mean value

para empty coefficient matrix
mnames empty method names vector

regmeth string specifying the regression-method

cimeth string specifying the confidence interval method

error.ratio for deming regression

alpha value specifying the 100(1-alpha) confidence-level

weight 1 for each data point

MCResultAnalytical.printSummary

Print Regression-Analysis Summary for Objects of class 'MCResult-

Analytical'.

## **Description**

Function prints a summary of the regression-analysis for objects of class 'MCResultAnalytical'.

#### Usage

```
MCResultAnalytical.printSummary(.Object)
```

## **Arguments**

. Object of class 'MCResultAnalytical'

MCResultBCa-class Class "MCResultBCa"

## **Description**

Result of a method comparison with BCa-bootstrap based confidence intervals.

## Objects from the Class

Object is typically created by a call to function mcreg. Object can be directly constructed by calling newMCResultBCa or new("MCResultBCa", data, para, xmean, mnames, regmeth, cimeth, bootcimeth, alpha, glo

#### Slots

```
glob.sigma: Object of class "numeric" ~~
xmean: Object of class "numeric" ~~
nsamples: Object of class "numeric" ~~
nnested: Object of class "numeric" ~~
B0: Object of class "numeric" ~~
B1: Object of class "numeric" ~~
sigmaB0: Object of class "numeric" ~~
sigmaB1: Object of class "numeric" ~~
```

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```
MX: Object of class "numeric" ~~

bootcimeth: Object of class "character" ~~

rng.seed: Object of class "numeric" ~~

rng.kind: Object of class "character" ~~

glob.coef: Object of class "numeric" ~~

B0jack: Object of class "numeric" ~~

B1jack: Object of class "numeric" ~~

data: Object of class "data.frame" ~~

para: Object of class "matrix" ~~

mnames: Object of class "character" ~~

regmeth: Object of class "character" ~~

cimeth: Object of class "character" ~~

error.ratio: Object of class "numeric" ~~

alpha: Object of class "numeric" ~~

weight: Object of class "numeric" ~~
```

#### **Extends**

```
Class "MCResultJackknife", directly. Class "MCResult", by class "MCResultJackknife", distance 2.
```

#### Methods

```
calcResponse signature(.Object = "MCResultBCa"): ...
printSummary signature(.Object = "MCResultBCa"): ...
```

#### Author(s)

Ekaterina Manuilova <ekaterina.manuilova@roche.com>, Andre Schuetzenmeister <andre.schuetzenmeister@roche.com> Fabian Model <fabian.model@roche.com>

#### **Examples**

```
showClass("MCResultBCa")
```

MCResultBCa.bootstrapSummary

Compute Bootstrap-Summary for 'MCResultBCa' Objects.

# **Description**

Function computes the bootstrap summary for objects of class 'MCResultBCa'.

## Usage

```
MCResultBCa.bootstrapSummary(.Object)
```

## Arguments

. Object of class 'MCResultBCa'

#### Value

matrix of bootstrap results

MCResultBCa.calcResponse

Caluculate Response

# Description

Calculate predicted values for given values of the reference-method.

## Usage

```
MCResultBCa.calcResponse(.Object, x.levels, alpha = 0.05,
bootcimeth = .Object@bootcimeth)
```

## **Arguments**

. Object of class 'MCResultBCa'

x.levels numeric vector specifying values of the reference method for which prediction

should be made

alpha significance level for confidence intervals

bootcimeth character string specifying the method to be used for bootstrap confidence inter-

vals

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```
MCResultBCa.initialize
```

Initialize Method for 'MCResultBCa' Objects.

## **Description**

Method initializes newly created objects of class 'MCResultBCa'.

#### Usage

```
MCResultBCa.initialize(.Object, data = data.frame(X = NA, Y = NA),
  para = matrix(NA, ncol = 4, nrow = 2), xmean = 0, mnames = c("unknown",
  "unknown"), regmeth = "unknown", cimeth = "unknown",
  bootcimeth = "unknown", alpha = 0.05, glob.coef = c(0, 0),
  glob.sigma = c(0, 0), nsamples = 0, nnested = 0, B0jack = 0,
  B1jack = 0, B0 = 0, B1 = 0, MX = 0, rng.seed = as.numeric(NA),
  rng.kind = "unknown", sigmaB0 = 0, sigmaB1 = 0, error.ratio = 0,
  weight = 1)
```

.Object	object to be initialized
data	empty data.frame
xmean	0 for init-purpose
para	empty coefficient matrix
mnames	empty method names vector
regmeth	string specifying the regression-method
cimeth	string specifying the confidence interval method
bootcimeth	string specifying the method for bootstrap confidence intervals
error.ratio	for deming regression
alpha	value specifying the 100(1-alpha) confidence-level
glob.coef	global coefficients
rng.seed	random number generator seed
rng.kind	type of the random number generator
glob.sigma	global sd values for regression parameters
nsamples	number of samples for resampling
nnested	number of inner simulation for nested bootstrap
B0jack	jackknife intercpet
B1jack	jackknife slope
В0	intercept
B1	slope

MX parameter

sigmaB0 SD for intercepts sigmaB1 SD for slopes

weight 1 for each data point

 ${\tt MCResultBCa.plotBootstrapCoefficients}$ 

Plot distriblution of bootstrap coefficients

# Description

Plot distriblution of bootstrap coefficients (slope and intercept).

## Usage

```
MCResultBCa.plotBootstrapCoefficients(.Object, breaks = 20, ...)
```

## **Arguments**

.0bject Object of class "MCResultBCa" breaks used in function 'hist' (see ?hist) ... further graphical parameters

MCResultBCa.plotBootstrapT

Plot distriblution of bootstrap pivot T

#### **Description**

Plot distribution of bootstrap pivot T for slope and intercept and compare them with t(n-2) distribution.

#### Usage

```
MCResultBCa.plotBootstrapT(.Object, breaks = 20, ...)
```

# Arguments

.0bject Object of class "MCResultBCa".breaks Number of breaks in histogram.... further graphical parameters

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```
MCResultBCa.printSummary
```

Print Regression-Analysis Summary for Objects of class 'MCResult-BCa'.

## **Description**

Functions prints a summary of the regression-analysis for objects of class 'MCResultBCa'.

#### Usage

```
MCResultBCa.printSummary(.Object)
```

# Arguments

```
.0bject of class 'MCResultBCa'
```

MCResultJackknife-class

Class "MCResultJackknife"

#### **Description**

Result of a method comparison with Jackknife based confidence intervals.

# Objects from the Class

Object is typically created by a call to function mcreg. Object can be directly constructed by calling newMCResultJackknife or new("MCResultJackknife", data, para, mnames, regmeth, cimeth, alpha, glob.coef

# Slots

```
glob.coef: Object of class "numeric" ~~

B0jack: Object of class "numeric" ~~

B1jack: Object of class "numeric" ~~

data: Object of class "data.frame" ~~

para: Object of class "matrix" ~~

mnames: Object of class "character" ~~

regmeth: Object of class "character" ~~

cimeth: Object of class "character" ~~

error.ratio: Object of class "numeric" ~~

alpha: Object of class "numeric" ~~

weight: Object of class "numeric" ~~
```

#### **Extends**

```
Class "MCResult", directly.
```

#### Methods

```
calcResponse signature(.Object = "MCResultJackknife"): ...
getRJIF signature(.Object = "MCResultJackknife"): ...
plotwithRJIF signature(.Object = "MCResultJackknife"): ...
printSummary signature(.Object = "MCResultJackknife"): ...
```

## Author(s)

Ekaterina Manuilova <ekaterina.manuilova@roche.com>, Andre Schuetzenmeister <andre.schuetzenmeister@roche.com> Fabian Model <fabian.model@roche.com>

## **Examples**

```
showClass("MCResultJackknife")
```

MCResultJackknife.calcResponse

Caluculate Response

## **Description**

Calculate predicted values for given values of the reference-method.

## Usage

```
MCResultJackknife.calcResponse(.Object, x.levels, alpha = 0.05)
```

abject of along 'MCP apult Inaldznifa'

#### **Arguments**

Object

.object	object of class Wickesultrackkille
x.levels	numeric vector specifying values of the reference method for which prediction should be made

alpha significance level for confidence intervals

MCResultJackknife.getJackknifeIntercept

Get-Method for Jackknife-Intercept Value.

# Description

Extracts the intercept value from objects of class 'MCResultJackknife'.

## Usage

```
MCResultJackknife.getJackknifeIntercept(.Object)
```

# Arguments

.Object

object of class 'MCResultJackknife'

#### Value

(numeric) jackknife-intercept

MCResultJackknife.getJackknifeSlope

Get-Method for Jackknife-Slope Value.

# Description

Extracts the slope value from objects of class 'MCResultJackknife'.

# Usage

```
MCResultJackknife.getJackknifeSlope(.Object)
```

## **Arguments**

.Object

object of class 'MCResultJackknife'

#### Value

(numeric) jackknife-slope

 $\begin{tabular}{ll} MCResult Jackknife.get Jackknife Statistics \\ \it Jackknife Statistics \\ \end{tabular}$ 

## **Description**

Calculate jackknife mean, bias and standard error.

## Usage

MCResultJackknife.getJackknifeStatistics(.Object)

## Arguments

.Object

object of class "MCResultJackknife" or "MCResultResampling"

#### Value

table with jackknife mean, bias and standard error for intercept and slope.

MCResultJackknife.getRJIF

Relative Jackknife Influence Function

#### **Description**

Calculate the value of relative jackknife function for each observation.

#### Usage

MCResultJackknife.getRJIF(.Object)

# **Arguments**

.Object

object of class "MCResultJackknife" or "MCResultResampling".

#### Value

a list of the following elements:

slope numeric vector containing the values of relative jackknife function of slope.

intercept numeric vector containing the values of relative jackknife function of intercept.

#### References

Efron, B. (1990) Jackknife-After-Bootstrap Standard Errors and Influence Functions. Technical Report, N 134.

MCResultJackknife.initialize

Initialize Method for 'MCResultJackknife' Objects.

# Description

Method initializes newly created objects of class 'MCResultAnalytical'.

# Usage

```
MCResultJackknife.initialize(.Object, data = data.frame(X = NA, Y = NA),
  para = matrix(NA, ncol = 4, nrow = 2), mnames = c("unknown", "unknown"),
  regmeth = "unknown", cimeth = "jackknife", alpha = 0.05,
  glob.coef = c(0, 0), B0jack = 0, B1jack = 0, error.ratio = 0,
  weight = 1)
```

## Arguments

.Object object to be initialized data empty data.frame

para empty coefficient matrix
mnames empty method names vector

regmeth string specifying the regression-method

cimeth string specifying the confidence interval method

error.ratio for deming regression

alpha value specifying the 100(1-alpha) confidence-level

glob.coef global coefficients
B0jack jackknife intercepts
B1jack jackknife slopes
weight 1 for each data point

MCResultJackknife.plotwithRJIF

Plotting the Relative Jackknife Influence Function

## Description

The function draws reference method vs. test method as scatter plot. Observations with high influence (relative jackknife influence function is greater than 2) are highlighted as red points.

#### Usage

```
MCResultJackknife.plotwithRJIF(.Object)
```

## Arguments

. Object of class "MCResultJackknife" or "MCResultResampling"

#### References

Efron, B. (1990) Jackknife-After-Bootstrap Standard Errors and Influence Functions. Technical Report, N 134.

#### **Examples**

MCResultJackknife.printSummary

Print Regression-Analysis Summary for Objects of class 'MCResult-Jackknife'.

#### **Description**

Functions prints a summary of the regression-analysis for objects of class 'MCResultJackknife'.

# Usage

```
MCResultJackknife.printSummary(.Object)
```

## **Arguments**

. Object of class 'MCResultJackknife'

```
MCResultResampling-class Class "MCResultResampling"
```

#### **Description**

Result of a method comparison with resampling based confidence intervals.

## **Objects from the Class**

Object is typically created by a call to function mcreg. Object can be directly constructed by calling newMCResultResampling or new("MCResultResampling", data, para, xmean, mnames, regmeth, cimeth, bootcimes, bootcimes, regmeth, cimeth, bootcimes, regmeth, regmeth,

#### Slots

```
glob.coef: Object of class "numeric" ~~
glob.sigma: Object of class "numeric" ~~
xmean: Object of class "numeric" ~~
nsamples: Object of class "numeric" ~~
nnested: Object of class "numeric" ~~
B0: Object of class "numeric" ~~
B1: Object of class "numeric" ~~
sigmaB0: Object of class "numeric" ~~
sigmaB1: Object of class "numeric" ~~
MX: Object of class "numeric" ~~
bootcimeth: Object of class "character" ~~
rng.seed: Object of class "numeric" ~~
rng.kind: Object of class "character" ~~
data: Object of class "data.frame" ~~
para: Object of class "matrix" ~~
mnames: Object of class "character" ~~
regmeth: Object of class "character" ~~
cimeth: Object of class "character" ~~
error.ratio: Object of class "numeric" ~~
alpha: Object of class "numeric" ~~
weight: Object of class "numeric" ~~
```

#### **Extends**

```
Class "MCResult", directly.
```

#### Methods

```
calcResponse signature(.Object = "MCResultResampling"): ...
printSummary signature(.Object = "MCResultResampling"): ...
```

#### Author(s)

Ekaterina Manuilova <ekaterina.manuilova@roche.com>, Andre Schuetzenmeister <andre.schuetzenmeister@roche.com> Fabian Model <fabian.model@roche.com>

#### **Examples**

```
showClass("MCResultResampling")
```

MCResultResampling.bootstrapSummary

Compute Bootstrap-Summary for 'MCResultResampling' Objects.

## **Description**

Function computes the bootstrap summary for objects of class 'MCResultResampling'.

#### Usage

```
MCResultResampling.bootstrapSummary(.Object)
```

## Arguments

```
. Object of class 'MCResultResampling'
```

## Value

matrix of bootstrap results

```
MCResultResampling.calcResponse
```

Caluculate Response

# Description

Calculate predicted values for given values of the reference-method.

# Usage

```
MCResultResampling.calcResponse(.Object, x.levels, alpha = 0.05,
bootcimeth = .Object@bootcimeth)
```

#### **Arguments**

. Object of class 'MCResultResampling'

x.levels numeric vector specifying values of the reference method for which prediction

should be made

alpha significance level for confidence intervals

bootcimeth bootstrap confidence interval method to be used

MCResultResampling.initialize

Initialize Method for 'MCResultAnalytical' Objects.

#### **Description**

Method initializes newly created objects of class 'MCResultAnalytical'.

#### Usage

```
MCResultResampling.initialize(.0bject, data = data.frame(X = NA, Y = NA),
    para = matrix(NA, ncol = 4, nrow = 2), xmean = 0, mnames = c("unknown",
    "unknown"), regmeth = "unknown", cimeth = "unknown",
    bootcimeth = "unknown", alpha = 0.05, glob.coef = c(0, 0),
    rng.seed = as.numeric(NA), rng.kind = "unknown", glob.sigma = c(0, 0),
    nsamples = 0, nnested = 0, B0 = 0, B1 = 0, MX = 0, sigmaB0 = 0,
    sigmaB1 = 0, error.ratio = 0, weight = 1)
```

#### **Arguments**

.Object object to be initialized data empty data.frame xmean 0 for init-purpose

para empty coefficient matrix
mnames empty method names vector

regmeth string specifying the regression-method

cimeth string specifying the confidence interval method

bootcimeth string specifying the method for bootstrap confidence intervals

error.ratio for deming regression

alpha value specifying the 100(1-alpha) confidence-level

glob.coef global coefficients

rng.seed random number generator seed
rng.kind type of the random number generator
glob.sigma global sd values for regression parameters

-	1 6 1 6 1:	
nsamples	number of samples for resampling	

nnested number of inner simulation for nested bootstrap

B0 resampling intercepts
B1 resampling slopes

MX Numeric vector with point estimations of (weighted-)average of reference method

values for each bootstrap sample.

sigmaB0 SD for 'B0' sigmaB1 SD for 'B1'

weight 1 for each data point

 ${\tt MCResultResampling.plotBootstrapCoefficients}$ 

Plot distriblution of bootstrap coefficients

#### **Description**

Plot distriblution of bootstrap coefficients (slope and intercept).

## Usage

```
MCResultResampling.plotBootstrapCoefficients(.Object, breaks = 20, ...)
```

## **Arguments**

.Object Object of class "MCResultResampling" breaks see function 'hist' (?hist) for details

... further graphical parameters

MCResultResampling.plotBootstrapT

Plot distriblution of bootstrap pivot T

# Description

Plot distribution of bootstrap pivot T for slope and intercept and compare them with t(n-2) distribution.

## Usage

```
MCResultResampling.plotBootstrapT(.Object, breaks = 20, ...)
```

#### **Arguments**

.0bject Object of class "MCResultResampling".

breaks Number of breaks in histogram.
... further graphical parameters

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MCResultResampling.printSummary

Print Regression-Analysis Summary for Objects of class 'MCResultResampling'.

## **Description**

Functions prints a summary of the regression-analysis for objects of class 'MCResultResampling'.

#### Usage

```
MCResultResampling.printSummary(.Object)
```

## **Arguments**

. Object of class 'MCResultResampling'

newMCResult

MCResult Object Constructor with Matrix in Wide Format as Input

## Description

MCResult Object Constructor with Matrix in Wide Format as Input

## Usage

```
newMCResult(wdata, para, sample.names = NULL, method.names = NULL,
  regmeth = "Unknown", cimeth, error.ratio, alpha = 0.05, weight = rep(1,
  nrow(wdata)))
```

#### **Arguments**

wdata measurement data in matrix format. First column reference method	ethod (x), second
--	-------------------

column test method (y).

para regression parameters in matrix form. Rows: Intercept, Slope. Cols: EST, SE,

LCI, UCI.

sample.names names of individual data points, e.g. barcodes of measured samples.

method. names names of reference and test method.

regmeth name of statistical method used for regression.

cimeth name of statistical method used for computing confidence intervals. error.ratio ratio between standard deviation of reference and test method.

alpha numeric value specifying the 100(1-alpha)% confidence level of confidence in-

tervals (Default is 0.05).

weight numeric vector specifying the weights used for each point

## Value

MCResult object containing regression results.

 $\begin{tabular}{ll} \textbf{mewMCResultAnalytical} & \textbf{\textit{MCResultAnalytical object constructor with matrix in wide format as input.} \\ \end{tabular}$ 

# Description

MCResultAnalytical object constructor with matrix in wide format as input.

# Usage

```
newMCResultAnalytical(wdata, para, xmean, sample.names = NULL,
method.names = NULL, regmeth = "Unknown", cimeth = "analytical",
error.ratio = error.ratio, alpha = 0.05, weight = rep(1, nrow(wdata)))
```

## **Arguments**

Measurement data in matrix format. First column reference method $(x)$ , second column comparator method $(y)$ .
Regression parameters in matrix form. Rows: Intercept, Slope. Cols: EST, SE, LCI, UCI.
Global (weighted) mean of x-values.
Names of individual data points, e.g. barcodes of measured samples.
Names of reference and comparator method.
Name of statistical method used for regression.
Name of statistical method used for computing confidence intervals.
Ratio between standard deviation of reference and comparator method.
1 - significance level for confidence intervals.
numeric vector specifying the weights used for each point

#### Value

MCResultAnalytical object containing regression results.

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newMCResultBCa	MCResultBCa object constructor with matrix in wide format as input.

# Description

MCResultBCa object constructor with matrix in wide format as input.

# Usage

```
newMCResultBCa(wdata, para, xmean, sample.names = NULL, method.names = NULL,
regmeth = "unknown", glob.coef, glob.sigma, cimeth = "unknown",
bootcimeth = "unknown", nsamples, nnested, rng.seed, rng.kind, B0jack,
B1jack, B0, B1, MX, sigmaB0, sigmaB1, error.ratio, alpha = 0.05,
weight = rep(1, nrow(wdata)))
```

wdata	Measurement data in matrix format. First column reference method (x), second column comparator method (y).
para	Regression parameters in matrix form. Rows: Intercept, Slope. Cols: EST, SE, LCI, UCI.
xmean	Global (weighted) mean of x-values
sample.names	Names of individual data points, e.g. barcodes of measured samples.
method.names	Names of reference and comparator method.
regmeth	Name of statistical method used for regression.
cimeth	Name of statistical method used for computing confidence intervals.
error.ratio	Ratio between standard deviation of reference and comparator method.
alpha	1 - significance level for confidence intervals.
glob.coef	Numeric vector of length two with global point estimations of intercept and slope.
glob.sigma	Numeric vector of length two with global estimations of standard errors of intercept and slope.
bootcimeth	Bootstrap based confidence interval estimation method.
nsamples	Number of bootstrap samples.
nnested	Number of nested bootstrap samples.
rng.seed	Seed used to call mcreg, NULL if no seed was used
rng.kind	RNG type (string, see set.seed for details) used, only meaningfull if rng.seed was specified
B0jack	Numeric vector with point estimations of intercept for jackknife samples.
B1jack	Numeric vector with point estimations of slope for jackknife samples.
В0	Numeric vector with point estimations of intercept for each bootstrap sample.

newMCResultJackknife 63

B1	Numeric vector with point estimations of slope for each bootstrap sample.
sigmaB0	Numeric vector with estimation of standard error of intercept for each bootstrap sample.
sigmaB1	Numeric vector with estimation of standard error of slope for each bootstrap sample.
MX	Numeric vector with point estimations of (weighted-)average of reference method values for each bootstrap sample.
weight	numeric vector specifying the weights used for each point

#### Value

MCResult object containing regression results.

 ${\tt newMCResultJackknife} \quad {\tt \it MCResultJackknife\ Object\ Constructor\ with\ Matrix\ in\ Wide\ Format\ as\ Input}$ 

# Description

MCResultJackknife Object Constructor with Matrix in Wide Format as Input

# Usage

```
newMCResultJackknife(wdata, para, sample.names = NULL, method.names = NULL,
regmeth = "Unknown", glob.coef, cimeth = "unknown", B0jack, B1jack,
error.ratio = error.ratio, alpha = 0.05, weight = rep(1, nrow(wdata)))
```

wdata	measurement data in matrix format. First column reference method $(x)$ , second column test method $(y)$ .
para	regression parameters in matrix form. Rows: Intercept, Slope. Cols: EST, SE, LCI, UCI.
sample.names	names of individual data points, e.g. barcodes of measured samples.
method.names	names of reference and test method.
regmeth	name of statistical method used for regression.
glob.coef	global coefficients
cimeth	name of statistical method used for computing confidence intervals.
B0jack	jackknife intercepts
B1jack	jeckknife slopes
error.ratio	ratio between standard deviation of reference and test method.
alpha	numeric value specifying the $100(1-alpha)\%$ confidence level of confidence intervals (Default is 0.05).
weight	numeric vector specifying the weights used for each point

## Value

MCResult object containing regression results.

newMCResultResampling MCResultResampling object constructor with matrix in wide format as input.

## **Description**

MCResultResampling object constructor with matrix in wide format as input.

## Usage

```
newMCResultResampling(wdata, para, xmean, sample.names = NULL,
method.names = NULL, regmeth = "unknown", glob.coef, glob.sigma,
cimeth = "unknown", bootcimeth = "unknown", nsamples, nnested, rng.seed,
rng.kind, B0, B1, MX, sigmaB0, sigmaB1, error.ratio, alpha = 0.05,
weight = rep(1, nrow(wdata)))
```

wdata	Measurement data in matrix format. First column reference method $(x)$ , second column comparator method $(y)$ .
para	Regression parameters in matrix form. Rows: Intercept, Slope. Cols: EST, SE, LCI, UCI.
xmean	Global (weighted) mean of x-values
sample.names	Names of individual data points, e.g. barcodes of measured samples.
method.names	Names of reference and comparator method.
regmeth	Name of statistical method used for regression.
cimeth	Name of statistical method used for computing confidence intervals.
error.ratio	Ratio between standard deviation of reference and comparator method.
alpha	1 - significance level for confidence intervals.
glob.coef	Numeric vector of length two with global point estimations of intercept and slope.
glob.sigma	Numeric vector of length two with global estimations of standard errors of intercept and slope.
bootcimeth	Bootstrap based confidence interval estimation method.
nsamples	Number of bootstrap samples.
nnested	Number of nested bootstrap samples.
rng.seed	Seed used to call mcreg, NULL if no seed was used
rng.kind	RNG type (string, see set.seed for details) used, only meaningfull if rng.seed was specified

В0	Numeric vector with point estimations of intercept for each bootstrap sample.
B1	Numeric vector with point estimations of slope for each bootstrap sample.
sigmaB0	Numeric vector with estimation of standard error of intercept for each bootstrap sample.
sigmaB1	Numeric vector with estimation of standard error of slope for each bootstrap sample.
MX	Numeric vector with point estimations of (weighted-)average of reference method values for each bootstrap sample.
weight	numeric vector specifying the weights used for each point

# Value

MCResult object containing regression results.

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